

BREMS – a program for calculating spectra and
angular distributions of electron-atom bremsstrahlung at
electron energies less than 30 MeV

v1.5.8.4

User's Manual

by Andrius Poškus

(Vilnius University, Institute of Chemical Physics)

2024-06-02

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E-mail: andrius.poskus@ff.vu.lt or andrius.poskus@live.com

Web: <https://web.vu.lt/ff/a.poskus/brems/> or
[https://www.researchgate.net/publication/332171944 BREMS](https://www.researchgate.net/publication/332171944_BREMS)

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1. Introduction

BREMS is a set of Fortran-90 codes for calculating the energy spectra and angular distributions of photons emitted due to atomic-field bremsstrahlung when fast electrons interact with neutral atoms or ions. The approximate energy range of the incident electron is from 10 eV to 30 MeV. BREMS was written by Andrius Poškus (Vilnius University, Faculty of Physics, Institute of Chemical Physics). BREMS is distributed under the GNU General Public License 3.

BREMS can be downloaded from <https://web.vu.lt/ff/a.poskus/brems/> or https://www.researchgate.net/publication/332171944_BREMS.

1.1. The theoretical basis

The theory and some of the numerical methods used in BREMS were developed in [1, 2]. The atom is represented by a static spherically symmetrical charge distribution of infinite mass. The elementary process of bremsstrahlung is described as a one-electron transition in the field of an atom (or an ion). The atom is described by a central potential. The electron continuum wave functions are calculated by solving the Dirac equation with one of several possible types of the interaction potential. The wave functions are expanded in partial wave series and the radial integrals are calculated numerically. The relativistic partial-wave formulation is currently the best available theory for calculating the cross sections of unpolarized electron-atom bremsstrahlung. The results of this theory are summarized in Section 1.1.1.

In addition to the relativistic partial-wave method, BREMS implements the analytical expressions of the differential cross sections, which are based on the first Born approximation (with or without the atomic form factor), and on the Sommerfeld-Maue (SM) wave functions (both in the leading-order-term approximation and with the next-to-leading-order correction, and with or without the screening correction). The atomic form factor (or the screening correction) is calculated using the approximation of the screening function by a linear combination of up to 200 decaying exponentials. The corresponding formulas are given in Sections 1.1.2 and 1.1.3.

The effect of the finite size of the nucleus on the differential cross sections is modeled using one of three analytical approximations of the nuclear charge distribution (uniform distribution, Helm's uniform-uniform distribution, or Fermi distribution). This charge distribution is integrated with respect to the radial coordinate, resulting in the "finite-nucleus correction" of the screening function. The overall screening function is calculated as a sum of the "point-nucleus screening function" (including the electron screening effects) and the mentioned finite-nucleus correction. In the case of the Born approximation, the nuclear size effects are included via the nuclear form factor.

BREMS allows selection of one of three central potentials for calculation of the mentioned point-nucleus screening function:

- 1) the point-Coulomb potential $-\alpha Z / r$ (the unscreened nucleus),
- 2) a linear combination of up to 200 decaying exponentials divided by r (in a special case, three exponential terms corresponding to the Thomas-Fermi-Csavinszky potential [3] are used),
- 3) an arbitrary function of the form $\bar{V}(r)/r$, where $\bar{V}(r)$ is a smooth negative-valued monotonous function that decays exponentially in the limit $r \rightarrow \infty$ and is equal to $-\alpha Z$ at $r = 0$. This function must be defined in tabular format. By default, the Kohn-Sham potential [4, 5] is used.

It is also possible to use the interaction potential corresponding to an ion. In such a case, the function $\bar{V}(r)$ mentioned above approaches a non-zero value in the limit $r \rightarrow \infty$, and the mentioned linear combination of decaying exponentials includes a constant term.

1.1.1. The relativistic partial-wave method

Unless otherwise specified, the relativistic units will be used throughout this text, i.e., the reduced Planck's constant, the speed of light and the electron's rest mass will be assumed to be equal to 1, and the elementary charge squared will be assumed to be equal to the fine-structure constant α . The relativistic unit of length is equal to the reduced Compton wavelength of the electron (0.3861592679588 pm). The partial waves constituting the initial and final states of the

electron will be labeled by the quantum number κ , which is defined in terms of the orbital angular momentum and the total angular momentum (quantum numbers l and j , respectively) as follows [6]:

$$\kappa = \begin{cases} l & \text{for } j = l - \frac{1}{2}, \\ -l - 1 & \text{for } j = l + \frac{1}{2}. \end{cases} \quad (1.1.1)$$

As it follows from Eq. (1.1.1),

$$|\kappa| = j + \frac{1}{2}. \quad (1.1.2)$$

The incident and final electron states will be labeled with the subscripts “1” and “2”, respectively. Energies and momenta will be denoted as follows:

E – total relativistic energy of the electron,

T – kinetic energy of the electron,

$p = |\mathbf{p}|$ – modulus of the momentum of the electron (\mathbf{p} is the momentum vector),

$k = |\mathbf{k}|$ – energy of the bremsstrahlung photon and modulus of its momentum vector \mathbf{k} .

The coordinate system is centered on the atomic nucleus, with the z -axis along \mathbf{k} , y -axis along $\mathbf{k} \times \mathbf{p}_1$, and x -axis in the $(\mathbf{k}, \mathbf{p}_1)$ plane. The angles defining the direction of emission of the bremsstrahlung photon will be denoted as follows:

θ – angle between the directions of the emitted photon and the incident electron,

ϕ – azimuth angle,

Ω_k – solid angle.

The expressions of the “double differential” cross section (proportional to the joint probability density of the direction and energy of bremsstrahlung photons) and of the photon energy spectrum (the “single differential” cross section, defined as the integral of the double differential cross section with respect to the solid angle of photon emission) are presented below [1, 7]:

$$\frac{k}{Z^2} \frac{d\sigma}{dk d\Omega_k} \equiv \sigma(k, \theta) = \lambda_0 \sum_{\kappa_1 \bar{\kappa}_1 \kappa_2} (-1)^{l_1 + \bar{l}_1} \cos(\delta_{\kappa_1} - \delta_{\bar{\kappa}_1}) \sum_{m=|m_2|} [A_+^+(m) \bar{A}_+^+(m) + A_+^-(m) \bar{A}_+^-(m) + A_-^+(m) \bar{A}_-^+(m) + A_-^-(m) \bar{A}_-^-(m)] \quad (1.1.3)$$

(in mb/sr), or, equivalently [7],

$$\frac{k}{Z^2} \frac{d\sigma}{dk d\Omega_k} \equiv \sigma(k, \theta) = \lambda_0 \sum_{\kappa_2, m=|m_2|} \left[\left| \sum_{\kappa_1} (-1)^{l_1} e^{i\delta_{\kappa_1}} A_+^+ \right|^2 + \left| \sum_{\kappa_1} (-1)^{l_1} e^{i\delta_{\kappa_1}} A_-^+ \right|^2 + \left| \sum_{\kappa_1} (-1)^{l_1} e^{i\delta_{\kappa_1}} A_+^- \right|^2 + \left| \sum_{\kappa_1} (-1)^{l_1} e^{i\delta_{\kappa_1}} A_-^- \right|^2 \right] \quad (1.1.4)$$

(in mb/sr), and

$$\frac{k}{Z^2} \frac{d\sigma}{dk} \equiv \sigma(k) = \lambda_0 \sum_{\kappa_2, \kappa_1, m=|m_2|} \{ [R_{\kappa_2 \kappa_1}^+(m)]^2 + [R_{\kappa_2 \kappa_1}^-(m)]^2 \} \quad (1.1.5)$$

(in mb), where the set of values of \bar{l}_1 and $\bar{\kappa}_1$ is the same as that of l_1 and κ_1 , respectively, m_2 is the magnetic quantum number corresponding to the partial wave κ_2 (i.e., $m_2 = -|\kappa_2| + \frac{1}{2}, -|\kappa_2| + \frac{3}{2}, \dots, |\kappa_2| - \frac{3}{2}, |\kappa_2| - \frac{1}{2}$),

$$\lambda_0 = [(3.861592679588)^2 \times 10^5] \frac{32\alpha}{Z^2 p_1} E_1 E_2 p_2 k^2 \quad (1.1.6)$$

(the factor in brackets is the reduced Compton wavelength squared, in mb),

$$A_{\pm}^+(m) = C_{\kappa_1, m-1}^{\pm} y_{l_1, m-1 \mp \frac{1}{2}}(\theta) R_{\kappa_2 \kappa_1}^+(m), \quad (1.1.7a)$$

$$A_{\pm}^-(m) = C_{\kappa_1, m+1}^{\pm} y_{l_1, m+1 \mp \frac{1}{2}}(\theta) R_{\kappa_2 \kappa_1}^-(m), \quad (1.1.7b)$$

$C_{\kappa, m}^{\pm}$ is the Clebsch-Gordan coefficient:

$$C_{\kappa, m}^{\pm} = C(l \frac{1}{2} j; m \mp \frac{1}{2}, \pm \frac{1}{2}) = \begin{cases} \mp [(l \mp m + \frac{1}{2}) / (2l + 1)]^{1/2} & \text{for } j = l - \frac{1}{2}, \\ [(l \pm m + \frac{1}{2}) / (2l + 1)]^{1/2} & \text{for } j = l + \frac{1}{2}, \end{cases} \quad (1.1.8)$$

$y_{lm}(\theta)$ is the preexponential factor of the spherical harmonic $Y_{lm}(\theta, \phi)$:

$$Y_{lm}(\theta, \phi) = y_{lm}(\theta)e^{im\phi}, \quad (1.1.9)$$

the bar over A_{\pm}^{\pm} corresponds to the replacement of κ_1 and l_1 with $\bar{\kappa}_1$ and \bar{l}_1 in Eqs. (1.1.7a,b),

$$R_{\kappa_2 \kappa_1}^{\pm}(m) = \sum_{n=1}^2 Q_n^{\pm}(m) \sum_l P_n^{\pm}(m) S_n, \quad (1.1.10)$$

and δ_{κ} is the electron phase shift for the partial wave κ . In Eq. (1.1.10), l is the orbital quantum number of the emitted photon, indicating its orbital angular momentum (not to be confused with the orbital quantum number of the electron, which is also denoted “ l ” in Eq. (1.1.1)). It runs from $|l'_2 - l_1|$ to $(l'_2 + l_1)$ in steps of 2 for $n = 1$, and from $|l_2 - l'_1|$ to $(l_2 + l'_1)$ in steps of 2 for $n = 2$. Here

$$l' = l + \eta_{\kappa}, \quad \eta_{\kappa} = -\kappa / |\kappa|, \quad (1.1.11)$$

$$Q_1^{\pm}(m) = \eta_{\kappa_2} (-1)^{m \mp 1/2} [(2l'_2 + 1)(2l_1 + 1)]^{1/2} C_{-\kappa_2, m}^{\pm} C_{\kappa_1, m \mp 1}^{\mp}, \quad (1.1.12a)$$

$$Q_2^{\pm}(m) = -\eta_{\kappa_1} (-1)^{m \mp 1/2} [(2l_2 + 1)(2l'_1 + 1)]^{1/2} C_{\kappa_2, m}^{\pm} C_{-\kappa_1, m \mp 1}^{\mp}, \quad (1.1.12b)$$

$$P_1^{\pm}(m) = (-1)^{(l'_2 + l_1 + l)/2} T(l'_2, l_1, l; m \mp \frac{1}{2}), \quad (1.1.13a)$$

$$P_2^{\pm}(m) = (-1)^{(l_2 + l'_1 + l)/2} T(l_2, l'_1, l; m \mp \frac{1}{2}), \quad (1.1.13b)$$

$$T(l_2, l_1, l; m) = (2l + 1) \begin{pmatrix} l_2 & l_1 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_1 & l \\ -m & m & 0 \end{pmatrix}, \quad (1.1.14)$$

where the last two factors are the Wigner 3j coefficients, and

$$S_1 = \int_0^{\infty} j_l(kr) g_{\kappa_1}(r) f_{\kappa_2}(r) dr, \quad (1.1.15a)$$

$$S_2 = \int_0^{\infty} j_l(kr) g_{\kappa_2}(r) f_{\kappa_1}(r) dr. \quad (1.1.15b)$$

In Eqs. (1.1.15a,b), j_l is the spherical Bessel function of the first kind, order l , and the functions g_{κ} and f_{κ} are defined as the radial continuum wave functions multiplied by r . The functions g_{κ} and f_{κ} correspond to the upper and lower spinors composing the four-component wave function of the electron (“bispinor”), respectively [6]. Those functions satisfy the coupled radial Dirac equations

$$\frac{dg_{\kappa}}{dr} = [E + 1 - V(r)] f_{\kappa}(r) - \frac{\kappa g_{\kappa}(r)}{r}, \quad (1.1.16a)$$

$$\frac{df_{\kappa}}{dr} = -[E - 1 - V(r)] g_{\kappa}(r) + \frac{\kappa f_{\kappa}(r)}{r}, \quad (1.1.16b)$$

where V is the central potential used to describe the target atom. The ratio of the screened and unscreened potentials is called the screening function. It will be denoted $\tilde{V}(r)$:

$$\tilde{V}(r) \equiv \frac{V(r)}{-Z\alpha/r}. \quad (1.1.17)$$

In the case of a neutral atom, $\tilde{V}(r)$ tends to zero when $r \rightarrow \infty$.

Although the two expressions of the double differential cross section (1.1.3) and (1.1.4) are mathematically equivalent, the expression (1.1.4) is more convenient for practical calculations, because it involves triple summation, whereas expression (1.1.3) involves quadruple summation. Consequently, the expression (1.1.4) is the one that is implemented in the code of BREMS.

At large r , the solution of the system of equations (1.1.16a,b) is asymptotically equal to [1]

$$\begin{aligned} g_{\kappa}(r) &= r \sqrt{\frac{E+1}{2E}} A_{\kappa} [\cos \bar{\delta}_{\kappa} j_{\kappa}(pr) - \sin \bar{\delta}_{\kappa} y_{\kappa}(pr)], \\ f_{\kappa}(r) &= r \sqrt{\frac{E-1}{2E}} A_{\kappa} [\cos \bar{\delta}_{\kappa} j_{\kappa-1}(pr) - \sin \bar{\delta}_{\kappa} y_{\kappa-1}(pr)], \end{aligned} \quad (1.1.18)$$

where $\bar{\delta}_{\kappa}$ is the phase shift and y_{κ} is the spherical Bessel function of the second kind, order κ (this notation differs from the notation of the spherical harmonic y_{lm} by the number of subscripts). The

wave functions are normalized by setting $A_\kappa = 1$. Those expressions define the phase-shifted free-field solution of the Dirac equation for the case of screening functions that tend to zero when $r \rightarrow \infty$. The phase shift $\bar{\delta}_\kappa$, which is used in Eqs. (1.1.18), is related to the phase shift δ_κ , which appears in Eq. (1.1.3) and Eq. (1.1.4), as follows [1]:

$$\delta_\kappa = \bar{\delta}_\kappa + (l - \kappa)\frac{1}{2}\pi = \begin{cases} \bar{\delta}_\kappa & \text{if } \kappa > 0, \\ \bar{\delta}_\kappa - (\kappa + \frac{1}{2})\pi & \text{if } \kappa < 0. \end{cases} \quad (1.1.19)$$

In the limit $k \rightarrow 0$, the values of the S integrals (1.1.15) grow indefinitely as $1/k$, whereas the factor λ_0 (1.1.6) approaches zero due to the presence of k^2 in the expression of λ_0 . As a result, an indeterminate form of the type $0 \times \infty$ appears in Eqs. (1.1.3), (1.1.4), and (1.1.5). Consequently, the definition of the factor λ_0 (1.1.6) in the case $k = 0$ must be modified by removing the factor k^2 , and the definition of the R factors (1.1.10) must be modified by replacing S_1 and S_2 with $\lim_{k \rightarrow 0}(kS_1)$ and $\lim_{k \rightarrow 0}(kS_2)$, respectively. The latter limits can be expressed analytically, using only the values of the electron energy $E = E_1 = E_2$ and the phase shifts corresponding to that energy (numerical integration is not required). The analytical expression of the mentioned limits is the following [8, 9]:

$$\begin{aligned} \lim_{k \rightarrow 0}(kS_1) = -\lim_{k \rightarrow 0}(kS_2) &= \frac{\sqrt{\pi}}{2^{l+3}} \frac{\Gamma(l+1)}{\Gamma(l+\frac{3}{2})} \frac{1}{E^2} \left(1 - \frac{1}{E^2}\right)^{\frac{l}{2}} F\left(\frac{l+2}{2}, \frac{l+1}{2}; l+\frac{3}{2}; 1 - \frac{1}{E^2}\right) \\ &\times \cos\left(\bar{\delta}_{\kappa_1} - \bar{\delta}_{\kappa_2} + (\kappa_2 - \kappa_1 + l)\frac{\pi}{2}\right), \end{aligned} \quad (1.1.20)$$

where F is the hypergeometric function.

It should be noted that the method of calculating the soft-photon cross sections described above (i.e., using expressions (1.1.4) and (1.1.5) in conjunction with Eq. (1.1.20)) is not the best one at electron energies higher than approximately 1 MeV, due to slowing down of convergence of the partial-wave series with increasing T_1 in the limit $k = 0$. A more efficient method is based on the known fact that the double and single differential cross sections of bremsstrahlung in the limit $k \rightarrow 0$ are equal to a weighted integral of the differential cross section of electron elastic scattering with respect to the electron's scattering angle [10, 11] (the expressions of double and single differential cross sections differ only by the functional form of the mentioned weighting factor, which depends on the angle of photon emission θ in the case of the double differential cross section [11], and does not depend on θ in the case of the single differential cross section [10]).

In order to apply Eqs. (1.1.18) in the case of the point-Coulomb field (unscreened nucleus), one should add a logarithmic term depending on r to the definition of the phase shift $\bar{\delta}_\kappa$ [6]:

$$\bar{\delta}_\kappa = \tilde{\delta}_\kappa + \nu \ln 2pr, \quad (1.1.21)$$

where

$$\nu \equiv Z\alpha E / p \quad (1.1.22)$$

(this factor is sometimes called “the Coulomb parameter”), and $\tilde{\delta}_\kappa$ is a constant whose analytical expression can be obtained, for example, from Eq. (5.75) in [6]. This expression is reproduced below in a form consistent with Eqs. (1.1.18):

$$\tilde{\delta}_\kappa = -\arg(\Gamma(\gamma + i\nu)) + \varepsilon - \frac{1}{2}\pi\gamma + (\kappa + 1)\frac{\pi}{2}, \quad (1.1.23)$$

$$\gamma \equiv (\kappa^2 - \alpha^2 Z^2)^{1/2}, \quad (1.1.24)$$

$$e^{2i\varepsilon} = -\frac{\kappa - i\nu/E}{\gamma + i\nu}. \quad (1.1.25)$$

The left-hand sides of Eqs. (1.1.3), (1.1.4), and (1.1.5) will be further referred to as the “scaled” differential cross sections (due to the presence of the scaling factor k/Z^2).

1.1.2. The Born approximation

The relativistic plane-wave Born approximation treats the interaction potential $V(r)$ as a small perturbation to free space, resulting in the expression of the electron continuum wave function as an infinite series of terms proportional to $Z\alpha$, $(Z\alpha)^2$, $(Z\alpha)^3$, ...:

$$\Psi = \psi_0 + (Z\alpha)\psi_1 + (Z\alpha)^2\psi_2 + \dots, \quad (1.1.26)$$

where ψ_0 is a plane wave. The first-order Born approximation is based on the assumption that the perturbation is weak enough to allow neglecting all second- and higher-order terms. Further on, following the usual convention, the attributes “plane-wave” and “first-order” before “Born approximation” will be omitted (they will be implied). The criterion for the validity of the Born approximation is [12]

$$\beta \gg Z\alpha, \quad (1.1.27)$$

where β is the ratio of the electron speed to the speed of light. This condition must be satisfied both for the initial and the final electron. Obviously, this condition is valid only in the case of low values of Z and with β not much less than 1, i.e., at relativistic speeds of the incident electron. In addition, since the condition (1.1.27) is applied to both the initial and the final electron, the Born approximation never works close to the “tip” of the photon energy spectrum (corresponding to $k=T_1$), independently of the incident electron energy. Since ψ_0 describes a free electron, which cannot emit a photon, the zero-order term ψ_0 does not contribute to the interaction matrix elements (and, consequently, to the interaction cross section). Consequently, the interaction cross sections in the first-order Born approximation are proportional to $(Z\alpha)^2$, whereas the scaled differential cross sections (as defined at the end of Section 1.1.1) do not depend on Z explicitly (they depend only on the screening function defined by Eq. (1.1.17)). The inclusion of the second-order term in Eq. (1.1.26) introduces terms proportional to Z and Z^2 into the expansions of the scaled differential cross sections in powers of Z . The inclusion of the third-order term in Eq. (1.1.26) modifies the term proportional to Z^2 and additionally introduces terms proportional to Z^3 and Z^4 into the expansions of the scaled differential cross sections in powers of Z .

In the framework of the Born approximation, the finite size of the nucleus and screening of the nuclear Coulomb potential by the electron cloud are taken into account by the use of the factor $(F_n - F_e)^2$ in the expression of the triple differential cross section (TDCS), where F_n and F_e are the nuclear form factor (NFF) and the atomic electron form factor (AFF), respectively [13, 14]:

$$\frac{k}{Z^2} \frac{d\sigma}{dk d\Omega_{\hat{k}} d\Omega_{\hat{p}_2}} = \frac{\alpha r_e^2}{(2\pi)^2} \frac{p_2}{p_1} \frac{[F_n(q) - F_e(q)]^2}{q^4} [8k^2 E_1 E_2 \xi \eta (\mathbf{u} - \mathbf{v})^2 + 16E_1^2 E_2^2 (\xi \mathbf{u} - \eta \mathbf{v})^2 - 4q^2 (E_1 \xi \mathbf{u} - E_2 \eta \mathbf{v})^2], \quad (1.1.28)$$

where r_e is the classical electron radius (if the relativistic units are used, then $r_e = \alpha$),

$$\mathbf{u} = \mathbf{p}_1 \times \hat{\mathbf{k}}, \quad \mathbf{v} = \mathbf{p}_2 \times \hat{\mathbf{k}}, \quad (1.1.29a)$$

where $\hat{\mathbf{k}}$ is the \mathbf{k} unit vector:

$$\hat{\mathbf{k}} = \mathbf{k} / k, \quad (1.1.29b)$$

and the other notations are defined as follows:

$$\xi = \frac{1}{2E_1 d_1}, \quad \eta = \frac{1}{2E_2 d_2}, \quad (1.1.29c)$$

$$d_1 = E_1 - p_1 \cos \theta_1, \quad d_2 = E_2 - p_2 \cos \theta_2, \quad (1.1.29d)$$

$$\mathbf{q} = \mathbf{p}_1 - \mathbf{p}_2 - \mathbf{k}, \quad (1.1.29e)$$

where θ_1 is the angle between \mathbf{p}_1 and \mathbf{k} , and θ_2 is the angle between \mathbf{p}_2 and \mathbf{k} . The vector \mathbf{q} is the momentum transferred to the nucleus that recoils after the emission of the photon. Its modulus is indicated by q and called the momentum transfer. The value of expression (1.1.28) would not change after rotating vectors \mathbf{u} and \mathbf{v} so that the angle between them does not change. Consequently, it may be more convenient to rotate both \mathbf{u} and \mathbf{v} around the direction of \mathbf{k} by 90° and redefine them as the component of \mathbf{p}_1 perpendicular to \mathbf{k} and the component of \mathbf{p}_2 perpendicular to \mathbf{k} , respectively.

The AFF is defined as follows:

$$F_c(q) = \frac{1}{Z} \int n(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3\mathbf{r} = \frac{4\pi}{Z} \int_0^\infty n(r) \frac{\sin qr}{qr} r^2 dr, \quad (1.1.30a)$$

where $n(\mathbf{r})$ is the electron density ($\int n(\mathbf{r}) d^3\mathbf{r} = Z$). The second equality in (1.1.30a) follows from the assumption of spherical symmetry of the electron cloud. The definition of the NFF can be obtained from the definition of the AFF (1.1.30a) by replacing the electron density with proton density $\rho(\mathbf{r})$:

$$F_n(q) = \frac{1}{Z} \int \rho(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3\mathbf{r} = \frac{4\pi}{Z} \int_0^\infty \rho(r) \frac{\sin qr}{qr} r^2 dr = \frac{4\pi}{Z} \int_0^{R_c} \rho(r) \frac{\sin qr}{qr} r^2 dr, \quad (1.1.30b)$$

where R_c is the cutoff radius of the nuclear charge distribution. As it follows from Eq. (1.1.30b), NFF can be significantly different from 1 only when the maximum momentum transfer q_{\max} is not much less than $1/R_c$. As it follows from Eq. (1.1.29e), $q_{\max} = p_1 + p_2 + k < 2p_1 = 2/\lambda_1$, where λ_1 is the reduced wavelength of the incident electron (the reduced wavelength is defined as the wavelength divided by 2π). Thus, if $2p_1 \ll 1/R_c$ (or, equivalently, $\lambda_1 \gg 2R_c$), then NFF may be assumed to be equal to 1 (i.e., the nucleus may be approximated by a point charge). Several analytical approximations of the radial dependence of the nuclear charge density and the corresponding expressions of the NFF will be given in Section 1.1.6.

Eq. (1.1.28) is mathematically equivalent to the Bethe-Heitler formula, which was originally derived in [15]. However, Eq. (1.1.28) is more convenient for practical calculations than the Bethe-Heitler formula. The double differential cross section (DDCS) may be calculated by double angular integration of the TDCS with respect to the two independent angles defining the direction of the outgoing electron – θ_2 and the angle between the vectors \mathbf{u} and \mathbf{v} , which will be denoted θ_3 :

$$\frac{d\sigma}{dkd\Omega_k} = \int \frac{d\sigma}{dkd\Omega_k d\Omega_{p_2}} d\Omega_{p_2} \equiv 2 \int_0^\pi d\theta_2 \sin\theta_2 \int_0^\pi \frac{d\sigma}{dkd\Omega_k d\Omega_{p_2}} d\theta_3. \quad (1.1.31a)$$

The integration with respect to θ_3 is from 0 to 2π , but the integrals from 0 to π and from π to 2π are equal to each other, hence Eq. (1.1.31a) includes the integral with respect to θ_3 from 0 to π multiplied by 2. The corresponding expression of the single differential cross section (SDCS) is

$$\frac{d\sigma}{dk} = \int \frac{d\sigma}{dkd\Omega_k} d\Omega_k \equiv 2\pi \int_0^\pi \frac{d\sigma}{dkd\Omega_k} \sin\theta_1 d\theta_1 = 4\pi \int_0^\pi d\theta_1 \sin\theta_1 \int_0^\pi d\theta_2 \sin\theta_2 \int_0^\pi \frac{d\sigma}{dkd\Omega_k d\Omega_{p_2}} d\theta_3. \quad (1.1.31b)$$

In order to determine the limiting behavior of the factor $(F_n - F_e)^2 / q^4$ in Eq. (1.1.28) at $q \rightarrow 0$, it is convenient to express it as $[(F_n - 1) / q^2 + (1 - F_e) / q^2]^2$. The term $(F_n - 1) / q^2$ is finite at $q = 0$. In the case of a neutral atom (or a truncated interaction potential), the term $(1 - F_e) / q^2$ is also finite at $q = 0$. In the case of the exact (not truncated) potential for an ion, the term $(1 - F_e) / q^2$ approaches infinity at $q \rightarrow 0$ as $(Z_i / Z) / q^2$, where Z_i is the ion charge, hence the scaled DDCS and SDCS for an ion diverge in the soft-photon limit (this also holds for the partial-wave result).

If $F_n(q) \equiv 1$ and $F_e(q) \equiv 0$ (the “no-screening approximation”), then the TDCS defined by Eq. (1.1.28) (or by the Bethe-Heitler formula) may be integrated analytically with respect to Ω_{p_2} (see Eq. (1.1.31a)), yielding the following expression of the scaled DDCS [16, 17]:

$$\begin{aligned} \frac{k}{Z^2} \frac{d\sigma}{dkd\Omega_k} &= \frac{\alpha r_e^2}{8\pi} \frac{p_2}{p_1} \left\{ \frac{8 \sin^2 \theta_1 (2E_1^2 + 1)}{p_1^2 d_1^4} - \frac{2(5E_1^2 + 2E_1 E_2 + 3)}{p_1^2 d_1^2} - \frac{2(p_1^2 - k^2)}{Q^2 d_1^2} + \frac{4E_2}{p_1^2 d_1} \right. \\ &+ \frac{1}{p_1 p_2} \ln \left(\frac{E_1 E_2 - 1 + p_1 p_2}{E_1 E_2 - 1 - p_1 p_2} \right) \left[\frac{4E_1 \sin^2 \theta_1 (3k - p_1^2 E_2)}{p_1^2 d_1^4} + \frac{4E_1^2 (E_1^2 + E_2^2)}{p_1^2 d_1^2} \right. \\ &+ \left. \left. \frac{2 - 2(7E_1^2 - 3E_1 E_2 + E_2^2)}{p_1^2 d_1^2} + \frac{2k(E_1^2 + E_1 E_2 - 1)}{p_1^2 d_1} \right] - \frac{4}{p_2 d_1} \ln \left(\frac{E_2 + p_2}{E_2 - p_2} \right) \right. \\ &+ \left. \frac{1}{Q p_2} \ln \left(\frac{Q + p_2}{Q - p_2} \right) \left[\frac{4}{d_1^2} - \frac{6k}{d_1} - \frac{2k(p_1^2 - k^2)}{Q^2 d_1} \right] \right\}, \quad (1.1.32) \end{aligned}$$

where d_1 is given by Eq. (1.1.29d), and

$$Q^2 = p_1^2 + k^2 - 2p_1k \cos \theta_1. \quad (1.1.33)$$

The analytical expression of the DDCS in the screened Born approximation is known only for the case of the screening function equal to a linear combination of N decaying exponentials:

$$\tilde{V}(r) = \sum_{i=1}^N a_i \exp(-b_i r), \quad (1.1.34a)$$

$$\sum_{i=1}^N a_i = 1. \quad (1.1.34b)$$

In this case, the AFF is equal to

$$F_e(q) = 1 - \sum_{i=1}^N a_i \frac{q^2}{q^2 + b_i^2}, \quad (1.1.35)$$

and the corresponding expression of the scaled DDCS is the following [14, 18]:

$$\frac{k}{Z^2} \frac{d\sigma}{dkd\Omega_k} = \sum_{i=1}^N a_i^2 I_1(b_i) + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{a_i a_j}{b_j^2 - b_i^2} [I_2(b_i) - I_2(b_j)], \quad (1.1.36)$$

where

$$\begin{aligned} I_1(b) = & \frac{\alpha r_e^2}{2\pi p_1} \left\{ 16p_2(4E_1^2 + b^2) \frac{p_1^2 \sin^2 \theta_1}{W^4} - \frac{2p_2}{W^2} \left[4E_1^2 + 2E_1E_2 - E_2 \frac{D_1}{k} + b^2 \left(1 - 2E_2 \frac{k}{D_1} \right) \right] \right. \\ & + \frac{2p_2}{W^2} \frac{D_1^2 + 2(E_1E_2 - 1)D_1 + b^2(D_1 - 2E_2k)}{(D_1 + b^2)^2 + 4p_2^2b^2} \left[\frac{1}{D_1} (16E_1E_2 - 4E_1^2b^2 - b^4) - \frac{4E_1^2 + b^2}{k^2W^2} \right. \\ & \times (D_1^2 + 2(E_1E_2 - 1)D_1 + b^2(D_1 - 2E_2k)) \left. \right] - \frac{2k^2p_2}{(D_1 + b^2)^2 + 4p_2^2b^2} \left[\frac{4}{D_1^2} (4E_2^2 + (1 - D_1)b^2) \right. \\ & + \frac{D_1^2 + 2(E_1E_2 - 1)D_1 + b^2(D_1 - 2E_2k)}{D_1(p_1 - k)^2} \left. \right] - \frac{4k}{D_1} \ln(E_2 + p_2) + \frac{L_1}{W} \left[2k + \frac{4k}{D_1} (E_1^2 + p_2^2 + b^2) \right. \\ & + \frac{2}{D_1W^2} (E_1D_1 - 2k + b^2k) \left(8E_1E_2 - \frac{D_1^2}{2} - b^2(2E_1^2 + 2p_2^2 + D_1) - b^4 \right) \\ & + \frac{2(2E_1^2 + b^2)(D_1 - 2E_2k) + D_1^2 + 2(E_1E_2 - 1)D_1}{kW^2} - \frac{3}{kW^4} (4E_1^2 + b^2) \left(E_1 \frac{D_1}{k} - 2 + b^2 \right) \\ & \left. \times (D_1^2 + 2(E_1E_2 - 1)D_1 + b^2(D_1 - 2E_2k)) \right] + \frac{k^2L_2}{D_1|\mathbf{p}_1 - \mathbf{k}|} \left[\frac{2}{D_1} - 2 + \frac{D_1 - 2E_2k}{2(p_1 - k)^2} \right] \left. \right\} \quad (1.1.37) \end{aligned}$$

and

$$\begin{aligned} I_2(b) = & -\frac{\alpha r_e^2}{2\pi p_1} \left\{ \frac{2p_2}{W^2} (4E_1^2 + b^2) \left(E_1 \frac{D_1}{k} - 2 + b^2 \right) + \frac{L_1}{W} \left[k(D_1 + 2b^2) + \frac{2k}{D_1} (b^4 + 2b^2(E_1^2 + p_2^2) - 8E_1E_2) \right. \right. \\ & + \frac{4E_1^2 + b^2}{kW^2} (D_1^2 + 2(E_1E_2 - 1)D_1 + b^2(D_1 - 2E_2k)) \left. \right] + \frac{k^2L_2}{D_1|\mathbf{p}_1 - \mathbf{k}|} \left[\frac{2}{D_1} (4E_2^2 + b^2(1 - D_1)) \right. \\ & \left. + \frac{D_1^2 + 2(E_1E_2 - 1)D_1 + b^2(D_1 - 2E_2k)}{2(p_1 - k)^2} \right] - \frac{4k}{D_1} b^2 \ln(E_2 + p_2) \left. \right\} \quad (1.1.38) \end{aligned}$$

with the auxiliary definitions

$$D_1 = 2k(E_1 - p_1 \cos \theta_1), \quad (1.1.39a)$$

$$W = \left[\left(p_1 \frac{D_1}{k} \right)^2 + 2b^2 \left(E_1 \frac{D_1}{k} - 2 \right) + b^4 \right]^{1/2}, \quad (1.1.39b)$$

$$L_1 = \ln \frac{(E_1 E_2 - 1)D_1 / k + E_2 b^2 + p_2 W}{(E_1 E_2 - 1)D_1 / k + E_2 b^2 - p_2 W}, \quad (1.1.39c)$$

$$L_2 = \ln \frac{(|\mathbf{p}_1 - \mathbf{k}| + p_2)^2 + b^2}{(|\mathbf{p}_1 - \mathbf{k}| - p_2)^2 + b^2}. \quad (1.1.39d)$$

1.1.3. The approximations based on the Sommerfeld-Maue wave functions

The Sommerfeld-Maue (SM) Coulomb wave functions [19, 20, 21] are a closed-form approximation to the continuum solutions of the Dirac equation in the case of a point-Coulomb potential (an exact solution of the Dirac equation for the continuum cannot be obtained in a closed form and can only be expressed as a sum of partial waves, even in the case of the point-Coulomb field). In terms of the perturbation theory, the dominant part of the SM wave function is the zero-order term of the perturbative expansion of the exact wave function in powers of αZ (see Eq. (1.1.26)), and the other part of the SM wave function is the first-order term of the mentioned expansion. Thus, the primary difference between the SM theory and the Born approximation is a different definition of the expansion point ψ_0 . In the Born approximation, ψ_0 is a plane wave describing a free electron, whereas in the SM theory ψ_0 is a zero-order approximation of the “distorted” wave describing an electron interacting with the point-Coulomb potential, and hence is more suited for the problem of calculating the differential cross section of bremsstrahlung.

The expression of the scaled TDCS of bremsstrahlung for the case of the point-Coulomb potential (i.e., in absence of screening by the atomic electrons) without any further approximations, beyond the use of the SM wave functions, was obtained by Elwert and Haug [21]. Following [14], this expression will be called the “leading-order” (LO) result. It is given below [14, 22]:

$$\begin{aligned} \frac{k}{Z^2} \frac{d\sigma_{\text{LO}}}{dk d\Omega_k d\Omega_{p_2}} &= \frac{\alpha r_e^2}{4\pi^2} \frac{p_2}{p_1} \frac{N}{q^4} \left\{ [E_1 E_2 - 1 - (\mathbf{p}_1 \cdot \hat{\mathbf{k}})(\mathbf{p}_2 \cdot \hat{\mathbf{k}})] |J_1|^2 + [E_1 E_2 + 1 + (\mathbf{p}_1 \cdot \hat{\mathbf{k}})(\mathbf{p}_2 \cdot \hat{\mathbf{k}})] (|J_2|^2 + |J_3|^2) \right. \\ &+ 2 \operatorname{Re}[(\mathbf{J}_3 - \mathbf{J}_2) \cdot (\mathbf{p}_1 (\mathbf{J}_2 \cdot \hat{\mathbf{k}}) (\mathbf{p}_2 \cdot \hat{\mathbf{k}}) - \mathbf{p}_2 (\mathbf{J}_3 \cdot \hat{\mathbf{k}}) (\mathbf{p}_1 \cdot \hat{\mathbf{k}})) - (E_1 E_2 + 1 + \mathbf{p}_1 \cdot \mathbf{p}_2) (\mathbf{J}_2 \cdot \hat{\mathbf{k}}) (\mathbf{J}_3^* \cdot \hat{\mathbf{k}}) \\ &+ (\mathbf{J}_2 \cdot \mathbf{p}_1) (\mathbf{J}_3^* \cdot \mathbf{p}_2) - (\mathbf{J}_2 \cdot \mathbf{p}_2) (\mathbf{J}_3^* \cdot \mathbf{p}_1) + E_1 J_1^* (\mathbf{J}_3 \cdot \mathbf{p}_2 - (\mathbf{J}_2 \cdot \hat{\mathbf{k}}) (\mathbf{p}_2 \cdot \hat{\mathbf{k}})) \\ &\left. + E_2 J_1^* (\mathbf{J}_2 \cdot \mathbf{p}_1 - (\mathbf{J}_3 \cdot \hat{\mathbf{k}}) (\mathbf{p}_1 \cdot \hat{\mathbf{k}})) + (\mathbf{J}_2 \cdot \mathbf{J}_3) (\mathbf{p}_1 \cdot \mathbf{p}_2 - (\mathbf{p}_1 \cdot \hat{\mathbf{k}}) (\mathbf{p}_2 \cdot \hat{\mathbf{k}})) \right\}, \quad (1.1.40) \end{aligned}$$

where

$$\hat{\mathbf{k}} = \mathbf{k} / k \quad (1.1.41)$$

and the other auxiliary quantities are defined as follows:

$$N = \frac{4\pi^2 a_1 a_2}{(e^{2\pi a_1} - 1)(1 - e^{-2\pi a_2})}, \quad (1.1.42a)$$

$$a_1 = (E_1 / p_1) \alpha Z, \quad (1.1.42b)$$

$$a_2 = (E_2 / p_2) \alpha Z, \quad (1.1.42c)$$

$$J_1 = 2 \left(\frac{E_2}{d_1} - \frac{E_1}{d_2} \right) (V + i a_2 x W) + i \frac{2W}{\mu} \left[E_1 a_2 \left(\frac{\mu}{d_2} - 2k \right) - E_2 a_1 \left(\frac{\mu}{d_1} + 2k \right) \right], \quad (1.1.42d)$$

$$\mathbf{J}_2 = \frac{V + i a_2 x W}{d_2} \mathbf{q} - \frac{i a_2 W}{\mu} \left[\left(\frac{\mu}{d_2} - 2k \right) \mathbf{q} - \frac{2k}{p_1} \mathbf{P} \right], \quad (1.1.42e)$$

$$\mathbf{J}_3 = \frac{V + i a_2 x W}{d_1} \mathbf{q} - \frac{i a_1 W}{\mu} \left[\left(\frac{\mu}{d_1} + 2k \right) \mathbf{q} - \frac{2k}{p_2} \mathbf{P} \right], \quad (1.1.42f)$$

$$\mu = 2(E_1 E_2 + p_1 p_2 - 1), \quad (1.1.42g)$$

$$\mathbf{P} = p_1 \mathbf{p}_2 + p_2 \mathbf{p}_1, \quad (1.1.42h)$$

$$V = F(-i a_1, i a_2; 1; x), \quad (1.1.42i)$$

$$W = F(1-ia_1, 1+ia_2; 2; x), \quad (1.1.42j)$$

$$x = 1 - \frac{4k^2 d_1 d_2}{\mu q^2}, \quad (1.1.42k)$$

and $d_{1,2}$ are defined by Eq. (1.1.29d). It should be noted that the definitions of J_1 , J_2 and J_3 (1.1.42d–f) differ from the corresponding definitions presented in [14, 22] by an additional factor $2kq^2$, whereas the expression (1.1.40) differs from the corresponding expression of [14, 22] by an additional overall factor $1/(4k^2 q^4)$, so that Eq. (1.1.40) is mathematically equivalent to the corresponding formula of [14, 22].

If the value of x defined by Eq. (1.1.42k) is close to 1, then the direct computation of the hypergeometric series in Eqs. (1.1.42i) and (1.1.42j) may become too time-consuming, because the convergence of the hypergeometric series slows down as its argument approaches 1. As suggested in [23], it is then advantageous to use the following transformation formula [24, Eq. (9.131.2)]:

$$\begin{aligned} F(a, b; c; x) &= \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} F(a, b; a+b-c+1; 1-x) \\ &+ (1-x)^{c-a-b} \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} F(c-a, c-b; c-a-b+1; 1-x). \end{aligned} \quad (1.1.43)$$

When x is close to 1, the argument of the two hypergeometric series on the right-hand side of Eq. (1.1.43) is close to 0, which ensures their fast convergence.

An expression of a correction to the expression (1.1.40) was derived in [23]. This correction was calculated by including the term proportional to $(\alpha Z)^2$ in the expression of the wave function. Unlike Eq. (1.1.40), the mentioned correction is valid only for high electron energies ($E_2 \gg 1$). As in the case of Eq. (1.1.40), the point-Coulomb potential is assumed. Following [14], this correction will be called the “next-to-leading-order” (NLO) result. It is given below [14]:

$$\begin{aligned} \frac{k}{Z^2} \frac{d\sigma_{\text{NLO}}}{dk d\Omega_k d\Omega_{p_2}} &= \alpha^2 Z r_e^2 \frac{p_2}{p_1} N \frac{(\mathbf{q} \cdot \hat{\mathbf{k}})}{4q d_1 d_2} \left\{ \frac{1}{\pi q^2} \text{Re} \left[((E_1 E_2 - 1 - (\mathbf{p}_1 \cdot \hat{\mathbf{k}})(\mathbf{p}_2 \cdot \hat{\mathbf{k}})) J_1 \right. \right. \\ &\left. \left. + E_1 (\mathbf{J}_3 \cdot \mathbf{p}_2 - (\mathbf{J}_2 \cdot \hat{\mathbf{k}})(\mathbf{p}_2 \cdot \hat{\mathbf{k}})) + E_2 (\mathbf{J}_2 \cdot \mathbf{p}_1 - (\mathbf{J}_3 \cdot \hat{\mathbf{k}})(\mathbf{p}_1 \cdot \hat{\mathbf{k}})) e^{i\Phi} \right] \right\}, \end{aligned} \quad (1.1.44)$$

where

$$\Phi = a_1 \ln \left(\frac{q^2}{2k d_2} \right) - a_2 \ln \left(\frac{\mu}{2k d_2} \right). \quad (1.1.45)$$

It should be noted that expression (1.1.44) does not include an extra “next-to-next-to-leading order” (NNLO) term, which includes the factor Z^2 and which is included in the original definition of the NLO correction [14, 23]. The mentioned NNLO term has been omitted, because it is known that inclusion of the NNLO term causes inaccuracies of the DDCS at large angles [25]. Those errors are caused by exclusion of other NNLO terms of the same order with respect to Z [25].

No analytical expression of the DDCS based on the SM wave functions is known. This means that the DDCS must be calculated by numerical integration of (1.1.40) (or of the sum of (1.1.40) and (1.1.44)) with respect to Ω_{p_2} (see Eq. (1.1.31a)).

The expressions of the TDCS (1.1.40) and (1.1.44) are valid only for the pure Coulomb field (without screening). As shown in [26], the screening correction of the DDCS at high energies (~ 1 MeV and higher) in the theory based on the SM wave functions is approximately the same as in the Born approximation. I.e., the screening of the nuclear charge by the electrons can be approximately taken into account by writing the DDCS of bremsstrahlung as follows [14, 26]:

$$\left(\frac{d\sigma}{dk d\Omega_k} \right)_{\text{exact}}^{\text{screened}} \approx \left(\frac{d\sigma}{dk d\Omega_k} \right)_{\text{exact}}^{\text{no screening}} + \left[\left(\frac{d\sigma}{dk d\Omega_k} \right)_{\text{Born}}^{\text{screened}} - \left(\frac{d\sigma}{dk d\Omega_k} \right)_{\text{Born}}^{\text{no screening}} \right], \quad (1.1.46)$$

where the subscript “exact” refers to the exact value of the DDCS calculated using the SM wave functions. This additivity rule cannot be applied to the TDCS [26].

Note: The analytical expression of the SM DDCS without screening (the first term on the right-hand side of Eq. (1.1.46)) is known only for the case of a point nucleus. In the code of BREMS, the first term in brackets in Eq. (1.1.46) may optionally correspond to a finite nucleus (with the nuclear form factor calculated according to Eq. (1.1.30b)). However, the second term in brackets always corresponds to the unscreened point-nucleus approximation, given by Eq. (1.1.32).

1.1.4. The Elwert factor

In the case of the pure Coulomb potential and non-relativistic speed of the outgoing electron, the Sommerfeld-Maue approximation is superior to the Born approximation, especially when $Z\alpha \ll 1$. However, a modification of the Born-approximation TDCS (1.1.28) suggested in [27] extends its usefulness to non-relativistic speeds of the electron. It consists in multiplication of the expression (1.1.28) by a factor depending only on the two values of the ‘‘Coulomb parameter’’ $\nu \equiv Z\alpha / \beta$ corresponding to the initial and final values of the electron speed. This factor, which is usually called the ‘‘Elwert factor’’, is equal to

$$f_E(\nu_1, \nu_2) = \frac{\nu_2}{\nu_1} \frac{1 - \exp(-2\pi\nu_1)}{1 - \exp(-2\pi\nu_2)}, \quad (1.1.47)$$

where

$$\nu_1 \equiv \frac{Z\alpha}{\beta_1} \equiv \frac{Z\alpha E_1}{p_1}, \quad \nu_2 \equiv \frac{Z\alpha}{\beta_2} \equiv \frac{Z\alpha E_2}{p_2}. \quad (1.1.48)$$

As explained in [28], this modification improves the accuracy of the Born approximation at low energies, especially in the ‘‘tip region’’ of the photon spectrum, i.e., when $T_2 \ll T_1$. Consequently, BREMS applies the Elwert factor to the Born-approximation TDCS, DDCS and SDCS by default, including the additive screening correction in the SM theory (the expression in brackets in Eq. (1.1.46)).

When the speed of the outgoing electron is relativistic, the application of the Elwert factor does not have a significant effect on the value of the differential cross section of bremsstrahlung, because then $\nu_1 \approx \nu_2 \approx Z\alpha$, so that $f_E \approx 1$. In the ‘‘soft-photon limit’’ $k = 0$, the Elwert factor is also equal to 1, because then ν_1 and ν_2 are equal to each other (independently of the electron speed).

1.1.5. The interaction potential in the point-nucleus approximation

One of the most accurate approximations of the interaction potential is the Kohn-Sham (KS) potential [4, 5], which was used for the calculations reported in [1] and in the subsequent works by Tseng and Pratt. According to the Kohn-Sham theory [4], the total potential acting upon an electron in an atom consists of three terms:

$$V(\mathbf{r}) = -\frac{\alpha Z}{r} + \alpha \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \mu_x(n(\mathbf{r})), \quad (1.1.49)$$

where the first term is the potential due to the point charge of the nucleus, the second term is the electrostatic potential due to all electrons of the atom (n is the electron density), and the third term is a local approximation to the exchange potential. As shown in [4] (using the variational principle), the assumption of a slowly varying electron density in conjunction with the approximation of an inhomogeneous electron gas leads to the following expression of the exchange potential:

$$\mu_x(n(\mathbf{r})) = -\alpha \frac{[3\pi^2 n(\mathbf{r})]^{1/3}}{\pi}. \quad (1.1.50)$$

An expression of the exchange potential differing from Eq. (1.1.50) only by an additional factor of $3/2$ had been earlier obtained by Slater [29] on the basis of the Hartree-Fock equations, using the approximation of free electron gas and the concept of an ‘‘exchange hole’’ (a decrease of the number of electrons with the same spin orientation as the investigated electron in the vicinity of the latter). It was proved in [4] formally that usage of the expression (1.1.50) for the estimation of the self-consistent potential $V(\mathbf{r})$ by iterative solution of the one-electron wave equation (or, equivalently, by

applying the variational principle) gives the exchange correction of the electron density that is more accurate than that obtained using the expression by Slater.

Due to the spherical symmetry of $n(\mathbf{r})$, Eq. (1.1.49) may be rewritten as follows:

$$V(r) = -\frac{\alpha Z}{r} + 4\pi\alpha \left[\frac{1}{r} \int_0^r n(r') r'^2 dr' + \int_r^\infty n(r') r' dr' \right] + \mu_x(n(r)). \quad (1.1.51)$$

Apart from the differences in notations and units, this expression coincides with Eq. (3.1d) in [1] (where the KS potential was referred to as the “modified Hartree-Fock-Slater” potential).

For comparison with the KS potential, the Thomas-Fermi-Csavinszky (TFC) potential [3] will be used (in [1], it was referred to as the “modified Thomas-Fermi” potential). The TFC potential is intended as a replacement for the Thomas-Fermi (TF) potential [30, 31, 32]. In the Thomas-Fermi atomic model, the electrons are regarded as forming an ideal gas satisfying the Fermi statistics and occupying the region of phase space of lowest energy. This region of phase space is assumed to be saturated, with two electrons with opposite spins in each unit volume, and the remainder is assumed to be empty. As noted in [3], a shortcoming of the TF theory is that it leads to a radial electron density which decreases as the inverse fourth power of the distance from the nucleus, whereas the quantum mechanics requires an exponential decrease. This shortcoming is overcome in [3] by replacing the TF differential equation for the screening function $\tilde{V}(r)$ with an equivalent variational principle (i.e., defining a functional $L(\tilde{V})$ such that the corresponding Euler-Lagrange equation coincides with the TF equation), choosing a trial function subject to the requirement that it both satisfies the boundary conditions of the TF equation and has the desirable asymptotic behavior, and then extremalizing the functional with respect to the unknown parameters of the trial function subject to the subsidiary condition that the electron density is normalized. The trial function that satisfies the mentioned requirements is the following three-parameter function:

$$\tilde{V}(r) = [c_1 e^{-c_2 a_0 r} + (1 - c_1) e^{-c_3 a_0 r}]^2, \quad (1.1.52)$$

where

$$a_0 = 2\left(\frac{3}{4}\pi\right)^{-2/3} \alpha Z^{1/3}. \quad (1.1.53)$$

After substituting the values of c_1 , c_2 and c_3 that extremalize the mentioned functional subject to the subsidiary condition, the following expression of the screening function is obtained [3]:

$$\tilde{V}(r) = (0.7111 e^{-0.175 a_0 r} + 0.2889 e^{-1.6625 a_0 r})^2, \quad (1.1.54)$$

so that the potential function is

$$V(r) \equiv -\frac{Z\alpha}{r} \tilde{V}(r) = -\frac{Z\alpha}{r} (0.7111 e^{-0.175 a_0 r} + 0.2889 e^{-1.6625 a_0 r})^2. \quad (1.1.55)$$

As shown in [3], the screening function defined by Eq. (1.1.54) is within 5% of the exact solution $\tilde{V}_0(a_0 r)$ of the TF equation (the so-called “Thomas-Fermi universal function”) at radii $r < 1.8 / a_0$, and within 15% at $r < 7.5 / a_0$. At greater radii, the exponential decrease of (1.1.54) becomes much faster than the decrease of $\tilde{V}_0(a_0 r)$. The simplicity of the TFC potential function (1.1.55) makes it attractive from the computational point of view for solving the system of differential equations (1.1.16a,b). However, since it is an approximation to the simplified TF model of the atom, it is less accurate than the KS potential. Consequently, BREMS uses the KS potential by default.

Applications of the Thomas-Fermi and Kohn-Sham potentials for atomic systems often include a so-called “tail correction” [5, 33, 34], whose purpose is to take into account absence of the electrostatic self-interaction of the electron. This is achieved by changing the asymptotic form of the potential function at large radii, i.e., by making it go to zero as $-\alpha/r$ (i.e., as the potential function of a positive elementary charge) rather than exponentially. A modification of the Kohn-Sham variational method by addition of the tail correction was described in [5, 34]. It consists in dividing the atom into two parts by a sphere centered on the nucleus, with the radius R chosen so that on the average there is one electron outside the sphere. Then the assumption of no self-interaction of the charge outside the sphere leads to the mentioned result (i.e., $V(r) = -\alpha/r$ when $r > R$). Clearly, the tail correction is not appropriate when describing interaction of an extraneous

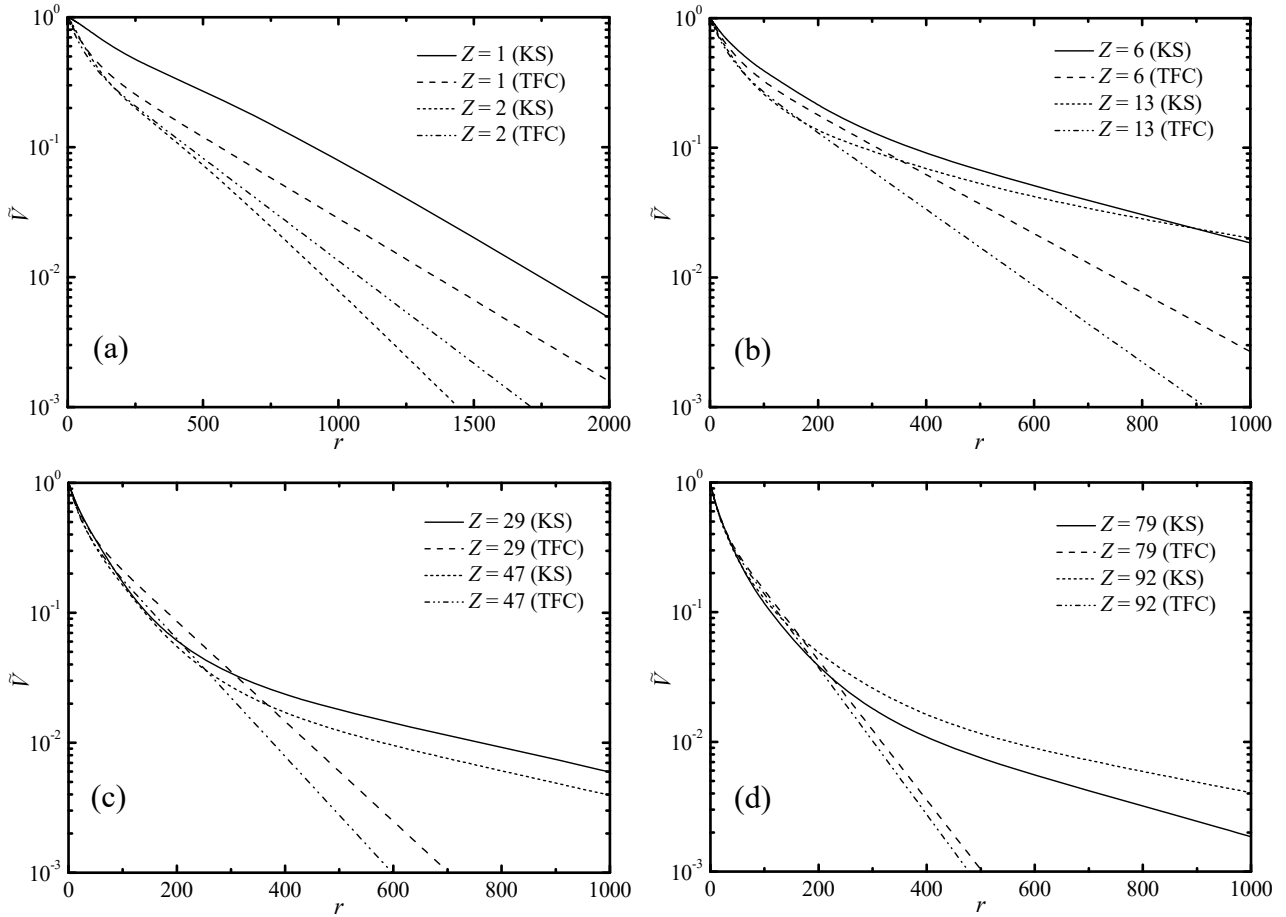


Fig. 1. Comparison of the Kohn-Sham (KS) and Thomas-Fermi-Csavinszky (TFC) screening functions for: (a) $Z = 1$ (hydrogen) and $Z = 2$ (helium), (b) $Z = 6$ (carbon) and $Z = 13$ (aluminum), (c) $Z = 29$ (copper) and $Z = 47$ (silver), (d) $Z = 79$ (gold) and $Z = 92$ (uranium).

electron with a neutral atom (for example, in the case of the hydrogen atom, $R = 0$ and the tail correction becomes equivalent to a complete absence of screening). The program described in [5], which was used for generating the tables with the values of the KS potential used by BREMS, has an option to calculate either the original KS potential (1.1.51), or the potential with the tail correction (thus modified KS potential is called “new potential” in [5, 34]). The KS potential used in BREMS, as well as the potential used in the works cited herein, was constructed according to the original definition (1.1.51) (which does not have the tail correction) by the relativistic (Dirac) self-consistent calculation with a local approximation to the exchange potential defined by Eq. (1.1.50).

Fig. 1 shows the KS and TFC screening functions (\tilde{V}_{KS} and \tilde{V}_{TFC} , respectively) as functions of r for 8 values of Z from 1 to 92. In all cases excluding $Z = 1$, the relative difference of the two functions at $r < 200$ is less than 30 %, and in most of those cases the relative difference is less than 10 % at $r < 200$. Since r is expressed in units of αa_{B} , where a_{B} is the Bohr radius, the mentioned range of r approximately corresponds to $r < 1.5 a_{\text{B}}$. At larger values of r , $\tilde{V}_{\text{KS}} > \tilde{V}_{\text{TFC}}$, except in the case $Z = 2$, when $\tilde{V}_{\text{KS}} < \tilde{V}_{\text{TFC}}$, and the ratio of the two functions increases exponentially with increasing r . The magnitude of this divergence increases with increasing Z . In the case $Z = 1$, the ratio $\tilde{V}_{\text{KS}} / \tilde{V}_{\text{TFC}}$ is roughly constant (between 2 and 3) when $r > 200$.

1.1.6. The finite-nucleus interaction potential and the nuclear form factor

The nuclear charge distribution may be taken into account by modifying Eq. (1.1.49) as follows:

$$V(\mathbf{r}) = \alpha \int \frac{n(\mathbf{r}') - \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \mu_x(\tilde{n}(\mathbf{r})), \quad (1.1.56)$$

where $\rho(\mathbf{r})$ is the proton density. Eq. (1.1.49) is a special case of Eq. (1.1.56), corresponding to the point-nucleus approximation $\rho(\mathbf{r}) = Z\delta(\mathbf{r})$, where $\delta(\mathbf{r})$ is the three-dimensional Dirac delta function. Eq. (1.1.56) can be written as a sum of electron potential $V_e(\mathbf{r})$ and nuclear potential $V_n(\mathbf{r})$:

$$V(\mathbf{r}) = V_e(\mathbf{r}) + V_n(\mathbf{r}), \quad (1.1.57)$$

where

$$V_e(\mathbf{r}) = \alpha \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' + \mu_x(n(\mathbf{r})), \quad (1.1.58)$$

$$V_n(\mathbf{r}) = -\alpha \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'. \quad (1.1.59)$$

Since $n(\mathbf{r})$ and $\rho(\mathbf{r})$ are spherically symmetric, Eqs. (1.1.58) and (1.1.59) can be written as follows:

$$V_e(r) = 4\pi\alpha \left[\frac{1}{r} \int_0^r n(r') r'^2 dr' + \int_r^\infty n(r') r' dr' \right] + \mu_x(n(r)), \quad (1.1.60)$$

$$V_n(r) = -4\pi\alpha \left[\frac{1}{r} \int_0^r \rho(r') r'^2 dr' + \int_r^\infty \rho(r') r' dr' \right]. \quad (1.1.61)$$

According to Eq. (1.1.57), the overall screening function can be written as a sum of the point-nucleus screening function $\tilde{V}_p(r)$ and the ‘‘finite-nucleus correction’’ $\Delta\tilde{V}_f(r)$:

$$\tilde{V}(r) \equiv \frac{V(r)}{-Z\alpha/r} = \tilde{V}_p(r) + \Delta\tilde{V}_f(r), \quad (1.1.62)$$

where

$$\tilde{V}_p(r) \equiv \frac{V_e(r)}{-Z\alpha/r} + 1, \quad (1.1.63)$$

$$\Delta\tilde{V}_f(r) \equiv \frac{V_n(r)}{-Z\alpha/r} - 1. \quad (1.1.64)$$

By substituting Eq. (1.1.61) into Eq. (1.1.64), the following expression of $\Delta\tilde{V}_f(r)$ is obtained:

$$\Delta\tilde{V}_f(r) = \frac{4\pi}{Z} \left[\int_0^r \rho(r') r'^2 dr' + r \int_r^\infty \rho(r') r' dr' \right] - 1. \quad (1.1.65)$$

This function increases monotonously from -1 at $r = 0$ to 0 at $r \geq R_c$, where R_c is the cutoff radius of the nuclear charge distribution. Consequently, $\tilde{V}(r)$ is identical to $\tilde{V}_p(r)$ outside the nucleus, i.e.,

$$\tilde{V}(r) \Big|_{r > R_c} \equiv \tilde{V}_p(r). \quad (1.1.66)$$

Since \tilde{V}_p is equal to 1 at $r = 0$, the overall screening function (1.1.62) is equal to zero at $r = 0$. Inside the nucleus (i.e., at $r < R_c$), $\tilde{V}(r)$ is monotonously increasing. Its maximum value is reached near the cutoff radius of the nuclear charge distribution (at $r \approx R_c$). When electron screening is present, the maximum value of \tilde{V} is slightly less than 1 , and $\tilde{V}(r)$ is monotonously decreasing outside the nucleus (i.e., at $r > R_c$).

As mentioned in Section 1.1.2, the point-nucleus approximation is acceptable if the reduced wavelength $\hat{\lambda}_1$ of the incident electron is much greater than the nuclear radius. In the code of BREMS, the point-nucleus approximation is applied by default when $\hat{\lambda}_1$ exceeds the mean nuclear radius R_n by a factor of at least 40 (values of T_1 corresponding to $\hat{\lambda}_1 / R_n = 40$ vary from 0.4 MeV for $Z = 100$ to 4 MeV for $Z = 1$). Otherwise, the Fermi distribution [35] is used by default:

$$\rho_F(r) = \frac{\rho_0}{\exp[(r - R_n)/z] + 1}, \quad z = t / (4 \ln 3). \quad (1.1.67a)$$

This charge density is nearly uniform near $r = 0$ and falls off smoothly at the surface of the nucleus. In Eq. (1.1.67a), R_n is the mean radius of the nucleus, t is the “skin thickness”, which is defined as the distance over which ρ_F drops from 90 % to 10 % of its maximum value, and ρ_0 is a normalization constant. The empirical values of R_n , t , and z are the following [35]:

$$R_n = 1.07 A^{1/3} \text{ fm}, \quad t = 2.4 \text{ fm}, \quad z = 0.546 \text{ fm}. \quad (1.1.67b)$$

In addition, following the example of the elastic-scattering code ELSEPA [36], BREMS provides an option to choose two other approximations of the radial dependence of the nuclear charge density. The simplest one is the uniform distribution [36], corresponding to the representation of the nucleus as a uniformly charged sphere of radius

$$R_U = R_n \sqrt{\frac{1 + (2.5s^2 / R_n^2)}{1 + (0.75s^2 / R_n^2)}} \quad (1.1.68a)$$

with

$$R_n = 1.07 A^{1/3} \text{ fm}, \quad s = 2 \text{ fm}. \quad (1.1.68b)$$

The corresponding proton density is

$$\rho_U(r)|_{r \leq R_U} = Z \frac{3}{4\pi R_U^3}. \quad (1.1.68c)$$

The third analytical approximation of the radial dependence of proton density implemented in BREMS is the so-called “uniform-uniform” (Uu) distribution proposed by Helm [37]. This function is defined as the convolution of two uniform distributions:

$$\rho_{Uu}(r) = Z \int \rho_1(\mathbf{r}') \rho_2(\mathbf{r} - \mathbf{r}') d\mathbf{r}', \quad (1.1.69a)$$

where ρ_1 and ρ_2 are uniform distributions (normalized to unity) over spheres of radii R_1 and R_2 . I.e., the expressions of ρ_1 and ρ_2 are obtained from Eq. (1.1.68c) with $Z = 1$, by replacing R_U with R_1 or R_2 , respectively. With the values

$$R_1 = 0.962 R_n + 0.435 \text{ fm}, \quad R_2 = 2 \text{ fm}, \quad (1.1.69b)$$

Helm’s uniform-uniform distribution gives nearly the same mean radius and skin thickness as the Fermi distribution (1.1.67a–b). If $R_1 > R_2$, then

$$\rho_{Uu}(r) = \begin{cases} \rho_{12} & \text{if } r < R_1 - R_2, \\ \rho_{12} \frac{[(r + R_1)^2 - R_2^2 + 2rR_1][(r - R_1)^2 - R_2^2]^2 + [(r + R_2)^2 - R_1^2 + 2rR_2][(r - R_2)^2 - R_1^2]^2}{32r^3 R_2^3} & \text{if } R_1 - R_2 < r < R_1 + R_2, \\ 0 & \text{if } r > R_1 + R_2, \end{cases} \quad (1.1.69c)$$

where ρ_{12} is a normalization constant. If $R_1 < R_2$, then the expression of $\rho_{Uu}(r)$ can be obtained by interchanging R_1 and R_2 in Eq. (1.1.69c).

The uniform distribution (1.1.68c) results in a simple analytical expression of the finite-nucleus correction (1.1.65):

$$\Delta \tilde{V}_{f,U}(r) = \begin{cases} \frac{r}{2R_U} \left[3 - \left(\frac{r}{R_U} \right)^2 \right] - 1 & \text{if } r \leq R_U, \\ 0 & \text{if } r > R_U. \end{cases} \quad (1.1.70)$$

The finite-nucleus corrections corresponding to the Fermi distribution (1.1.67a) and Helm’s Uu distribution (1.1.69c) are obtained in BREMS by numerical calculation of the integrals in Eq. (1.1.65) (the Helm’s Uu distribution (1.1.69c) can also be integrated analytically, but the resulting expression of $\Delta \tilde{V}_f(r)$ is too cumbersome).

By substituting Eq. (1.1.68c) into the expression of the nuclear form factor (1.1.30b), the following expression of the NFF corresponding to the uniform proton density is obtained:

$$F_{n,U}(R_U; q) = \frac{4\pi}{Z} \int_0^{R_U} \rho_U(r) \frac{\sin qr}{qr} r^2 dr = \frac{3}{(R_U q)^3} [\sin(R_U q) - R_U q \cos(R_U q)]. \quad (1.1.71)$$

Since the form factor of a convolution of any two distributions is equal to the product of the corresponding two form factors, the analytical expression of the NFF corresponding to the Helm's Uu distribution (1.1.69a) is calculated as a product of form factors of two uniform distributions (1.1.68c), where R_U is replaced with R_1 and R_2 , respectively:

$$F_{n, Uu}(q) = F_{n, U}(R_1; q) F_{n, U}(R_2; q), \quad (1.1.72)$$

where the two factors on the right-hand side are calculated according to Eq. (1.1.71). In the case of the default Fermi distribution, the general expression of the NFF (1.1.30b) is calculated by numerical quadrature.

1.2. The numerical methods

When $k \neq 0$, the calculation of the S integrals (1.1.15) is the most time-consuming part. By default, the system (1.1.16a,b) of ordinary differential equations (ODEs) is solved by expanding the functions g_κ and f_κ in powers of the radial coordinate r at discrete values of r [9]. The power-series coefficients are calculated using the recurrence relations derived from the coupled Dirac equations (1.1.16a,b) and from the power-series expansion of the screening function (1.1.17), similarly to the approach applied in [38, 39, 40]). The mentioned system of ODEs is solved simultaneously for the entire range of values of κ_1 and κ_2 specified by the user (i.e., multiple systems of ODEs corresponding to both values of E and all values of κ are solved simultaneously). If $k \neq 0$, then the S integrals (1.1.15) are calculated (i.e., incremented in predefined steps of r) for the user-specified range of values of κ_1 , κ_2 and l simultaneously with the process of solving the ODEs. The solutions of (1.1.16a,b) are periodically compared with the asymptotic form (1.1.18). As proposed in [2], the range of validity of the asymptotic expressions (1.1.18) can be extended to smaller values of r by assuming that A_κ and $\bar{\delta}_\kappa$ are not constants, but are functions of r instead, tending to constant values at $r \rightarrow \infty$ if $|V(r)|$ decreases faster than $1/r$. These functions have a well-defined form, making it possible to determine the limiting values of A_κ and $\bar{\delta}_\kappa$ without excessive computation time, which would be needed for numerical integration of the system of equations (1.1.16a,b) to large values of r , where A_κ and $\bar{\delta}_\kappa$ become practically constant. In addition, the assumption that $\bar{\delta}_\kappa$ is a function of r makes it possible to use Eqs. (1.1.18) in the case of unscreened point-Coulomb potential, too, by choosing an appropriate form of $\bar{\delta}_\kappa(r)$ (see Eq. (1.1.21)). Both A_κ and $\bar{\delta}_\kappa$ include a constant term and an oscillating term with the oscillation period equal to π/p and the oscillation amplitude tending to zero with increasing r [2] (the average value of the oscillating term is zero). In addition, $\bar{\delta}_\kappa$ includes a monotonously increasing term Q , which is called the ‘‘phase correction integral’’ [2]:

$$\bar{\delta}_\kappa = \tilde{\delta}_\kappa + Q(r), \quad (1.2.1)$$

where

$$Q(r) = \begin{cases} \nu \ln 2pr & \text{for point-Coulomb field,} \\ -\nu \int_r^\infty \frac{\tilde{V}(w)}{w} dw & \text{for screened fields.} \end{cases} \quad (1.2.2)$$

Further on, notation $\tilde{\delta}_\kappa$ will be used to mean the average value of the first term in Eq. (1.2.1), i.e., its value at large r , where the oscillation amplitude has decayed to zero (for screened potentials, thus defined $\tilde{\delta}_\kappa$ is equal to the limiting value of $\bar{\delta}_\kappa$, because in this case $\lim_{r \rightarrow \infty} Q(r) = 0$). Similarly, notation A_κ will be used to mean the constant term in the oscillating factor $A_\kappa(r)$ in Eqs. (1.1.18), i.e., the average value of that factor. When it is determined that the asymptotic form has been attained for a particular combination of values of E and κ (i.e., when the range of variation of the estimates of A_κ and $\tilde{\delta}_\kappa$ over the last 10 ‘‘test’’ points becomes less than the predefined tolerances), the value of $\tilde{\delta}_\kappa$ is stored in the array of phase shifts, the corresponding wave function is normalized by multiplying it (and the S integrals using it) by $1/A_\kappa$, and the program switches from the numerical solution algorithm to the expressions (1.1.18) for calculation of the corresponding wave

function (the factor A_κ cancels out, because the wave function is multiplied by $1/A_\kappa$). The algorithm used for calculating the spherical Bessel functions of the first kind $j_n(pr)$ in Eqs. (1.1.18) depends on the values of pr and $\max(n)$. When $pr \leq \max(n)$, $j_n(pr)$ are calculated using backward recursion, otherwise $j_n(pr)$ are calculated using forward recursion [41, 42]. The spherical Bessel functions of the second kind $y_n(pr)$ are always calculated using forward recursion. Both $j_n(pr)$ and $y_n(pr)$ are calculated using quadruple precision arithmetic.

The spherical Bessel functions $j_l(kr)$, which appear in the integrands of the S integrals (1.1.15), are calculated in the same way as the electron wave functions g_κ and f_κ , i.e., by the power-series method. The corresponding differential equations can be obtained from the well-known expressions of derivatives of the spherical Bessel functions, or by making the following changes in the coupled radial Dirac equations (1.1.16a,b): (a) “ $(E \pm 1)$ ” is replaced by the photon energy k , (b) $V(r) \equiv 0$, (c) $\kappa = l$ (assuming that $l \geq 1$). Then the “ g_l ” and “ f_l ” components of the solution are proportional to $j_l(kr)$ and $j_{l-1}(kr)$, respectively (this is obvious from the expressions (1.1.18) with $\bar{\delta}_\kappa = 0$). In comparison with the recursion methods, the power-series method is much less prone to the accumulation of rounding errors and hence is more accurate.

The integrals are calculated using the 10th order Newton-Cotes (NC) formula (as in [1]). The default initial step size of the NC integration is $\Delta r_{\text{NC}} = \min(0.1/p_1, 0.1)$. This step size is based on a trade-off between accuracy and performance (the indicated NC integration step size is approximately the same as in [1], where it was $\pi/(32p_1)$). It may be modified by the user. A decrease of the step size would make the numerical integration more accurate, but also proportionally longer. As reported in [1], variation of the NC integration step from $\pi/(128p_1)$ to $\pi/(16p_1)$ caused fluctuation of the results by $O(0.1\%)$ for $\sigma(k)$, $O(1\%)$ for $\sigma(k, \theta)$ with small and large photon angles, and $O(0.1\%)$ for intermediate angles (here, “ $O(x)$ ” means the order of x).

The first part of the integration ends after all wave functions attain the asymptotic form (1.1.18) and (in the case of screened interaction potentials) after the absolute values of both phase correction integrals Q (corresponding to energies E_1 and E_2) become less than the predefined small value (10^{-8} by default). It is also possible to end the first part of the integration at a user-specified value of $r = r_0$. In the case of the point-Coulomb field, $Q(r)$ does not have a limiting value. This is one of the reasons why the point-Coulomb interaction potential usually has to be “truncated”, i.e., set to zero for $r > R_a$. A judicious choice of the cutoff radius R_a may cause a significant decrease of the processing time without a significant effect on the accuracy of the results (not only in the case of the point-Coulomb potential, but also in the case of screened potentials). If $r_0 \geq R_a$, then the iterative phase matching described above becomes unnecessary: if $r \geq R_a$, then expressions (1.1.18) are exact and the values of A_κ and $\bar{\delta}_\kappa$ do not oscillate, hence they are determined from the values of g_κ and f_κ at $r = R_a$ (in order to ensure maximum accuracy of A_κ and $\bar{\delta}_\kappa$, the values of the spherical Bessel functions at $r = R_a$ are calculated by forward recursion, using multiple precision arithmetic with precision level of 5000 digits). However, the asymptotic form (1.1.18) can sometimes be reached at $r < R_a$. Consequently, BREMS applies the method of iterative phase matching in the region of space where $V \neq 0$ regardless of whether the interaction potential is truncated or not. In the case of a truncated potential, the phase correction integral in Eq. (1.2.1) has to be calculated as follows:

$$Q(r)|_{r < R_a} = \begin{cases} \nu \ln \frac{r}{R_a} & \text{for truncated point-Coulomb field,} \\ -\nu \int_r^{R_a} \frac{\tilde{V}(w)}{w} dw & \text{for truncated screened fields,} \end{cases} \quad (1.2.3)$$

and $Q(r) \equiv 0$ when $r \geq R_a$. [The second expression of (1.2.2) is obtained by taking the limit $R_a \rightarrow \infty$ in the second expression of (1.2.3). Conversely, the exact point-Coulomb phase correction integral, which is given by the first expression of (1.2.2), cannot be obtained by taking the limit $R_a \rightarrow \infty$ in the first expression of (1.2.3). If R_a is very large (such that the contribution of the region $r > R_a$ to the interaction cross section is negligible), then the replacement of Eq. (1.2.2) with Eq. (1.2.3) in the

case of the point-Coulomb potential shows up only as a constant term $\nu \ln(2pR_a)$ added to the phase shifts of all partial waves corresponding to a given energy of the electron. A change of all phase shifts by adding a constant term does not alter the physical state of the electron, hence the values of the cross sections calculated using the truncated point-Coulomb potential in the limit $R_a \rightarrow \infty$ are the same as the values calculated using the exact point-Coulomb potential.]

The screening function of an ion has a constant term, which has the meaning of the ratio of the ion charge and the nuclear charge (i.e., the unscreened fraction of the nuclear charge). Thus, the screening function of an ion can be defined as follows:

$$\tilde{V}_i(r) \equiv \frac{V_i(r)}{-\alpha Z/r} = i + (1-i)\tilde{V}_p(r) + \Delta\tilde{V}_f(r), \quad (1.2.4a)$$

where $V_i(r)$ is the potential function of the ion, i is the mentioned constant term, \tilde{V}_p is the variable part of the point-nucleus screening function (1.1.63), which is normalized to 1 (i.e., \tilde{V}_p is equal to 1 at $r=0$ and asymptotically approaches zero in the limit $r \rightarrow \infty$), and $\Delta\tilde{V}_f$ is the finite-nucleus correction of the screening function (1.1.64). As mentioned in Section 1.1.6, $\Delta\tilde{V}_f$ is equal to 0 outside the nucleus, hence the overall screening function becomes identical to the point-nucleus screening function outside the nucleus:

$$\tilde{V}_i(r)|_{r>R_c} = i + (1-i)\tilde{V}_p(r), \quad (1.2.4b)$$

where R_c is the cutoff radius of the nuclear charge distribution. As a matter of programming convenience, when $i \neq 1$, the “normalized” variable part of the overall screening function is defined in the code of BREMS as follows:

$$\tilde{V}(r) \equiv \tilde{V}_p(r) + \frac{\Delta\tilde{V}_f(r)}{1-i}. \quad (1.2.4c)$$

In the case of a neutral atom (when $i=0$), this definition is consistent with the expression of the overall screening function (1.1.62). Using definition (1.2.4c), the screening function of an ion (1.2.4a) can be written in the form (1.2.4b) at all values of r (not only outside the nucleus):

$$\tilde{V}_i(r) = i + (1-i)\tilde{V}(r). \quad (1.2.5)$$

A side effect of definition (1.2.4c) is that the values of $\tilde{V}(r)$ calculated according to Eq. (1.2.4c) with $i \neq 0$ do not have a clear physical meaning inside the nucleus (for example, when $0 < i < 1$, $\tilde{V}(r)$ changes sign inside the nucleus and is negative at $r=0$). However, all physical calculations use only the values calculated according to Eq. (1.2.5), which have the meaning of the true screening function at all values of r (i.e., $\tilde{V}_i(r) = V_i(r)/(-Z\alpha/r)$).

As it follows from the expression of the screening function of an ion (1.2.5), the phase correction integral $Q(r)$ must be calculated in this case as a superposition of the logarithmic term and of the integral of $\tilde{V}(r)/r$ (see Eqs. (1.2.2) and (1.2.3)). I.e., if the interaction potential of an ion is not truncated, then the phase correction integral is equal to

$$Q(r) = \nu \left[i \ln 2pr - (1-i) \int_r^\infty \frac{\tilde{V}(w)}{w} dw \right], \quad (1.2.6a)$$

and in the case of a truncated potential, the phase correction integral at $r \leq R_a$ is equal to

$$Q(r)|_{r \leq R_a} = \nu \left[i \ln \frac{r}{R_a} - (1-i) \int_r^{R_a} \frac{\tilde{V}(w)}{w} dw \right]. \quad (1.2.6b)$$

In addition to the mentioned method of the power-series solution, two other methods are optionally available for solving the system of first-order ODEs (1.1.16a,b): the Hamming’s fourth-order modified predictor-corrector (P-C) method (see [43, p. 95–109] and [44]), and the method based on the Runge-Kutta formula pair (7,8), except in the vicinity of $r=0$, where the power-series solution (based on the Taylor series expansion of the point-nucleus screening function $\tilde{V}(r)$) is

always applied. The method of the power-series solution at small r is similar to the method used in [1, 2]. However, the default method of the iterative solution of the system of ODEs (1.1.16a,b) at larger values of r , which is implemented in BREMS, is different from the method used in [1, 2], where the 4th order Runge-Kutta method was used in the case of the interaction potentials defined in tabular format (such as the Kohn-Sham potential, whose expression is given in Section 1.1.5).

All three mentioned methods of solving the system of ODEs (1.1.16a,b) are essentially equivalent in terms of accuracy, but the default method (based on the power-series expansion of the wave function) is usually faster than the other two methods, because it is specifically tailored for solving the system of ODEs (1.1.16). The Runge-Kutta method is the least efficient of the mentioned methods. The P-C methods for solving the systems of ODEs are in general more efficient than the Runge-Kutta methods in terms of the balance between speed and accuracy [45], and the Hamming's method in particular was demonstrated to be superior to the other popular P-C methods (such as the Adams P-C method) [46]. Testing has shown that in the case of the exact (not truncated) point-Coulomb field the phase shifts calculated using BREMS converge to the exact phase shifts given by Eq. (1.1.23), whereas the normalization factors A_κ converge to their exact value (it is equal to 1 due to the choice of the initial values of $r^{-\gamma}g$ and $r^{-\gamma}f$, which are finite at $r = 0$, for the solution of the system of ODEs (1.1.16a,b) in BREMS).

The result of the first part of the integration is a set of the initial parts of S integrals (1.1.15), i.e., the values of the integrals from 0 to a certain value r_0 . Further on, those integrals will be called “numerical integrals” in order to distinguish them from the second part (integration from r_0 to ∞), which is based on the analytical expressions presented below.

The integration from r_0 to ∞ relies on the assumption that the coefficients $\cos \bar{\delta}_\kappa$ and $\sin \bar{\delta}_\kappa$ in Eqs. (1.1.18) are constant, i.e., that the phase correction integrals (1.2.2) are zero. This means that the interaction potential is either “truncated” at $r = R_a \leq r_0$ (i.e., that $V(r) \equiv 0$ at $r > r_0$), or at least negligibly small at $r > r_0$. Then each of the integrals from r_0 to ∞ is equal to a linear combination of four integrals of this general form:

$$\begin{aligned} S_{11} &\equiv \int_{r_0}^{\infty} j_l(kr) j_{N_1}(p_1 r) j_{N_2}(p_2 r) r^2 dr, & S_{12} &\equiv \int_{r_0}^{\infty} j_l(kr) j_{N_1}(p_1 r) y_{N_2}(p_2 r) r^2 dr, \\ S_{21} &\equiv \int_{r_0}^{\infty} j_l(kr) y_{N_1}(p_1 r) j_{N_2}(p_2 r) r^2 dr, & S_{22} &\equiv \int_{r_0}^{\infty} j_l(kr) y_{N_1}(p_1 r) y_{N_2}(p_2 r) r^2 dr. \end{aligned} \quad (1.2.7)$$

The mentioned linear combinations are obtained after substituting Eqs. (1.1.18) into the definition of the S integrals (1.1.15a,b) with the lower bound replaced by r_0 . The spherical Bessel functions of negative orders, which appear in Eqs. (1.1.18) when $\kappa < 0$, are expressed via the spherical Bessel functions of non-negative orders N_1 and N_2 by making use of the “reflection identities” $j_{-n}(z) = (-1)^n y_{n-1}(z)$ and $y_{-n}(z) = (-1)^{n+1} j_{n-1}(z)$ [47, Eq. (10.47.3) and Eq. (10.47.4)]. In order to calculate the integrals (1.2.7), the three spherical Bessel functions in the integrand are replaced by their closed-form expressions in terms of products of powers of $1/r$ and trigonometric functions. The closed-form expressions of the spherical Bessel functions of non-negative order are given below (see also [47, Eq. (10.49.1), Eq. (10.49.2), and Eq. (10.49.4)]):

$$j_l(z) = \sum_{n=0}^l \sin(z - \frac{1}{2}(l-n)\pi) \frac{a_n(l + \frac{1}{2})}{z^{n+1}}, \quad (1.2.8a)$$

$$y_l(z) = - \sum_{n=0}^l \cos(z - \frac{1}{2}(l-n)\pi) \frac{a_n(l + \frac{1}{2})}{z^{n+1}}, \quad (1.2.8b)$$

where

$$a_n(l + \frac{1}{2}) = \begin{cases} \frac{(l+n)!}{2^n n! (l-n)!}, & n = 0, 1, \dots, l, \\ 0, & n = l+1, l+2, \dots \end{cases} = \begin{cases} 1, & n = 0, \\ \frac{(l-n+1) \cdot \dots \cdot (l+n)}{2^n n!}, & n = 1, \dots, l, \\ 0, & n = l+1, l+2, \dots \end{cases} \quad (1.2.9)$$

After replacing the spherical Bessel functions in Eqs. (1.2.7) by the corresponding closed-form expressions (1.2.8a,b), each of the integrals (1.2.7) is expressed as a sum of such terms:

$$\pm \frac{1}{4} a_{n_1} (N_1 + \frac{1}{2}) a_{n_2} (N_2 + \frac{1}{2}) a_{n_3} (l + \frac{1}{2}) p_1^{-n_1-1} p_2^{-n_2-1} k^{-n_3-1} \int_{r_0}^{\infty} \frac{\sin p'r}{r^{n'}} dr = CI_1(p'r_0, n') \quad (1.2.10a)$$

or

$$\pm \frac{1}{4} a_{n_1} (N_1 + \frac{1}{2}) a_{n_2} (N_2 + \frac{1}{2}) a_{n_3} (l + \frac{1}{2}) p_1^{-n_1-1} p_2^{-n_2-1} k^{-n_3-1} \int_{r_0}^{\infty} \frac{\cos p'r}{r^{n'}} dr = CI_2(p'r_0, n'), \quad (1.2.10b)$$

where p' is one of the four values

$$p' \equiv p_1 \pm p_2 \pm k \quad (1.2.11)$$

(the sign “ \pm ” in Eq. (1.2.11) is not correlated with the sign “ \pm ” in Eqs. (1.2.10a,b)),

$$n' \equiv n_1 + n_2 + n_3 + 1, \quad (1.2.12)$$

$$C \equiv \pm \frac{1}{4} a_{n_1} (N_1 + \frac{1}{2}) a_{n_2} (N_2 + \frac{1}{2}) a_{n_3} (l + \frac{1}{2}) p_1^{-n_1-1} p_2^{-n_2-1} k^{-n_3-1} p'^{n'-1}, \quad (1.2.13)$$

and $I_{1,2}$ are the integrals defined below:

$$I_1(p'r_0, n') \equiv \int_{p'r_0}^{\infty} \frac{\sin z}{z^{n'}} dz, \quad (1.2.14a)$$

$$I_2(p'r_0, n') \equiv \int_{p'r_0}^{\infty} \frac{\cos z}{z^{n'}} dz. \quad (1.2.14b)$$

Each of the terms (1.2.10a,b) is a result of multiplying r^2 and three factors proportional to $\sin(z)/z^n$ or $\cos(z)/z^n$, where $z = p_{1,2}r$ or kr , $n = n_{1,2}$ or n_3 respectively, the sign “ \pm ” in Eqs. (1.2.10a,b) and (1.2.13) appears due to eliminating the term $-\frac{1}{2}(l-n)\pi$ from the argument of the sine and cosine functions in Eqs. (1.2.8a,b), and summing is done over all values of n_1 , n_2 and n_3 from 0 to N_1 , N_2 and l , respectively. All the integrals that appear in Eqs. (1.2.10a,b) can be calculated beforehand, once the value of r_0 is known. The maximum number of those integrals is $8n_{\max}$, where n_{\max} is the maximum value of n' , and the factor 8 appears because there are two types of the I integral (sine and cosine) and four values of p' (1.2.11), i.e., four values of the lower bound in Eqs. (1.2.14a,b). The values of I_1 and I_2 corresponding to $n' > 1$ are expressed in terms of the sine and cosine integrals

$$\text{si}(p'r_0) = -I_1(p'r_0, 1), \quad (1.2.15a)$$

$$\text{ci}(p'r_0) = -I_2(p'r_0, 1), \quad (1.2.15b)$$

using the known formulas [24, Eqs. (2.639.1–4)]. This means that there are actually only 8 trigonometric integrals that have to be calculated numerically. All other I integrals are expressed analytically in terms of those 8 integrals. Thus, apart from the standard methods for calculating the sine and cosine integrals (1.2.15a,b), the integration from r_0 to ∞ does not require any specialized numerical algorithms. This second part of the integration will be therefore called “analytical integration”.

In the case $k = 0$, the values of $\lim_{k \rightarrow 0}(kS_1)$ and $\lim_{k \rightarrow 0}(kS_2)$ are calculated instead of S_1 and S_2 .

Since the mentioned limits are given by the analytical formula (1.1.20), the numerical integration is not required. Thus, the value of r corresponding to transition from the “numerical” part of the calculation to the “analytical” part should be defined in the case $k = 0$ as the point where all needed phase shifts can be evaluated with sufficient accuracy, i.e., where all wave functions have attained the asymptotic form (1.1.18).

The Wigner $3j$ coefficients in Eq. (1.1.14) are calculated using the Racah formula [48]. Since this formula involves summation of a very large number of alternating terms that are similar in absolute value, extended-precision arithmetic has to be used when $l_1 > 80$ or $l_2 > 80$ in order to avoid cancellation errors.

1.3. The use of multiple-precision arithmetic and the methods of improving the performance

1.3.1. The use of multiple-precision arithmetic in BREMS

A problem that must be solved for an accurate analytical integration of a product of r^2 and three spherical Bessel functions from r_0 to ∞ when $k \neq 0$ is a strong cancellation of terms in the resulting alternating series. If this cancellation is almost exact, the final result may be dominated by rounding errors. This problem is solved in BREMS by using multiple-precision (MP) arithmetic [49, 50], whereby the number of significant digits is increased beyond the “native” double precision (DP) of the compiler (the double precision corresponds to 15–17 significant digits, typically 16). Since the calculations using the available MP systems are extremely slow (slower by a factor of more than 100 than the equivalent calculations using DP) and may require a prohibitive amount of computer memory, BREMS uses quadruple-precision (QP) arithmetic [51] when the required number of significant digits is between 18 and 30. The implementation of QP in BREMS is the so-called “double-double arithmetic”, whereby QP values are implemented as pairs of DP values. The calculations using this implementation of QP are slower by a factor of 6–10 than the equivalent calculations using DP, and usually do not require much more memory.

In order to determine if the current precision level is sufficient, the capability of the MP system to change the precision level at runtime is employed. In addition, the known fact that the S integrals corresponding to the largest absolute values of κ_1 , κ_2 and l are the ones that are most susceptible to the cancellation errors is employed (this is because the number of terms of the type (1.2.10a,b) in the expressions of those S integrals is largest). Thus, if accurate values of the analytical integrals are obtained for the largest κ_1 , κ_2 and l , then one can be certain that the current precision level is sufficient to obtain accurate values of all needed analytical integrals. In order to test the current precision level, the values of the four integrals (1.2.7) corresponding to the largest value of the sum $N_1 + N_2 + l$ are calculated at a different precision level. If the relative difference of the values obtained at both precision levels is less than 10^{-6} , this means that the current precision is sufficient. By repeating this procedure at different precision levels, it is possible to “optimize” the precision level, i.e., to find the lowest precision level needed to obtain the values of the analytical integrals with sufficient precision. This makes it possible to decrease the calculation time. When the number of significant digits is of the order of 100 or greater, the time of the analytical integration is roughly proportional to the precision level. At a lower precision, the dependence of the calculation time on the precision level becomes weaker.

Since the “ I ” integrals (1.2.14a,b) are calculated before starting the mentioned optimization procedure, this method will work only if the I integrals are sufficiently accurate. In order to ensure the accuracy of the I integrals, they are calculated at the precision level of 3000 digits (or 4000 digits in the case of the sine and cosine integrals (1.2.15a,b)), keeping track of the rounding errors accumulated in their calculation procedure. If the maximum accumulated relative uncertainty of I_1 and I_2 is greater than 10^{-n_d} , where n_d is the required number of significant digits, the program quits with an error message. In the case of the sine and cosine integrals (1.2.15a,b), $n_d = 3000$. In the case of the higher-degree I_1 and I_2 integrals (1.2.14a,b), n_d is equal to the initial precision level of the analytical integration (300 or 100 by default).

1.3.2. Truncation of the sum with respect to l

The calculation time may also be reduced by decreasing the number of l values included in the sum (1.1.10), i.e., by decreasing the number of the S integrals calculated for each pair of values of κ_1 and κ_2 . The absolute values of the S integrals decrease with increasing l , so that the S integrals corresponding to the largest l usually have no significant influence on the final values of the cross sections, if $T_1 \leq 10$ MeV (see Fig. 2c). However, at the stage of calculating the S integrals it is not possible to determine how this truncation of the sum with respect to l will affect the accuracy of the final values of the cross sections. Consequently, this is determined later by calculating the cross sections with two different values of l_{\max} (i.e., the maximum value of l) in Eq. (1.1.10). Since the sum with respect to l has a finite number of terms, and since it is known that the terms

corresponding to larger l have a progressively weaker influence on the magnitude of the sum, the estimate of the mentioned truncation error can be obtained by comparing the values of the cross sections obtained with two values of l_{\max} (for a more detailed discussion, see the beginning of Section 6.16). In addition to reducing the number of S integrals that have to be calculated, the decrease of l causes a decrease of the optimal precision level.

The decrease of the absolute value of S integrals as a function of l slows down with increasing T_1 (see Fig. 2c). Consequently, when $T_1 > 10$ MeV, one has to consider the entire range of values of l in Eq. (1.1.10).

1.3.3. Cubic spline interpolation of S integrals with respect to l

When T_2 is of the order of 1 MeV or greater, the number of S integrals that have to be calculated exactly (for example, using the method described in Section 1.2) may be reduced considerably (typically by a factor of 3 to 4) by employing the fact that the set of S_1 or S_2 integrals corresponding to a particular pair of κ_1 and κ_2 , but to different values of l (with adjacent values of l differing by ± 2) form an alternating sequence such that the absolute values of the S_1 or S_2 integrals lie on a smooth curve (see Fig. 2). This means that some of the S integrals can be calculated by cubic spline interpolation using l as the argument of the spline. By default, this method is applied in BREMS only when $T_1 > 3$ MeV and $l > 80$. I.e., the values of S integrals for $l \leq 80$ are always calculated exactly. For sufficiently small values of κ_1 , κ_2 and l , the logarithmic interpolation is most suitable, i.e., the interpolated function is the logarithm of the absolute value of the envelope of the

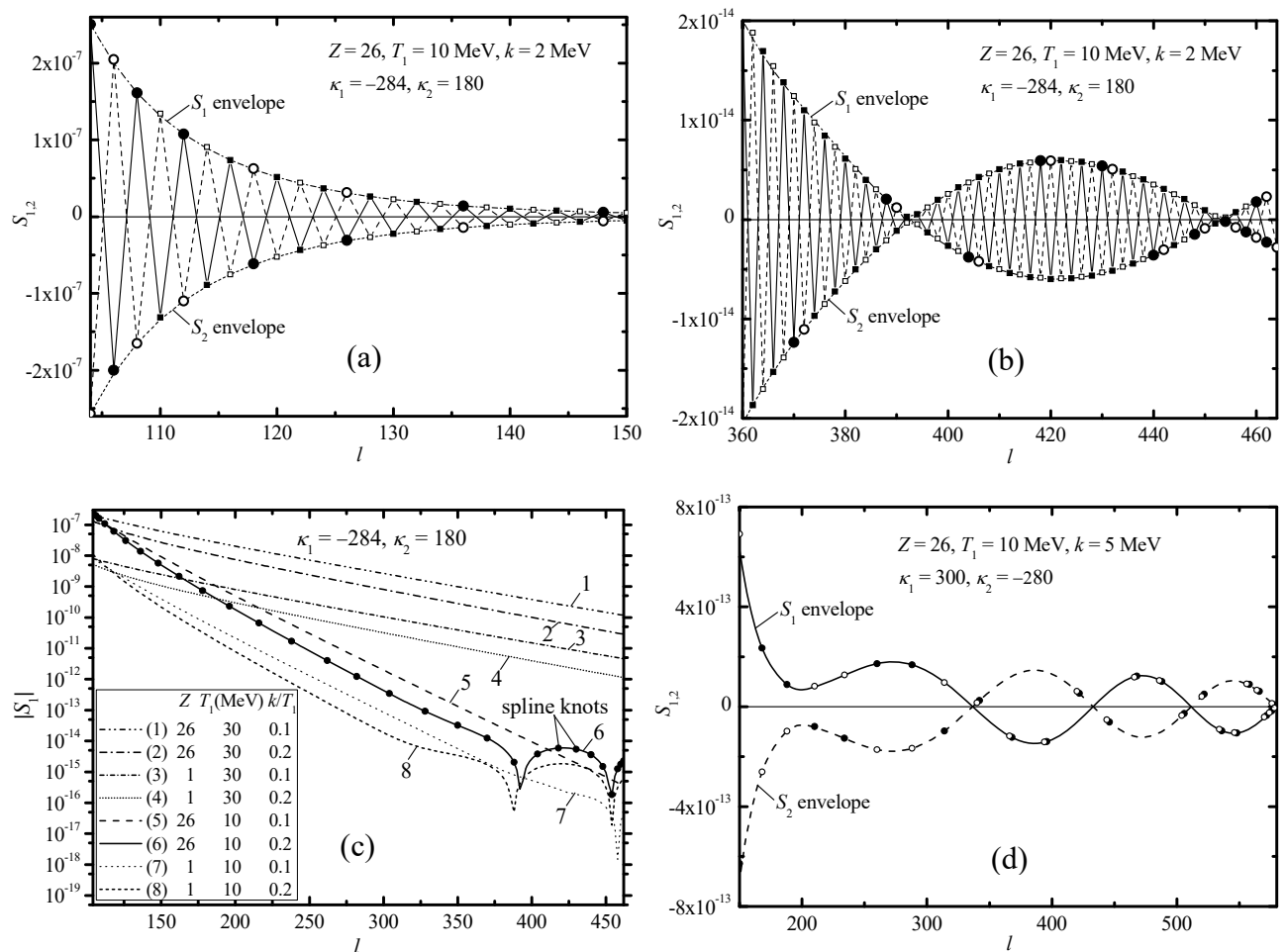


Fig. 2. Values of S_1 and S_2 integrals corresponding to different values of l , but the same pair of κ_1 and κ_2 . The physical parameters and the values of κ_1 and κ_2 are indicated in each graph. The Kohn-Sham potential is used. The values of S_1 integrals are shown by solid symbols, and the values of S_2 integrals are shown by open symbols. The values corresponding to the grid points (“knots”) of the cubic spline interpolation are shown by round symbols, and the exact values of the S integrals are shown by smaller square symbols. In (a) and (b), the interpolated envelope for S_1 and S_2 integrals is shown by the dash-dotted and short-dashed lines, respectively. In (d), the interpolated envelope for S_1 and S_2 integrals is shown by the solid and dashed lines, respectively.

set of S integrals (see Fig. 2c). Near the values of l where the envelope changes sign (as in Fig. 2b and Fig. 2d), the interpolated function must be the value of the mentioned envelope itself. Thus, the total interpolated envelope consists in general of a sequence of alternating logarithmic and linear segments. In the logarithmic segments, the spline is constructed using the “natural spline” boundary condition (zero second derivative at the endpoints). The same boundary condition is also applied at the minimum and maximum value of l for a given pair of κ_1 and κ_2 . At the other endpoints of the linear segments (i.e., the endpoints that are adjacent to a logarithmic segment), the first derivative of the spline in the linear segment is set equal to its value obtained by natural spline interpolation in the adjacent logarithmic segment. The density of grid points (further called “knots”) is highest near the minimum and maximum values of l , in order to deal with the situation when the S integrals at one or both endpoints are very close to zero and the logarithmic scale is used in most of the interval. Going towards the center of the interval of l , the difference of adjacent knots increases in an arithmetic progression: 2, 4, 6, etc., until a predefined maximum difference is reached (58 by default). The positions of the knots are symmetric with respect to the center of the interval of l where the interpolation is applied. If l_{\max} and l_{\min} denote the maximum and minimum values of l for a particular pair of κ_1 and κ_2 , and if $l_{\min} < 78$, then all values of l in the range $l_{\min} \leq l < 76$ are treated as knots of the spline, and the remaining knots are symmetric with respect to the center of the interval $76 \leq l \leq l_{\max}$ when the values of l are even, or $77 \leq l \leq l_{\max}$ when the values of l are odd.

During the cubic spline interpolation mentioned above, the following three additional rules are applied in order to improve the accuracy, particularly when $|\kappa_2| \ll |\kappa_1|$ (the S integrals corresponding to such pairs of κ_1 and κ_2 are especially important at high energies and close to the tip of the spectrum, i.e., when T_1 is of the order of 10 MeV or greater and $T_2 / T_1 < 0.05$):

- (a) if the second grid point of the $S(l)$ envelope corresponding to a particular pair of κ_1 and κ_2 is an extremum point, or if the absolute value of the first S integral exceeds the absolute values of all remaining S integrals corresponding to the same pair of κ_1 and κ_2 by a factor greater than 5, then the first point of the $S(l)$ envelope is excluded from the further cubic spline interpolation (and from the set of grid points referred to in the next two rules);
- (b) if the $S(l)$ envelope does not change sign, then the cubic spline interpolation is performed using a single logarithmic spline segment;
- (c) if the $S(l)$ envelope changes sign and the second grid point of the $S(l)$ envelope is not an extremum point, whereas the ratio of the two maximum absolute values of the $S(l)$ envelope of either sign is greater than 5 or less than 0.2, then a constant term is added to all values of the envelope, such that they all have the same sign and the minimum absolute value becomes equal to the absolute value of the corresponding grid point of the original envelope (i.e., the absolute value of the mentioned offset of the $S(l)$ envelope is equal to twice the smaller one of the two maximum absolute values corresponding to each of the two subsets of grid points with the same sign, and the sign of the offset is opposite to the sign of the corresponding grid point of the original envelope). After that, the interpolation is performed using a single logarithmic spline segment, and then the mentioned constant term is subtracted from the interpolated values, yielding the final interpolated $S(l)$ envelope.

However, even with these additional rules, the interpolation with respect to l may cause a significant bias (up to 20 %) of the final DCS at large angles, if $\max|\kappa_2|$ is of the order of 10 and $\max|\kappa_1| \gg \max|\kappa_2|$. Consequently, the mentioned interpolation is by default applied only when $|\kappa_2| > 30$ (the latter threshold value of $|\kappa_2|$ may be adjusted by the user).

1.3.4. Partial-wave interpolation method

Yet another method of improving the performance is based on decomposing the sums in Eqs. (1.1.4) and (1.1.5) into terms that are smooth functions of $|\kappa_1|$ or $|\kappa_2|$ (or l_1 or l_2). Then it may be sufficient to calculate only some of those terms exactly, and the missing terms may be obtained by interpolation. This method is called the “partial-wave interpolation method”. It was applied in [52], where the single differential cross section (SDCS) (1.1.5) was expressed as

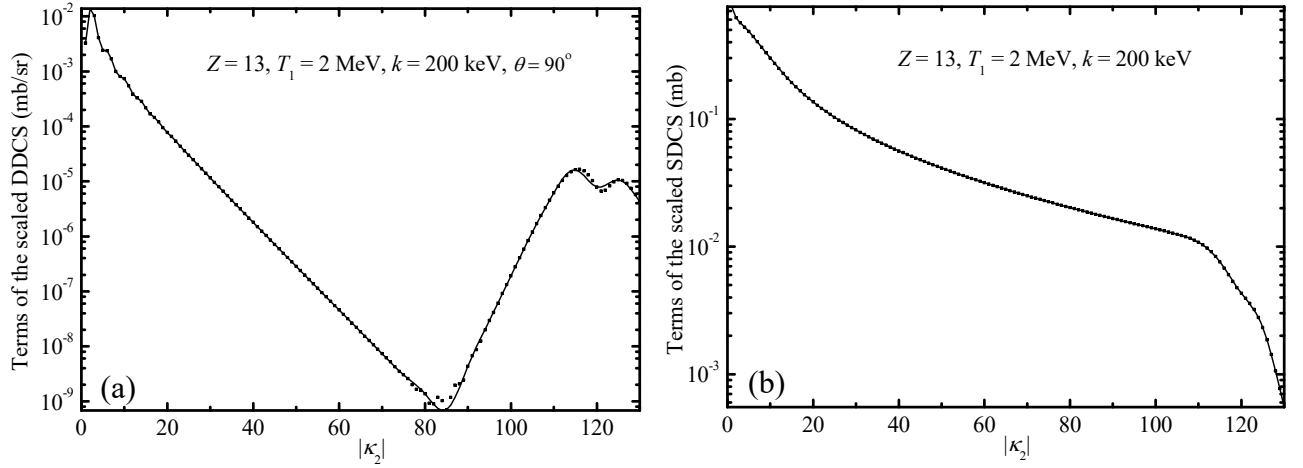


Fig. 3. Values of the first 130 terms of the expression of (a) scaled double differential cross section (DDCS) and (b) scaled single differential cross section (SDCS), where the summation is done with respect to $|\kappa_2|$. The physical parameters are indicated in the graphs. The Kohn-Sham potential is used. The scaled cross sections have been calculated using (1.1.3) and (1.1.5), where the summation indices κ_1 and $\bar{\kappa}_1$ run from -130 to $+130$, and the sum (1.1.10) is truncated at $l = 130$. The exact values of the terms are shown by squares. Starting from the term No. 31, the solid line shows the values obtained by cubic spline interpolation between the exact values of the logarithm of the terms with sequence numbers from 30 to 130 in increments of 5.

$$\sigma(k) = \sum_{l_1, l_2} \sigma_{l_1, l_2}(k) = \sum_{l_1} \sigma_{l_1}(k). \quad (1.3.1)$$

However, the interpolation with respect to l_1 (or $|\kappa_1|$) cannot be applied to the expression of the double differential cross section (DDCS) (1.1.3) or (1.1.4), because the latter expressions include a *double* sum with respect to the values of κ_1 (in Eq. (1.1.3), the corresponding summation indices are denoted κ_1 and $\bar{\kappa}_1$, whereas in Eq. (1.1.4) the mentioned double sum appears due to the squaring of the four single sums with respect to κ_1). This means that interpolation of the DDCS with respect to l_1 (or $|\kappa_1|$) would have to be two-dimensional, and such interpolation would be much less accurate than one-dimensional interpolation. Conversely, the sum with respect to κ_2 is simple (not double) both in the expression of the DDCS (1.1.3) (or (1.1.4)) and in the expression of the SDCS (1.1.5). In addition, as shown in Fig. 3a and Fig. 3b, after replacing the sum with respect to κ_2 by the sum with respect to $|\kappa_2|$ (i.e., treating each pair of terms corresponding to opposite values of κ_2 as a single term), the terms of both those sums become smooth functions of $|\kappa_2|$. Consequently, BREMS allows “skipping” some of the values of κ_2 when calculating the set of the S integrals (1.1.15a,b). The values of the logarithm of the missing terms in the sums of Eqs. (1.1.4) and (1.1.5) are subsequently calculated by cubic spline interpolation. By default, this method is applied in BREMS only when $|\kappa_2|_{\max} \geq 80$ (if $k \neq 0$), or when $|\kappa_2|_{\max} \geq 120$ (if $k = 0$), and the first skipped value of $|\kappa_2|$ is equal to 31 (i.e., the starting value of $|\kappa_2|$ for the mentioned interpolation is equal to 30). If $|\kappa_1|_{\max} / |\kappa_2|_{\max} < 2$ and $|\kappa_2|_{\max} \leq 300$, or $|\kappa_1|_{\max} / |\kappa_2|_{\max} \geq 2$ and $|\kappa_2|_{\max} < 250$, then the default difference of the adjacent retained values of $|\kappa_2|$ in the interval $30 \leq |\kappa_2| \leq |\kappa_2|_{\max}$ is constant and equal to 5 (possibly excluding the last two values of $|\kappa_2|$, whose difference will be less than 5 if $|\kappa_2|_{\max}$ is not a multiple of 5). If $|\kappa_1|_{\max} / |\kappa_2|_{\max} < 2$ and $|\kappa_2|_{\max} > 300$, or $|\kappa_1|_{\max} / |\kappa_2|_{\max} \geq 2$ and $|\kappa_2|_{\max} \geq 250$, then the default difference of the adjacent retained values of $|\kappa_2|$ is 10. In addition, there is an option to use a set of values of $|\kappa_2|$ whose differences increase in an arithmetic progression.

1.3.5. Truncation of the interaction potential

A method of decreasing the computation time based on “truncation” of the interaction potential $V(r)$ should also be mentioned. The cutoff radius R_a (or “atomic radius”), which is defined as the value of the radial coordinate where V drops to zero (i.e., $V(r) \equiv 0$ when $r > R_a$), can be calculated using the known fact that in momentum space the largest contribution to the radiation

cross section originates from the region where the momentum transferred to the nucleus is smallest [12]. In coordinate space, this corresponds to a distance from the nucleus of the order

$$r = 1/|\mathbf{q}_{\min}|, \quad (1.3.2)$$

where $|\mathbf{q}_{\min}|$ is the minimum momentum transfer (see Eq. (1.1.29e)), which is equal to

$$|\mathbf{q}_{\min}| = |\mathbf{p}_1| - |\mathbf{p}_2| - |\mathbf{k}| \equiv p_1 - p_2 - k = \sqrt{E_1^2 - 1} - \sqrt{E_2^2 - 1} - k. \quad (1.3.3)$$

It is reasonable to expect that if the value of R_a exceeds the value of r (1.3.2) by an order of magnitude or more, then the mentioned truncation will not have a significant effect on the values of the DDCS and the SDCS. However, the decrease of the computation time caused by the truncation of the potential function may be quite dramatic, because the value of the cutoff radius R_a may be much less than the radius r_0 where the asymptotic form would be attained without this truncation (this is usually the case when the kinetic energy of the incident electron is of the order of 1 MeV or greater). The asymptotic expression of the wave function (1.1.18) (with constant values of the phase shift $\bar{\delta}_\kappa$ and the normalization factor A_κ) is known to be exact in the region of space where $V(r) \equiv 0$. Consequently, by truncating the potential function, one can decrease the region of the numerical integration and thus shorten the processing time. By default, BREMS calculates R_a by multiplying the value of (1.3.2) by 20 when $T_1 < 1$ MeV, or by 13 when $T_1 \geq 1$ MeV. In addition, the default value of R_a is not allowed to become less than a certain minimum value $R_{a,\min}$. I.e., if the radius obtained as described previously is less than $R_{a,\min}$, then R_a is set equal to $R_{a,\min}$. If $T_1 \leq 3$ MeV, then $R_{a,\min} = \max(800, 126/p_2)$ (i.e., either approximately six Bohr radii or twenty wavelengths of the outgoing electron, whichever is greater). If $T_1 > 3$ MeV, then $R_{a,\min} = \max(1200, 126/p_2)$. When $k = 0$, the interaction potential is not truncated. The user can modify this default behavior.

1.3.6. Reusing the integrals from r_0 to ∞ for different Z

Since each integral from r_0 to ∞ (the ‘‘analytical’’ integral) is expressed as a linear combination of the four integrals defined by Eqs. (1.2.7), it is possible to decrease the total time of analytical integration by reusing the values of those four integrals for different values of Z , if a fixed set of values of T_1 and k is used for all Z . The values of the mentioned four integrals depend on T_1 , k and r_0 , but do not depend on Z explicitly. If the values of the radial coordinate corresponding to the transition from the numerical integration to the analytical integration (i.e., the lower integration bound r_0 in Eqs. (1.2.7)) are also defined independently of Z (for example, if $r_0 = R_a$, where the cutoff radius R_a is calculated as described in Section 1.3.5), then it is possible to reuse the values of the mentioned four integrals and thus to skip the stage of the analytical integration for some combinations of Z , T_1 and k . In such a case, a change of Z requires only recalculating the coefficients of the mentioned linear combination, which depend on the phase shifts calculated by numerical solution of the system of ODEs (1.1.16a,b). As a result, the total time of the analytical integration is decreased by a factor equal to the number of chemical elements, for which the cross sections are computed. For example, if BREMS is used for generation of a data library for all Z from 1 to 100, then the total time of the analytical integration can be reduced to the point where it is only a small fraction of the total processing time.

1.4. The numerical errors

The errors in the final values of the cross sections are caused by the inaccuracies of the numerical methods used to evaluate the expressions presented in Section 1.1.1. The sources of errors are the following:

- 1) errors of the numerical solution of the system of ODEs (1.1.16a,b),
- 2) errors of the numerical integration due to the finite step size,
- 3) errors caused by truncation of the series (1.1.4) and (1.1.5) at finite values of κ_1 and κ_2 .

The combined effect of the errors of the first and second types on the numerical integrals is estimated by calculating the so-called ‘‘test’’ numerical integrals, i.e., by redoing the numerical integration with all tolerances and step sizes increased by a factor of two. The output data files

created at the stage of calculating the S integrals contain not only the values of the total integrals (from 0 to ∞), but also the values of both numerical integrals (corresponding to the initial numerical integration from 0 to the cutoff radius r_0 and the test integration with the same bounds). The difference of the latter two integrals serves as the estimate of the error of the numerical integration. The uncertainty of the phase shifts $\tilde{\delta}_\kappa$ caused by errors of the first type affects the accuracy of the analytical integrals (from r_0 to ∞), too, because the asymptotic expressions of the radial wave functions (1.1.18) depend on the mentioned phase shifts. In the case of screened (exponentially decaying) or “truncated” interaction potentials, the effect of the uncertainty of the phase shifts on the analytical integrals is estimated by calculating three estimates of each analytical integral:

- 1) the one corresponding to the original (i.e., average) phase shifts $\tilde{\delta}_{\kappa_1}$ and $\tilde{\delta}_{\kappa_2}$,
- 2) the one obtained after incrementing $\tilde{\delta}_{\kappa_1}$ by the uncertainty of $\tilde{\delta}_{\kappa_1}$,
- 3) the one obtained after incrementing $\tilde{\delta}_{\kappa_2}$ by the uncertainty of $\tilde{\delta}_{\kappa_2}$.

The mentioned “uncertainty of $\tilde{\delta}_\kappa$ ” is the range of variation (i.e., the difference of the maximum and minimum values) of $\tilde{\delta}_\kappa$ over the last 10 “test” points (see also Section 1.2). After performing the test integration, the overall range of variation of $\tilde{\delta}_\kappa$ is obtained by combining the ranges of variation corresponding to the original and test integrations. The absolute value of the maximum difference of these three estimates of the analytical integral serves as the estimate of the error of the analytical integral due to uncertainty of the phase shift. In the case of the exact (non-truncated) point-Coulomb potential (or in the case of an ion), the phase shift $\bar{\delta}_\kappa$ in Eqs. (1.1.18) is unknown due to an undefined value of the phase correction integral (see Eqs. (1.2.1), (1.2.2), and (1.2.6a)). Consequently, the uncertainty of the S integrals caused by the uncertainty of the phase shift is estimated in this case as twice the absolute value of the largest of the four integrals (1.2.7), multiplied by the product of the two corresponding square-root factors before the brackets in Eqs. (1.1.18), i.e., by $\sqrt{(E_1+1)(E_2-1)/(4E_1E_2)}$ for S_1 integrals, or by $\sqrt{(E_1-1)(E_2+1)/(4E_1E_2)}$ for S_2 integrals.

The mentioned errors of the analytical integrals caused by the uncertainty of the phase shift are also included in the S integral data files. The overall error (i.e., uncertainty) of each S integral is obtained by combining the error of the numerical integration and the error of the analytical integral caused by uncertainty of the phase shifts (these two errors are assumed to be independent, hence they are combined by adding them in quadrature). It should be noted that the overall relative errors of the S integrals are usually greater than the relative errors of the separate numerical and analytical integrals by several orders of magnitude due to a strong cancellation of those two integrals.

The effect of the truncation of the series (1.1.4) and (1.1.5) may be ameliorated by extrapolation as described in Section 1.5.

1.5. Refining the estimates of cross sections by extrapolation to $\kappa_{\max} \rightarrow \infty$

1.5.1. The stretched exponential approximation

In the following text, the cross section that is differential in photon energy and angle (1.1.4) will be called simply “differential cross section” (DCS), and the cross section that is differential in photon energy only (1.1.5) will be called simply “cross section” (CS). It has been noticed that if the truncation error is not too large and if the summation in the truncated series (1.1.4) and (1.1.5) is symmetrical with respect to positive and negative values of the summation indices κ_1 and κ_2 (i.e., if for every term corresponding to a particular pair of indices (κ_1, κ_2) there are two terms corresponding to the pairs of indices $(-\kappa_1, \kappa_2)$ and $(\kappa_1, -\kappa_2)$), then the dependence of both the DCS and the CS on the maximum value of $|\kappa_1|$ and $|\kappa_2|$ used in the sum may be approximated by the following five-parameter expression:

$$(D)CS = c \pm \exp(a + b\kappa_{\max}^{d+h\kappa_{\max}}), \quad (1.5.1)$$

where $b < 0$, $d > 0$, $h \geq 0$, and κ_{\max} is the largest value of $|\kappa_2|$ included in the series (1.1.4) and (1.1.5), i.e., the ‘‘truncation value’’ of $|\kappa_2|$:

$$\kappa_{\max} \equiv \kappa_{2\max} \equiv \max(|\kappa_2|) = \kappa_{1\max} / n, \quad (1.5.2)$$

where $\kappa_{1\max} \equiv \max(|\kappa_1|)$, and n is a constant positive integer. This means that an increase of $\kappa_{2\max}$ by 1 is accompanied by an increase of $\kappa_{1\max}$ by $n \geq 1$. I.e., the set of terms added to the truncated partial-wave series (Eq. (1.1.4) or Eq. (1.1.5)) as a result of each such increment consists of all the terms corresponding to the following pairs of κ_1 and κ_2 :

$$\begin{aligned} 1 \leq |\kappa_1| \leq n\kappa_{\max} - n, \quad |\kappa_2| = \kappa_{\max}, \\ n\kappa_{\max} - n + 1 \leq |\kappa_1| \leq n\kappa_{\max}, \quad 1 \leq |\kappa_2| \leq \kappa_{\max}. \end{aligned}$$

This condition is needed in order to ensure smoothness of the dependence of (D)CS on κ_{\max} in the entire investigated range of κ_{\max} . Specifically, it is needed in order to accommodate the case $T_2 \ll T_1$, when $\kappa_{1\max}$ has to be much greater than $\kappa_{2\max}$, and to avoid the situation when in some intervals of κ_{\max} only one of the two numbers $\kappa_{1\max}$ and $\kappa_{2\max}$ is varied, whereas in other intervals of κ_{\max} both $\kappa_{1\max}$ and $\kappa_{2\max}$ are varied. In the code of BREMS, the default value of n in Eq. (1.5.2) is equal to the rounded value of the ratio of the initial and final momenta of the electron (p_1 / p_2), which approaches the ratio of the corresponding kinetic energies T_1 / T_2 as the speed of the outgoing electron approaches the speed of light. Depending on T_1 and T_2 , the mentioned rounded value is either the nearest integer or the largest integer that does not exceed p_1 / p_2 . When $n = 1$, an increase of κ_{\max} by 1 implies adding all the terms where one of the two summation indices (either κ_1 or κ_2) is equal to $\pm\kappa_{\max}$, and the other one is equal to all non-zero integer values from $-\kappa_{\max}$ to $+\kappa_{\max}$ ($\kappa_{1,2}$ cannot be zero according to Eq. (1.1.2)).

As it follows from Eq. (1.5.1), the (D)CS approaches the limiting value c as a stretched exponential of κ_{\max} , with the stretching exponent depending on κ_{\max} linearly. Approximation (1.5.1) is applicable when the magnitude of the truncation error corresponding to a given value of κ_{\max} (i.e., the absolute value of the relative deviation of the value of the truncated series (1.1.4) or (1.1.5) from the value corresponding to $\kappa_{\max} \rightarrow \infty$) is less than approximately 30 % and the shape of the actual dependence of the CS or DCS on κ_{\max} is consistent with Eq. (1.5.1), i.e., a monotonous increase or decrease with a tendency to saturation.

Equation (1.5.1) defines a prescription for improving the accuracy of the final estimates of CS and DCS: the dependence of CS and DCS on κ_{\max} must be fitted by the nonlinear function (1.5.1) in the range of values of κ_{\max} where the CS or DCS is sufficiently close to the saturation value. The optimal value of c (i.e., the value obtained by nonlinear fitting) is the estimate of the CS or the DCS. The fitting is performed by minimizing the sum of squared differences between the fitting function (1.5.1) and the actual values over the last N_{fit} values of κ_{\max} , i.e., in the range $K - N_{\text{fit}} < \kappa_{\max} \leq K$, where K is the upper bound on the value of κ_{\max} to be used in the analysis:

$$K \equiv \max(\kappa_{\max}). \quad (1.5.3)$$

In the case of the DCS, this fitting is performed independently for each value of the photon emission angle θ . If the partial-wave interpolation method described in Section 1.3.4 is applied, then the logarithmic cubic spline interpolation mentioned in Section 1.3.4 must be done for each value of κ_{\max} independently, because a change of κ_{\max} causes not only the change of the number of terms retained in the sums with respect to $|\kappa_2|$, but also a change of values of all terms in those sums (due to the change of the limits of summation with respect to κ_1 and $\bar{\kappa}_1$).

If

$$(d + h \kappa_{\max}) \ln \kappa_{\max} \ll 1, \quad (1.5.4)$$

then the expression of the (D)CS (1.5.1) becomes approximately equal to

$$(D)CS \approx c \pm \exp[a + b + b(d + h\kappa_{\max}) \ln \kappa_{\max}]. \quad (1.5.5)$$

Parameter b appears in Eq. (1.5.5) only as a term in the sum $a + b$ and as a factor in two products: bd and bh . This means that the fitting model is ‘‘over-parameterized’’: the four parameters a , b , d

and h should be replaced by three parameters having the meaning of $a + b$, bd , and bh . Equivalently, parameter b could be fixed at any convenient value (for example, -1). By setting parameter b equal to -1 and assuming that the condition (1.5.4) is true, the following approximation of the (D)CS is obtained:

$$(\text{D})\text{CS} \approx c \pm \exp(a-1) \kappa_{\max}^{-d-h\kappa_{\max}}. \quad (1.5.6)$$

Thus, in the special case defined by inequality (1.5.4), the five-parameter stretched exponential approximation (1.5.1) is replaced by a four-parameter power-function approximation with the exponent equal to a linear function of κ_{\max} (see Eq. (1.5.6)).

For any triplet of values of parameters c , d and h , the optimal values of parameters a and b in Eq. (1.5.1) are calculated by linear least squares fitting of $\ln|(\text{D})\text{CS} - c|$ as a function of $\kappa_{\max}^{d+h\kappa_{\max}}$. Thus, parameters a and b are expressed analytically in terms of independent parameters c , d and h , so that the latter three parameters are the only ones that have to be varied during the iterative fitting procedure. Alternatively, $\exp(b\kappa_{\max}^{d+h\kappa_{\max}})$ may be used as the argument of the linear regression, in which case parameters $\pm \exp(a)$ and c in Eq. (1.5.1) would have the meaning of the slope and intercept, respectively. Then parameters a and c are expressed analytically in terms of parameters b , d and h , so that the latter three parameters are the only ones that have to be varied independently during the iterative fitting procedure. In BREMS, both these approaches are applied consecutively: at first, the optimal values of all parameters are calculated using the first approach (with c , d and h as independent varied parameters), and then the second optimization is performed using b , d and h as independent parameters, whose initial values are obtained by the previous optimization. In the special case (1.5.4), (D)CS becomes a linear function of $\kappa_{\max}^{-d-h\kappa_{\max}}$ (see Eq. (1.5.6)), with the intercept equal to c and the slope equal to $\pm \exp(a-1)$, so that only d and h have to be varied during the iterative fitting procedure.

The Nelder-Mead simplex method [53] is used in BREMS for minimizing the sum of squared differences between the fitting function (1.5.1) and the original (unfitted) CS or DCS. In order to ensure the inequalities $b < 0$, $d > 0$ and $h \geq 0$, the iterative simplex procedure uses the transformed parameters b' , d' and h' , which are related to b , d and h as follows:

$$b = -\exp(b'), \quad d = \exp(d'), \quad h = (h')^2. \quad (1.5.7)$$

Testing has shown that the improvement of the fitting accuracy caused by inclusion of h into the set of varied parameters (as opposed to using $h = 0$ in Eq. (1.5.1)) is significant only when the (D)CS is an increasing function of κ_{\max} (which is always true in the case of the CS). However, in the latter case the polynomial approximation is significantly faster while ensuring a comparable or even better accuracy than the stretched exponential approximation, especially at large relative corrections of the DCS due to the κ_{\max} -fitting (see Section 1.5.2). Consequently, parameter h is used by default only when fitting the dependence of CS on κ_{\max} . When fitting the DCS, $h = 0$.

1.5.2. The polynomial approximation

An alternative fitting model for extrapolation of the κ_{\max} -dependence of the truncated PW (D)CS to $\kappa_{\max} \rightarrow \infty$ is based on the assumption that the mentioned dependence at large values of κ_{\max} is a smooth function of

$$x \equiv \exp(b\kappa_{\max}^{d+h\kappa_{\max}}), \quad (1.5.8)$$

where the b , d and h are constants ($b < 0$, $d > 0$, $h \geq 0$). Then the saturation value (c) of the (D)CS is the zero-degree term of the Taylor expansion of the (D)CS in the vicinity of $x = 0$:

$$(\text{D})\text{CS} = c + c_1 x + c_2 x^2 + c_3 x^3 + \dots \quad (1.5.9)$$

Accordingly, a possible approximation of the κ_{\max} -dependence of the (D)CS is a polynomial of x :

$$(\text{D})\text{CS} = c + \sum_{m=1}^M c_m x^m, \quad (1.5.10)$$

where M is the degree of the approximating polynomial. It has been determined that the mentioned polynomial approximation works best in the case of large positive corrections of the (D)CS due to

the κ_{\max} -fitting ($> 20\%$). Consequently, the polynomial approximation is applied in BREMS by default only when the relative correction of the (D)CS by the stretched exponential approximation (1.5.1) is positive and greater than 0.2. Testing has shown that satisfactory accuracy is achieved when $d = 0.5$, $h = 0$, and b is determined by least squares fitting at $M = 1$ (this stage of the calculations is described in Section 1.5.1). The optimal degree M of the polynomial is determined by performing the polynomial fitting for a set of increasing values of M (with b , d and h fixed) and then combining two criteria: 1) smallest relative uncertainty of c , 2) smallest total length of $M + 2$ longest runs of constant sign of the residuals [54]. By default, the maximum allowed value of M is 6. The optimal degree is either the maximum degree $M = M_{\max}$ of all polynomials with the relative uncertainty of c less than 5%, or the value of M corresponding to the smallest total length of $M + 2$ longest runs of constant sign of the residuals (the latter value of M will be denoted M'). If $M' < M_{\max}$, then M' is preferred to M_{\max} only when the corresponding total lengths of $M' + 2$ and $M_{\max} + 2$ longest runs of constant sign of the residuals are less than $0.5N_{\text{fit}}$ and greater than $0.7N_{\text{fit}}$, respectively, where N_{fit} is the number of values of κ_{\max} in the fitting interval.

1.5.3. Limits of applicability of the stretched exponential or polynomial approximation

By default, the stretched exponential fitting described above (using Eq. (1.5.1), or its special-case approximation (1.5.6), or the polynomial approximation (1.5.10)) is performed using the value of N_{fit} equal to

$$N_{\text{fit}} = \frac{K}{4} + 1.2\sqrt{K}. \quad (1.5.11a)$$

There is also an option use a fitting interval that is narrower by half, i.e.,

$$N_{\text{fit}} = \frac{K}{8} + 0.6\sqrt{K}, \quad (1.5.11b)$$

or to apply Eq. (1.5.1) or Eq. (1.5.6) with both values of N_{fit} (1.5.11a,b). In the latter case, the (D)CS is calculated as a weighted average of the two corresponding values of c (see also Section 1.6). If the polynomial approximation (1.5.10) has been applied in one or both of the two fitting intervals, then only the result corresponding to the wider interval is used. This choice of N_{fit} is largely arbitrary. If the fitting model defined by Eq. (1.5.1) or Eq. (1.5.10) was perfectly accurate, then one should fit the values of (D)CS corresponding to all values of κ_{\max} from 1 to K . However, the fitting equation becomes less accurate with decreasing κ_{\max} , hence the number of fitted data points N_{fit} is chosen on the basis of an empirical tradeoff between the accuracy of the fitting model and the rounding errors during the calculation of the original data and during the fitting procedure (the mentioned rounding errors tend to decrease with increasing N_{fit}).

Before performing the fitting of the data as a function of κ_{\max} by the methods described in Sections 1.5.1 and 1.5.2 (the “ κ_{\max} -fitting”), the dependences $\text{CS}(\kappa_{\max})$ and $\text{DCS}(\kappa_{\max})$ are smoothed. The smoothing with respect to κ_{\max} is implemented by replacing each value of (D)CS with the average of several values corresponding to consecutive values of κ_{\max} , where the last value is the current one. I.e., the dependence of the (D)CS on κ_{\max} is replaced by its moving average (MA). Accordingly, the value of κ_{\max} in the fitting equations (1.5.1) and (1.5.8) is less than the value of κ_{\max} corresponding to the endpoint of the corresponding MA interval by 0.5 times the MA interval reduced by 1. For example, if the MA interval is equal to 10, then the mentioned offset is equal to -4.5 . If the partial-wave (PW) interpolation method has been applied for generation of the (D)CS data (see Section 1.3.4), then the default MA interval for smoothing the (D)CS is equal to the magnitude of the increment of κ_2 used for the PW interpolation. If the PW interpolation method has not been applied, then the default MA interval is equal to 5 (in this case, the moving average is calculated only when $K \geq 80$).

The overall error of the final estimates of the CS or DCS obtained by applying the extrapolation techniques described above is usually less than the original truncation error at least by an order of magnitude. However, in the case of the DCS, the applicability of the approximation (1.5.1) or (1.5.10) is limited by the fact that the dependence of the DCS on κ_{\max} at a fixed non-zero

value of θ is sometimes oscillatory in a wide interval of values of κ_{\max} , when those values are insufficiently large. The mentioned oscillations are especially pronounced in the case of large values of T_1 (> 3 MeV) and k/T_1 (> 0.6). Those oscillations manifest themselves as wiggles in the angular dependence of the final DCS. As κ_{\max} is increased, the amplitude of those oscillations decreases and eventually the DCS becomes a monotonous function of κ_{\max} , which is approximately described by Eq. (1.5.1) or Eq. (1.5.10). The approximation (1.5.1) or (1.5.10) can be applied only when the dependence of the DCS on κ_{\max} is not oscillatory, or when the largest investigated values of κ_{\max} are well outside the oscillatory interval. If the largest value of κ_{\max} belongs to the oscillatory interval, then it is better to skip the nonlinear fitting, i.e., to use the original (unfitted) value of the DCS instead of the fitted value. BREMS checks the shape of the dependence of the DCS on κ_{\max} before the nonlinear fitting, and if it is determined that it is not consistent with Eq. (1.5.1), then the fitting is not performed, i.e., the final value of the DCS is set equal to the original value.

At high electron energies, or when k/T_1 is very close to 1, the values of the DCS at large angles are less by several orders of magnitude than at small and intermediate angles, and those values are especially sensitive to the truncation of the sums (1.1.4) and (1.1.10) with respect to $|\kappa_1|$, $|\kappa_2|$ and l . The nonlinear fitting described above is not always successful in eliminating the distortions of the function $\text{DCS}(\theta)$ at large values of θ . As a result, the angular dependence of the fitted DCS at large angles ($\theta > 140^\circ$) is sometimes non-monotonous when T_1 is of the order of 1 MeV or greater (at those conditions, the correct angular dependence of the DCS at large angles is a monotonous decrease with increasing θ). Examples of such distortions are given in Fig. 4 and Fig. 8a,b. Those distortions may be eliminated by polynomial or spline fitting for extrapolation of the fitted angular dependence of the DCS from the angular range where it has a “regular” shape to large angles (this method will be described in Section 1.7). A completely different approach to calculation of the angular dependence of the DCS at large angles (typically in the range $20^\circ \leq \theta \leq 180^\circ$) is based on an empirical observation that the PW DCS, as a function of κ_{\max} , has a practically identical shape for all angles inside a wide angular interval, if T_2 is sufficiently large (typically greater than 1 MeV). This approach is described in Section 1.5.4.

1.5.4. Extrapolation of the partial-wave DCS to $\kappa_{\max} \rightarrow \infty$ by linear rescaling

At sufficiently high energies of the incident electron ($T_1 > 1$ MeV), truncation of the partial-wave (PW) series (1.1.4) causes distortions in the approximation of the DCS by the truncated PW series, especially at large angles ($\theta > 100^\circ$). There is also some distortion at small angles ($\theta < 10^\circ$), but it is typically less pronounced than at large angles (see Fig. 4). Fig. 4a and Fig. 4b correspond to the two special cases when the exact calculation of the DCS (and the exact evaluation of the mentioned distortions) is feasible:

- I. Fig. 4a corresponds to the following set of physical parameters: $Z = 92$, $T_1 = 8$ MeV, $k = 6.4$ MeV, $T_2 = T_1 - k = 1.6$ MeV. If the value of T_2 is sufficiently small (as in Fig. 4a, where $T_2 = 1.6$ MeV), then the converged value of the PW series (1.1.4) at all values of the photon emission angle θ can be attained using a relatively small number of partial waves. In the case of Fig. 4a, the mentioned convergence is practically achieved using $\max(|\kappa_2|) \equiv \kappa_{\max} = 125$ and $\max(|\kappa_1|) = 500$ (these values correspond to $n = 4$ in Eq. (1.5.2)).
- II. Fig. 4b corresponds to the following set of physical parameters: $Z = 1$, $T_1 = 30$ MeV, $k = 6$ MeV, $T_2 = T_1 - k = 24$ MeV. In this case, the Born approximation should be sufficiently accurate (see Section 1.1.2). The criterion for the validity of the Born approximation is (1.1.27). The value of $Z = 1$ corresponds to $Z\alpha = 0.0073$, and the value of $T_2 = 24$ MeV corresponds to $\beta = 0.99978 \gg Z\alpha$. In this case, the relative error of the Born approximation is expected to be at most 1 % or so at all angles, so that the Born-approximation DCS may be treated as the exact DCS.

In both cases, the Kohn-Sham interaction potential and point-nucleus approximation are used (see Section 1.1.5). As shown in Fig. 4, the original DCS, which is equal to the truncated PW series

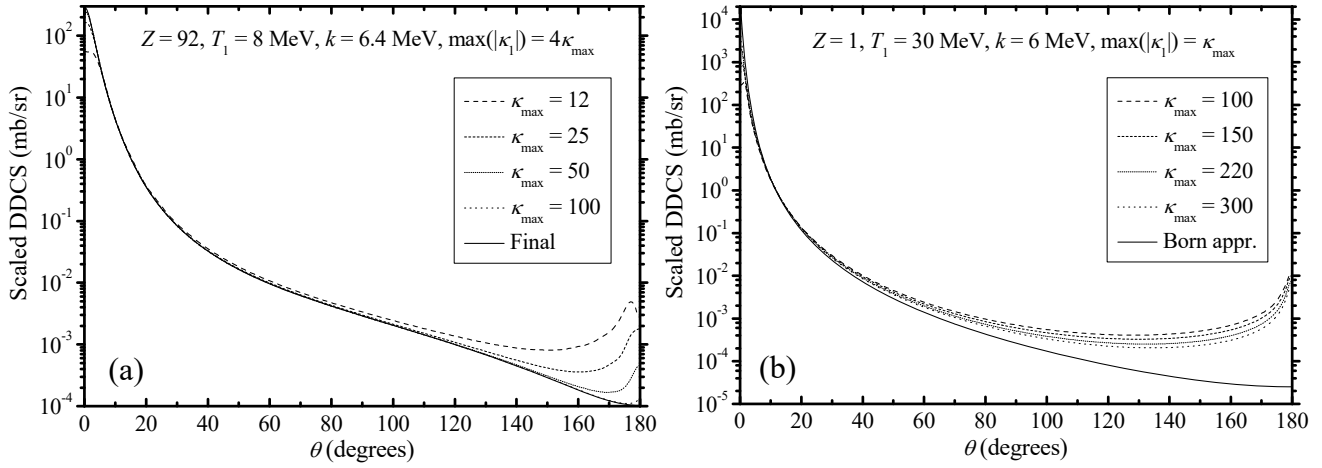


Fig. 4. The calculated angular dependence of the DCS for two sets of physical parameters: (a) $Z = 92$, $T_1 = 8$ MeV, $k = 6.4$ MeV, and (b) $Z = 1$, $T_1 = 30$ MeV, $k = 6$ MeV. The Kohn-Sham interaction potential and point-nucleus approximation are used in both cases. The dashed and dotted curves show the DCS obtained by truncating the sum in Eq. (1.1.4) (“partial-wave DCS” or “PW DCS”) at four values of κ_{\max} defined by Eq. (1.5.2), and the solid curve shows the exact theoretical DCS (corresponding to $\kappa_{\max} \rightarrow \infty$), obtained either by analyzing the data at sufficiently large values of $\max(|\kappa_1|)$ and $\max(|\kappa_2|)$ (in the case “(a)”, $\kappa_{\max} \equiv \max(|\kappa_2|) = 125$ and $\max(|\kappa_1|) = 500$), or using the Elwert-Born-form factor (EBF) approximation, which is the screened Born approximation (1.1.36) multiplied by the Elwert factor (1.1.47) (in the case “(b)”, the Elwert factor is practically equal to 1, and the Born approximation is accurate to better than 1 %).

(further called “partial-wave DCS”, or “PW DCS”), is typically greater than the exact DCS at large angles, and typically less than the exact DCS at small angles. Obviously, those distortions decrease with increasing value of κ_{\max} (defined by Eq. (1.5.2)), and the PW DCS at intermediate angles ($10^\circ < \theta < 100^\circ$) is less dependent on κ_{\max} and closer to the exact DCS (shown by the solid line in Fig. 4) than at large angles.

In the remainder of this subsection, several transforms of the data corresponding to the same two sets of physical parameters as in Fig. 4a and Fig. 4b will be discussed and illustrated in several graphs. As in Fig. 4, the “a” graphs will correspond to the case $Z = 92$, $T_1 = 8$ MeV, $k = 6.4$ MeV, and the “b” graphs will correspond to the case $Z = 1$, $T_1 = 30$ MeV, $k = 6$ MeV.

As shown in Fig. 5, the shape of the dependence of the PW DCS on κ_{\max} at different angles in a wide angular interval (typically $20^\circ \leq \theta \leq 170^\circ$) is practically constant, meaning that the mentioned dependence at a particular angle inside the mentioned angular interval can be obtained by a linear rescaling of a similar dependence at any other angle from the same angular interval [55]. Although Fig. 5 compares only the data for two values of θ , practically identical curves would be obtained at all intermediate values of θ (the scales of the left and right vertical axes in Fig. 5a and Fig. 5b have been intentionally displaced in order to make it possible to distinguish the two curves visually). This property of the PW DCS can be stated mathematically using the expression of the value of the PW DCS at a particular value of κ_{\max} as a linear combination of the values of the PW DCS at two other values of κ_{\max} , equal to K and K' :

$$\text{DCS}(\kappa_{\max}, \theta) = \text{DCS}(K', \theta) + \mu(\kappa_{\max}, \theta) (\text{DCS}(K, \theta) - \text{DCS}(K', \theta)). \quad (1.5.12a)$$

Obviously, $0 \leq \mu \leq 1$ when $K' \leq \kappa_{\max} \leq K$ (with the values $\mu = 0$ and $\mu = 1$ corresponding to $\kappa_{\max} = K'$ and $\kappa_{\max} = K$, respectively), and $\mu > 1$ when $\kappa_{\max} > K$. The mentioned property of the PW DCS implies that the “scale factor” μ in Eq. (1.5.12a) does not depend on the photon emission angle θ if the same values of κ_{\max} , K , and K' are used for all values of θ inside the mentioned angular interval. If this property of the PW DCS holds up to $\kappa_{\max} \rightarrow \infty$, then the problem of calculating the exact theoretical DCS (i.e., the PW DCS corresponding to $\kappa_{\max} \rightarrow \infty$) is reduced to calculation of the constant factor μ in the following expression:

$$\text{DCS}_\mu(\theta) \equiv \text{DCS}(\kappa_{\max} \rightarrow \infty, \theta) = \text{DCS}(K'', \theta) + \mu (\text{DCS}(K, \theta) - \text{DCS}(K'', \theta)), \quad (1.5.12b)$$

where K is the absolute maximum value of κ_{\max} in the data used for the analysis (defined by Eq. (1.5.3)), whereas K' and K'' are (largely arbitrary) “base” values of κ_{\max} , which must be smaller

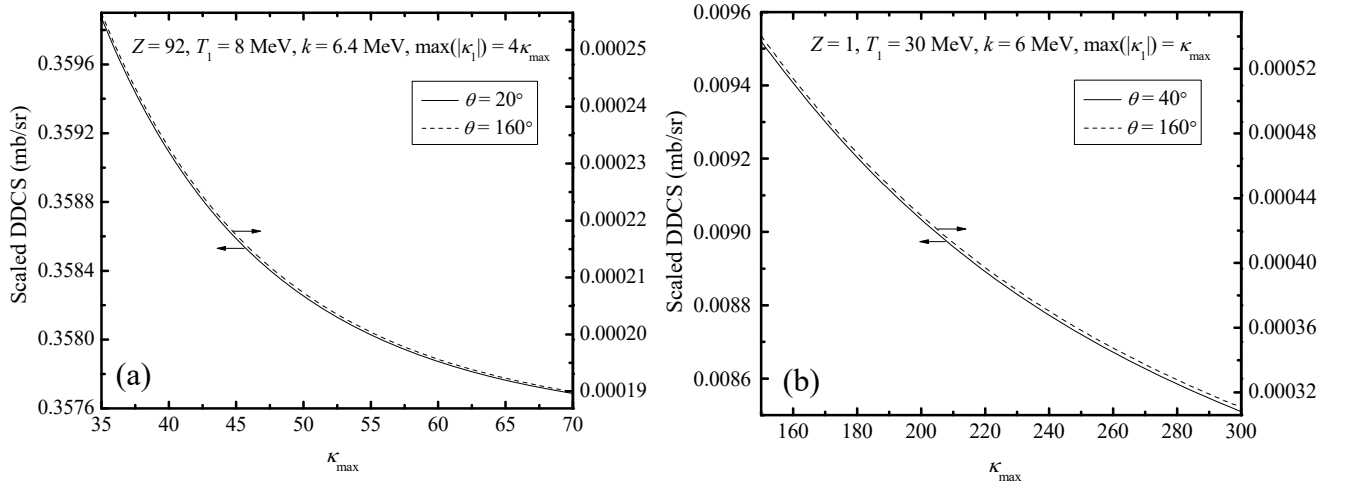


Fig. 5. Comparison of the dependence of the partial-wave DCS on κ_{\max} at two values of the photon emission angle θ . The two dependences on κ_{\max} are plotted for two sets of physical parameters: (a) $Z = 92$, $T_1 = 8$ MeV, $k = 6.4$ MeV, and $\max(|\kappa_1|) = 4\kappa_{\max}$, and (b) $Z = 1$, $T_1 = 30$ MeV, $k = 6$ MeV, and $\max(|\kappa_1|) = \kappa_{\max}$. In each case, the dependences of PW DCS on κ_{\max} at the two angles are plotted on different vertical axes, whose scales have been chosen so as to demonstrate the similarity of the two curves. Curves of practically identical shape are also obtained at all angles that are between the two indicated values of θ . The intervals of κ_{\max} are (a) $35 \leq \kappa_{\max} \leq 70$, and (b) $150 \leq \kappa_{\max} \leq 300$.

than K (but not too small, because μ ceases to be independent of the angle if K' or K'' is reduced below a certain threshold value).

The testing of the mentioned property of the PW DCS must be performed using values of K and K' that are sufficiently different from each other, so that nonlinearity of the function $\text{DCS}(\kappa_{\max})$ inside the interval $K' \leq \kappa_{\max} \leq K$ becomes apparent. Otherwise, the constancy of the factor μ in Eq. (1.5.12a) for different angles would become trivial (any two linear functions can be transformed into each other by a linear rescaling). However, after determining the angular range where the factor μ in Eq. (1.5.12a) is constant, the value of K'' in Eq. (1.5.12b) may be chosen to be arbitrarily close to the value of K (with the maximum possible value equal to $K'' = K - 1$). The rounding errors in the values of $\text{DCS}(\kappa_{\max})$ may again make a larger difference of K and K'' preferable (but not because of the approximate linearity of $\text{DCS}(\kappa_{\max})$ in the range $K'' \leq \kappa_{\max} \leq K$, which would not cause any problems in this case).

In the code of BREMS, the testing of the angle-independence of the scale factor μ in Eq. (1.5.12a) is by default performed inside the interval $K/2 \leq \kappa_{\max} \leq K$, where K is equal to the maximum value of κ_{\max} in the analyzed data. Thus, K' is by default equal to $K/2$. When $4 \text{ MeV} \leq T_1 \leq 30 \text{ MeV}$ and $T_2 \geq 1 \text{ MeV}$, the optimal value of K (in the sense of a tradeoff between the computation time and the magnitude of errors in the final values of the DCS) is such that the absolute maximum of $|\kappa_1|$ in the available data (which is equal to nK , according to Eqs. (1.5.2) and (1.5.3)) is usually inside the interval $200 \leq nK \leq 400$, with larger values of T_2 requiring larger values of nK . In Fig. 5, the values of K and $K' = K/2$ correspond to the endpoint and starting point of the κ_{\max} axis, respectively. This constancy of μ is clearly seen from comparison of the *differential* of $\text{DCS}(\kappa_{\max})$, which is defined as follows:

$$\Delta \text{DCS}(\kappa_{\max}, \theta) \equiv \text{DCS}(\kappa_{\max}, \theta) - \text{DCS}(\kappa_{\max} - 1, \theta), \quad (1.5.13)$$

for different values of θ . As it is obvious from Eq. (1.5.12a) and from the definition of $\Delta \text{DCS}(\kappa_{\max}, \theta)$ (Eq. (1.5.13)), it is proportional to the differential of μ as a function of κ_{\max} (bearing in mind that K and K' are constants):

$$\Delta \text{DCS}(\kappa_{\max}, \theta) \equiv \Delta \mu(\kappa_{\max}, \theta) (\text{DCS}(K, \theta) - \text{DCS}(K', \theta)), \quad (1.5.14)$$

where

$$\Delta \mu(\kappa_{\max}, \theta) \equiv \mu(\kappa_{\max}, \theta) - \mu(\kappa_{\max} - 1, \theta). \quad (1.5.15)$$

In order to test the angle-independence of the scale factor μ (i.e., of its differential $\Delta \mu$), the differential of $\text{DCS}(\kappa_{\max})$ should be “normalized” so that its dependence on θ is entirely caused by

the dependence of μ on θ . This can be achieved, e.g., by defining the normalized differential of the DCS as follows:

$$\Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta) \equiv \Delta\text{DCS}(\kappa_{\text{max}}, \theta) / (\Delta\text{DCS}_{\text{max}}(\theta) - \Delta\text{DCS}_{\text{min}}(\theta)), \quad (1.5.16)$$

where $\Delta\text{DCS}_{\text{max}}(\theta)$ and $\Delta\text{DCS}_{\text{min}}(\theta)$ are, respectively, the maximum and minimum values of $\Delta\text{DCS}(\kappa_{\text{max}}, \theta)$ over all values of κ_{max} from K' to K for a given value of θ .

$$\Delta\text{DCS}_{\text{max}}(\theta) \equiv \max_{K' \leq \kappa_{\text{max}} \leq K} \Delta\text{DCS}(\kappa_{\text{max}}, \theta), \quad \Delta\text{DCS}_{\text{min}}(\theta) \equiv \min_{K' \leq \kappa_{\text{max}} \leq K} \Delta\text{DCS}(\kappa_{\text{max}}, \theta). \quad (1.5.17)$$

By substituting expressions (1.5.14) and (1.5.17) into Eq. (1.5.16), the following expression is obtained:

$$\Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta) \equiv \Delta\mu(\kappa_{\text{max}}, \theta) / (\Delta\mu_{\text{max}}(\theta) - \Delta\mu_{\text{min}}(\theta)), \quad (1.5.18)$$

where $\Delta\mu_{\text{max}}(\theta)$ and $\Delta\mu_{\text{min}}(\theta)$ are, respectively, the maximum and minimum values of $\Delta\mu(\kappa_{\text{max}}, \theta)$ over all values of κ_{max} from K' to K for a given value of θ .

$$\Delta\mu_{\text{max}}(\theta) \equiv \max_{K' \leq \kappa_{\text{max}} \leq K} \Delta\mu(\kappa_{\text{max}}, \theta), \quad \Delta\mu_{\text{min}}(\theta) \equiv \min_{K' \leq \kappa_{\text{max}} \leq K} \Delta\mu(\kappa_{\text{max}}, \theta). \quad (1.5.19)$$

As it is obvious from Eq. (1.5.18), the dependence of $\Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta)$ on θ is entirely caused by the dependence of μ on θ . The angle-independence of μ can therefore be tested by calculating the range of variation of expression (1.5.16) over all values of θ in a given angular interval at a given value of κ_{max} . Although the same objective could be achieved using a simpler method of “normalization” (for example, division of $\Delta\text{DCS}(\kappa_{\text{max}}, \theta)$ by $\text{DCS}(K, \theta) - \text{DCS}(K', \theta)$, which, according to Eq. (1.5.14), would yield the value of $\Delta\mu(\kappa_{\text{max}}, \theta)$), the expression (1.5.16) (or, equivalently, (1.5.18)) is more convenient for evaluating the degree of stability of the scale factor μ as a function of θ , because the range of variation of $\Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta)$ as a function of κ_{max} inside the interval $K' \leq \kappa_{\text{max}} \leq K$ at any fixed value of θ is equal to 1. Consequently, the difference of values of $\Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta)$ corresponding to different θ at a fixed value of κ_{max} can be interpreted as a *relative* difference (in reference to the total range of variation of $\Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta)$ as a function of κ_{max} at a fixed value of θ), and the condition of approximate angle-independence of μ can be formulated as follows:

$$\max_{K' \leq \kappa_{\text{max}} \leq K} \left[\max_{\theta_{\text{start}} \leq \theta \leq \theta_{\text{end}}} \Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta) - \min_{\theta_{\text{start}} \leq \theta \leq \theta_{\text{end}}} \Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta) \right] \ll 1, \quad (1.5.20)$$

where θ_{start} and θ_{end} are the endpoints of the angular range where the values of $\Delta\text{DCS}(\kappa_{\text{max}}, \theta)$ are calculated. In addition, the definition (1.5.16) has the advantage of making it possible to test not only the angle-independence of the scale factor μ , but also the degree of nonlinearity of the dependence of DCS on κ_{max} (which, as mentioned, is one of the prerequisites for a meaningful test of the angle-independence of the scale factor μ in Eq. (1.5.12a)). If the dependence $\text{DCS}(\kappa_{\text{max}})$ is linear, then $\Delta\text{DCS}_{\text{max}}(\theta) = \Delta\text{DCS}_{\text{min}}(\theta)$, so that the value of the denominator in expression (1.5.16) becomes zero and the mentioned expression becomes undefined. If the dependence $\text{DCS}(\kappa_{\text{max}})$ is nonlinear, but this nonlinearity is relatively weak, then the magnitude of the denominator in expression (1.5.16) is strongly affected by the random rounding errors in the estimates of $\Delta\text{DCS}_{\text{max}}(\theta)$ and $\Delta\text{DCS}_{\text{min}}(\theta)$, causing a relatively large value of the total range of variation of $\Delta\text{DCS}_{\text{norm}}$ (i.e., of the left-hand side of inequality (1.5.20)) and a consequent failure of the test for the angle-independence of the scale factor μ . A larger nonlinearity of $\text{DCS}(\kappa_{\text{max}})$ implies a greater value of $\Delta\text{DCS}_{\text{max}}(\theta) - \Delta\text{DCS}_{\text{min}}(\theta)$ in Eq. (1.5.16) and thus a reduced sensitivity of the values of $\Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta)$ to the mentioned rounding errors, so that those values reflect the actual shape of $\text{DCS}(\kappa_{\text{max}})$ rather than the rounding errors. Fig. 6 shows the maximum and minimum values of the normalized differential of $\text{DCS}(\kappa_{\text{max}})$ (defined according to Eq. (1.5.16) or, equivalently, according to Eq. (1.5.18)) over all angles in the indicated angular range for each value of κ_{max} from $K' = K/2$ to K . I.e., the two quantities plotted in each of Fig. 6a and Fig. 6b are defined as follows:

$$\max_{\theta_{\text{start}} \leq \theta \leq \theta_{\text{end}}} \Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta), \quad \min_{\theta_{\text{start}} \leq \theta \leq \theta_{\text{end}}} \Delta\text{DCS}_{\text{norm}}(\kappa_{\text{max}}, \theta) \quad (1.5.21)$$

(the values of θ_{start} and θ_{end} are indicated in Figs. 6a and 6b). The similarity of the maximum and minimum normalized differential of $\text{DCS}(\kappa_{\text{max}})$ shown in Figs. 6a and 6b is a clear demonstration of

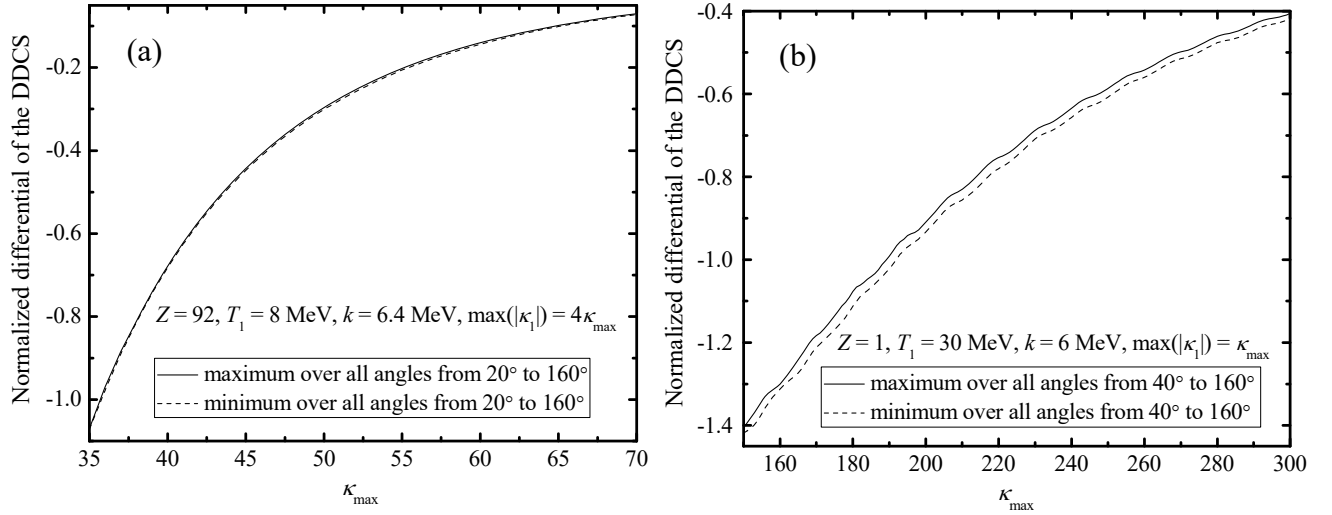


Fig. 6. The maximum and minimum normalized differential of the DDCS over all angles in the indicated angular interval for two sets of the physical parameters: (a) $Z = 92$, $T_1 = 8$ MeV, $k = 6.4$ MeV, and (b) $Z = 1$, $T_1 = 30$ MeV, $k = 6$ MeV. The intervals of κ_{\max} are (a) $35 \leq \kappa_{\max} \leq 70$, and (b) $150 \leq \kappa_{\max} \leq 300$.

the fact that the scale factor μ in Eq. (1.5.12a) is approximately angle-independent (the maximum difference of the solid and dashed curves, i.e., the left-hand side of inequality (1.5.20), is equal to 0.0085 in the case of Fig. 6a, and 0.038 in the case of Fig. 6b).

After determining the angular interval where the scale factor μ in Eq. (1.5.12a) is approximately angle-independent, the theoretical value of the DCS in this angular interval can be determined by evaluating expression (1.5.12b), if the constant factor μ is known. If the DCS is a decreasing function of κ_{\max} , then the value of the latter factor can be determined by minimizing the large-angle distortion in the angular dependence of DCS_μ (defined by Eq. (1.5.12b)). The latter distortion shows up as an increase of the PW DCS at large angles (see Fig. 4). If μ is smaller than optimal, then this type of distortion appears in $\text{DCS}_\mu(\theta)$, too (see curve 3 in Figs. 7a and 7b). If μ is greater than optimal, then the mentioned increase of the PW DCS causes a *decrease* of $\text{DCS}_\mu(\theta)$ at large angles, and $\text{DCS}_\mu(\theta)$ becomes negative starting from some value of μ (see curve 5 in Figs. 7a and 7b). The effect of those large-angle distortions can be reduced by replacing the large-angle part of the angular dependence of DCS_μ by angular extrapolation of the same function $\text{DCS}_\mu(\theta)$ from an angular range ending at a suitably small angle. Testing has shown that consistently accurate results (with accuracy of a few percent or better) are obtained when the mentioned angular extrapolation is performed by least squares fitting of $\text{DCS}_\mu(\theta)$ or of the ratio of $\text{DCS}_\mu(\theta)$ and an analytical “reference” DCS by a polynomial of $\cos \theta$. The mentioned “reference” DCS is obtained either from the screened Born approximation (see Section 1.1.2), or from the Sommerfeld-Maue (SM) approximation with the screening correction and with the next-to-leading-order (NLO) correction (see Section 1.1.3). Thus, the fitting function (which is used for the mentioned angular extrapolation) is defined as follows:

$$\text{DCS}_{\text{ext}}(\theta) = \text{DCS}_{\text{ref}}(\theta) \sum_{m=0}^L a_m \cos^m \theta, \quad (1.5.22)$$

where $\text{DCS}_{\text{ref}}(\theta)$ is either equal to 1, or the reference DCS corresponding to one of the two mentioned analytical approximations, L is the degree of the fitting polynomial, and a_i ($m = 0, 1, \dots, L$) are the polynomial coefficients, which are obtained by minimizing the sum of squared relative deviations (SSRD) of DCS_{ext} from DCS_μ :

$$\text{SSRD} \equiv \sum_{i=i'}^{i''} \left(\frac{\text{DCS}_{\text{ext}}(\theta_i)}{\text{DCS}_\mu(\theta_i)} - 1 \right)^2, \quad (1.5.23)$$

where the summation is performed over a set of discrete equidistant values of θ , numbered in an ascending order (the summation index i is the sequence number of a value of θ in the mentioned set,

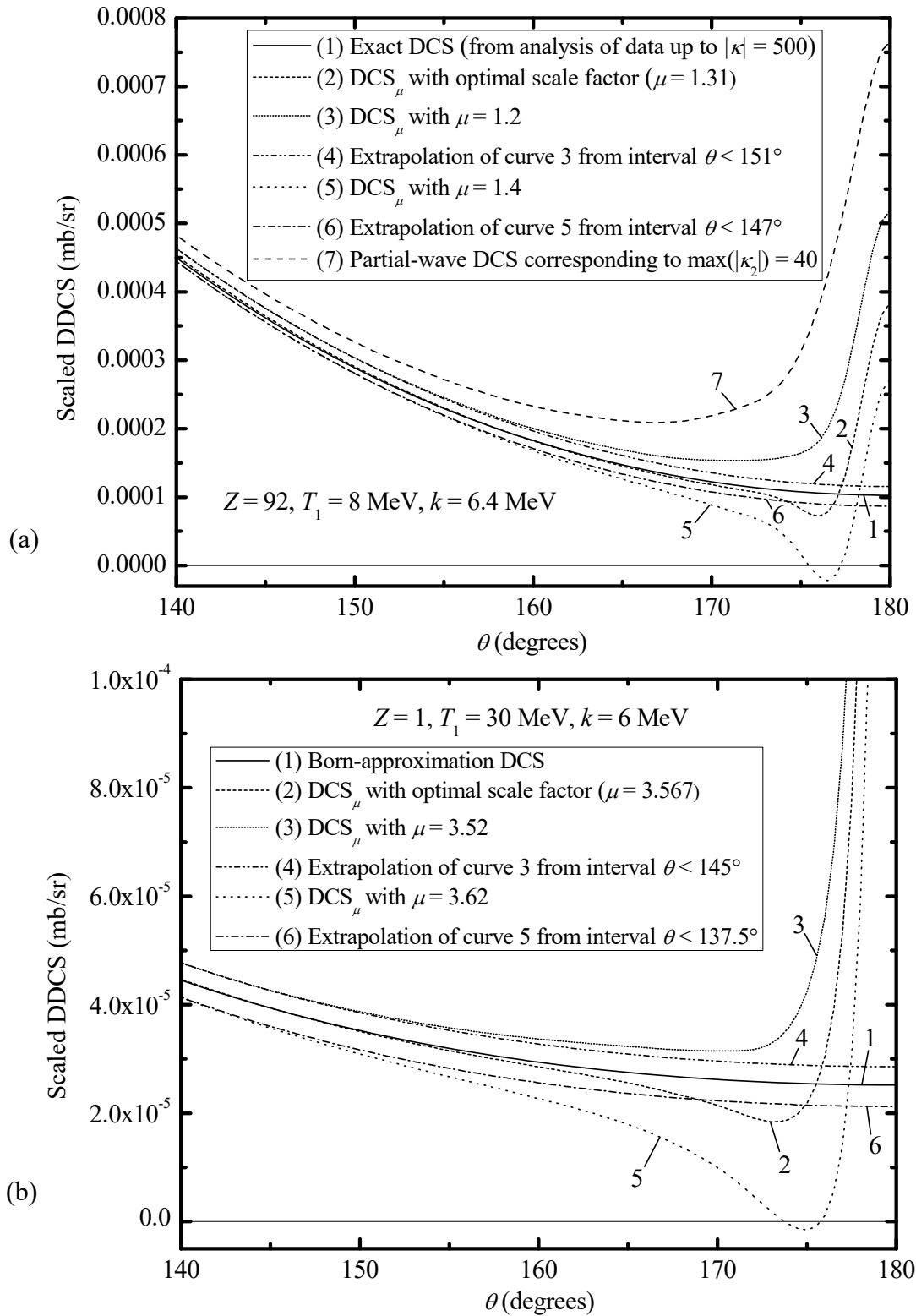


Fig. 7. Comparison of the exact DCS with the function $\text{DCS}_\mu(\theta)$ defined by Eq. (1.5.12b), calculated using three values of the scale factor μ : the optimal one, a smaller-than-optimal one, and a larger-than-optimal one, for two sets of physical parameters: (a) $Z = 92, T_1 = 8 \text{ MeV}, k = 6.4 \text{ MeV}$, and (b) $Z = 1, T_1 = 30 \text{ MeV}, k = 6 \text{ MeV}$. In the case of non-optimal μ , the angular extrapolation of the function $\text{DCS}_\mu(\theta)$ from the angular interval starting at 100° and ending at the indicated angle is shown, too. The angular extrapolation has been performed by fitting the ratio of $\text{DCS}_\mu(\theta)$ and the analytical “reference” DCS with a third-degree polynomial of $\cos \theta$ (see Eq. (1.5.22)). The endpoint of the polynomial fitting interval is less than the angle of the first irregularity (a minimum or an inflection) of the function $\text{DCS}_\mu(\theta)$ by 20° . The values of K and K'' in Eq. (1.5.12b) are either (a) 40 and 23, or (b) 300 and 205, respectively. The values of K'' have been calculated using the formula $K'' = K - [(K/4) + 1.2\sqrt{K}] + 1$, which is largely arbitrary (practically identical results would be obtained using other values of K''). The reference DCS has been calculated using the SMNLO approximation in the case of Fig. 7a, and the Born approximation in the case of Fig. 7b.

and the latter value is denoted θ_i). By default, the polynomial fitting interval starts at $\theta = \theta_i \equiv \theta' = 90^\circ$ and ends at an angle $\theta = \theta_i'' \equiv \theta''$ that is less than the angle of the first irregularity (a minimum or an extra inflection point) of the function $\text{DCS}_\mu(\theta)$ by 20° to 30° . As shown in Fig. 7 (where $\theta' = 100^\circ$ and $L = 3$), thus extrapolated curve is quite close to the exact angular dependence even when the value of μ is not optimal (see curves 4 and 6 in Fig. 7a and 7b). The choice of the optimal value of L and of the optimal reference DCS is based on two criteria: (a) the quality of the polynomial fit inside the fitting interval ($\theta' \leq \theta \leq \theta''$), and (b) the degree of stability of the polynomial fit in the range $\theta' \leq \theta \leq 180^\circ$ as a function of the endpoint of the fitting interval θ'' . Each of these criteria is implemented by calculating the corresponding standard deviation (over all data points inside the mentioned angular interval in the case (a), and over all values of θ'' in the case (b)). Then those two standard deviations are combined in quadrature, yielding the overall standard deviation. The set of parameters corresponding to the minimum overall standard deviation (balancing quality of the fit and insensitivity of the final results to the value of θ'') is chosen. The values of $\text{DCS}_\mu(\theta)$ and of the fitting polynomial for each value of θ are averaged over all values of θ'' that were used for testing the stability of the optimal polynomial as a function of θ'' . Those average values are then used for constructing the final “ μ -corrected” DCS.

The previous discussion and Fig. 7 suggest a criterion for determining the optimum value of the scale factor μ in Eq. (1.5.12b) when the DCS is decreasing function of κ_{\max} : it is the value that corresponds to the minimum deviation of $\text{DCS}_\mu(\theta)$ from the extrapolated DCS (i.e., $\text{DCS}_{\text{ext}}(\theta)$) at large angles. In the case discussed, the exact meaning of the quantity that should be minimized can be inferred from the requirement that the optimal value of μ should cause the extrapolated DCS to coincide with the exact DCS, and from the fact that $\text{DCS}_\mu(\theta)$ is completely above the extrapolated DCS when μ is too small (compare curves 3 and 4 in Figs. 7a and 7b), or mostly below the extrapolated DCS when μ is too large (compare curves 5 and 6 in Figs. 7a and 7b). The large-angle distortion usually does not disappear completely at any value of μ : even when μ is equal to the optimal value, $\text{DCS}_\mu(\theta)$ intersects with the extrapolated DCS at one or more points (see curve 2 in Figs. 7a and 7b). Bearing in mind that the SDCS is equal to the integral of the DCS with respect to $\cos \theta$ multiplied by 2π (see Eq. (1.1.31b)), it is natural to require that the integral of the difference between $\text{DCS}_\mu(\theta)$ and the extrapolated DCS with respect to $\cos \theta$ and with the lower bound corresponding to the starting point θ' of the polynomial fitting interval should be equal to zero when μ is optimal:

$$\int_{\theta'}^{\pi} (\text{DCS}_\mu(\theta) - \text{DCS}_{\text{ext}}(\theta)) \sin \theta d\theta = 0. \quad (1.5.24a)$$

The method described above is also applicable in the “soft-photon limit” $k = 0$ (assuming that the soft-photon DCS is calculated using Eq. (1.1.4) in conjunction with Eq. (1.1.20), rather than as a weighted integral of the elastic-scattering DCS [11]). In the case $k = 0$ (and possibly in the case of sufficiently small non-zero k), the angular interval characterized by approximately constant scale factor in Eq. (1.5.12a) is located at small angles, where the DCS is an increasing function of κ_{\max} . Consequently, the positions of the polynomial fitting interval and the angular extrapolation interval with respect to each other are reversed: the function $\text{DCS}_\mu(\theta)$ is extrapolated to small angles. In other respects, the method of determining the optimum value of μ is the same as in the case when the DCS decreases with κ_{\max} . I.e., the deviation of $\text{DCS}_\mu(\theta)$ from the function obtained by polynomial fitting and extrapolation to small angles ($\text{DCS}_{\text{ext}}(\theta)$) must be as small as possible, and this is achieved by numerical solution of the following equation:

$$\int_0^{\theta''} (\text{DCS}_\mu(\theta) - \text{DCS}_{\text{ext}}(\theta)) \sin \theta d\theta = 0, \quad (1.5.24b)$$

where θ'' is the endpoint of the polynomial fitting interval. The distortion of the PW DCS at small angles is less pronounced than at large angles, and it usually cannot be detected by locating a minimum or an extra inflection point (see Fig. 4). Consequently, the position of the mentioned

distortion cannot be used for defining the polynomial fitting interval (unlike in the case when the DCS is a decreasing function of κ_{\max}), and the starting point of the mentioned interval (θ) is equal to the starting point of the angular interval with angle-independent μ in Eq. (1.5.12a).

If the relative correction of the DCS due to the κ_{\max} -fitting by the stretched-exponential approximation (Eq. (1.5.1)) or by the polynomial approximation (Eq. (1.5.10)) is sufficiently small, then the mentioned approximations are sufficiently accurate, so that the value of the scale factor μ in Eq. (1.5.12b) can be calculated directly from Eq. (1.5.12b) as follows:

$$\mu = (\text{DCS}(\kappa_{\max} \rightarrow \infty, \theta) - \text{DCS}(K'', \theta)) / (\text{DCS}(K, \theta) - \text{DCS}(K'', \theta)), \quad (1.5.25)$$

where “ $\text{DCS}(\kappa_{\max} \rightarrow \infty, \theta)$ ” should be interpreted as the κ_{\max} -fitted value of the DCS at a given value of θ . The final value of μ should then be calculated by averaging the right-hand-side of Eq. (1.5.25) over all points that belong to the angular range where μ is approximately angle-independent. However, it has been determined empirically that an even more accurate estimate of μ can be obtained by replacing “ $\text{DCS}(\kappa_{\max} \rightarrow \infty, \theta)$ ” in Eq. (1.5.25) with the partial-wave DCS corresponding to a particular value of κ_{\max} and a given value of θ (i.e., “ $\text{DCS}(\kappa_{\max}, \theta)$ ”), then calculating the mentioned average (over θ) for each value of κ_{\max} in the range $K'' \leq \kappa_{\max} \leq K$, and then extrapolating the sequence of values of the average μ (as a function of κ_{\max}) to $\kappa_{\max} \rightarrow \infty$. Thus, each element of the mentioned sequence is defined as follows:

$$\mu(\kappa_{\max}) \equiv \text{Avg}_{\theta_{\text{start}} \leq \theta \leq \theta_{\text{end}}} [(\text{DCS}(\kappa_{\max}, \theta) - \text{DCS}(K'', \theta)) / (\text{DCS}(K, \theta) - \text{DCS}(K'', \theta))], \quad (1.5.26)$$

where θ_{start} and θ_{end} are the starting and ending angles of the interval where μ is approximately angle-independent. In order to be consistent with the stretched-exponential fitting of the DCS as a function of κ_{\max} (see Section 1.5.1), a similar stretched-exponential model is applied for fitting the function $\mu(\kappa_{\max})$. The two conditions

$$\mu(K'') = 0 \quad \text{and} \quad \mu(K) = 1 \quad (1.5.27)$$

cause a reduction of the number of unknown parameters from four to two, and the following expression of the “theoretical” dependence of μ on κ_{\max} is obtained:

$$\mu_{\text{theor}}(\kappa_{\max}) = \frac{\exp(-\lambda K''^C) - \exp(-\lambda \kappa_{\max}^C)}{\exp(-\lambda K''^C) - \exp(-\lambda K^C)}, \quad (1.5.28)$$

where $\lambda > 0$ and $C > 0$ are the two unknown parameters. Their values are determined by nonlinear least squares fitting, i.e., by minimizing the sum of squared errors (SSE):

$$\text{SSE} \equiv \sum_{\kappa_{\max}=K''}^K (\mu(\kappa_{\max}) - \mu_{\text{theor}}(\kappa_{\max}))^2. \quad (1.5.29)$$

The final value of the scale factor μ in Eq. (1.5.12b) is calculated by substituting the least-squares estimates of λ and C into Eq. (1.5.28) and taking the limit $\kappa_{\max} \rightarrow \infty$:

$$\mu = \mu_{\text{theor}}(\kappa_{\max} \rightarrow \infty) = \frac{\exp(-\lambda K''^C)}{\exp(-\lambda K''^C) - \exp(-\lambda K^C)}. \quad (1.5.30)$$

One of the consequences of calculating μ by this method is that the mentioned polynomial fitting by the function (1.5.22), which is performed at each value of the degree L and for each value of the endpoint θ'' of the polynomial fitting interval, plays no role in estimation of μ . This polynomial fitting has to be performed only to extrapolate the μ -corrected DCS to the angular range where the κ_{\max} -fitted DCS is not sufficiently accurate (i.e., where the relative correction due to the κ_{\max} fitting is too large), and to optimize L , whereas the iterative numerical solution of Eq. (1.5.24a) requires the polynomial fitting to be performed at each step of the iterative solution procedure. In the code of BREMS, such an approach (defined by Eqs. (1.5.26) – (1.5.30)) is applied by default if an angular interval with the values of the mentioned relative correction less than 0.3 is found, and if it is sufficiently wide (at least 20° , and with at least 30 data points inside it), and if the maximum absolute deviation of the empirical scale factor (1.5.25) from 1 inside the mentioned angular interval is less than 0.1. In such a case, the mentioned interval is used to calculate the angular average (1.5.26) (i.e., the endpoints of this interval are used in place of θ_{start} and θ_{end} in

Eq. (1.5.26)), and the value of the scale factor μ in Eq. (1.5.12b) is set equal to the least-squares estimate (1.5.30).

In the case of the two sets of physical parameters corresponding to the examples illustrated by Figs. 4 – 7, it is possible to check the accuracy of the previously-described method of calculating the DCS, because the “exact” theoretical DCS is known in both cases (see the beginning of the current subsection). In Figs. 7a and 7a, the exact DCS is shown by curve 1 (the solid line). The “ μ -corrected” DCS is equal to $\text{DCS}_\mu(\theta)$ (with the optimal μ determined by numerical solution of Eq. (1.5.24a)) in the angular interval $\theta_{\text{start}} \leq \theta < \theta'$, where θ_{start} is the starting angle of the interval where μ is approximately angle-independent, and to the corresponding “extrapolated” DCS_{ext} (obtained by applying the mentioned polynomial fitting and extrapolation) in the angular interval $\theta' \leq \theta \leq 180^\circ$. The absolute value of the relative deviation of the μ -corrected DCS from the exact DCS is less than 3.4 % at all angles greater than 20° in the case $Z = 92$, $T_1 = 8$ MeV, $k = 6.4$ MeV, and less than 1.1 % at all angles greater than 40° in the case $Z = 1$, $T_1 = 30$ MeV, $k = 6$ MeV. In Figs. 7a and 7b, the μ -corrected DCS corresponding to the optimal μ would be practically indistinguishable from the solid line showing the exact DCS. **Note:** Curve 2 (corresponding to optimal μ) in Figs. 7a and 7b has been obtained without the mentioned optimization of the degree of the fitting polynomial L (based on sensitivity of the function $\text{DCS}_{\text{ext}}(\theta)$ to the value of the endpoint θ' of the fitting interval), because a single value of θ' is used. If this optimization is applied, then the accuracy of the μ -corrected DCS is further improved, especially in the case of Fig. 7a ($Z = 92$, $T_1 = 8$ MeV, $k = 6.4$ MeV), where a larger value of L is preferable.

All results presented in this subsection have been obtained without the interpolation of S integrals with respect to l (see Section 1.3.3). The mentioned interpolation does not change the results significantly. In the case $Z = 92$, $T_1 = 8$ MeV, $k = 6.4$ MeV, the relative change of the μ -corrected DCS due to the mentioned interpolation with respect to l is less than 0.05 % at all angles greater than 20° . In the case $Z = 1$, $T_1 = 30$, $k = 6$ MeV, the relative change of the μ -corrected DCS due to the interpolation of S integrals with respect to l is less than 3.4 % at all angles greater than 40° (the maximum relative deviation of the μ -corrected DCS from the Born-approximation DCS changes sign and becomes equal to 2.3 %).

In the code of BREMS, the value of K'' in Eq. (1.5.12b) used for optimization of the scale factor μ is equal to the starting point of the κ_{max} -fitting interval, i.e.,

$$K'' = K - N_{\text{fit}} + 1, \quad (1.5.31)$$

where N_{fit} is calculated according to Eq. (1.5.11a).

In the code of BREMS, the values of DCS_μ calculated according to Eq. (1.5.12b) replace the values calculated by nonlinear κ_{max} -fitting described in Sections 1.5.1 and 1.5.2, if the angular interval with approximately constant μ is sufficiently wide and the range of variation of μ in this interval is sufficiently small. In order to apply the “ μ -correction” defined by Eq. (1.5.12b), the range of variation of the normalized differential of $\text{DCS}(\kappa_{\text{max}})$ (defined by Eq. (1.5.16)) for different angles and for all values of κ_{max} in the interval $K' \leq \kappa_{\text{max}} \leq K$ (i.e., the left-hand side of inequality (1.5.20)) is required to be less than a predefined tolerance (0.1 by default).

The determination of the angular interval of angle-independent scale factor μ in Eq. (1.5.12a) and the subsequent μ -correction of the partial-wave DCS according to Eq. (1.5.12b) are by default performed using the moving average of the original PW DCS (see Section 1.5.3), which is additionally smoothed by the angular spline fitting described in Section 1.7.1. The mentioned μ -correction is applied only when an irregularity (a minimum or an inflection point) is found at large angles in the smoothed angular dependence of the moving average of the PW DCS corresponding to $\kappa_{\text{max}} = K$ or $\kappa_{\text{max}} = K'$ (see Fig. 4a,b for an example of such an irregularity).

If the angular interval of constant scale factor μ is found, then additional moving-average smoothing of the angular dependence of the normalized PW DCS is by default applied inside the mentioned angular interval prior to the κ_{max} -fitting or μ -correction. The “normalization” of the PW DCS is such that the normalized PW DCS, as a function of κ_{max} , always varies from 0 (at $\kappa_{\text{max}} = K''$)

to 1 (at $\kappa_{\max} = K$). If μ is constant, then the values of the normalized PW DCS at a particular value of κ_{\max} should be identical for all values of the angle θ that belong to the mentioned angular interval (this fact justifies the mentioned angular moving-average smoothing). The exact definition of the smoothed normalized PW DCS is similar to Eq. (1.5.26), with the only difference that the averaging is performed over a predefined number of adjacent points (rather than over the entire interval $\theta_{\text{start}} \leq \theta \leq \theta_{\text{end}}$). Because of this additional moving-average smoothing, the κ_{\max} -dependence of the smoothed PW DCS inside the angular interval of constant μ is typically more accurate than outside this interval, so that the results of the κ_{\max} -fitting are also more reliable than in absence of the mentioned moving-average smoothing.

1.6. Calculation of the uncertainties of the fitted single- and double differential cross sections

The calculation of the confidence interval of c in BREMS follows the standard procedure adopted in nonlinear least squares fitting (see, for example, [56]). It involves calculation of the matrix of second partial derivatives of the sum of squared differences $\text{SSD}(\mathbf{x})$ between the fitting function and the actual values, where \mathbf{x} denotes the set of varied parameters (the ‘‘parameter vector’’). The mentioned second derivatives are calculated at the ‘‘optimal’’ parameter values ($\mathbf{x} = \mathbf{x}_0$), which correspond to the minimum value of SSD . Elements of that matrix are

$$G_{ij} = \frac{1}{2} \frac{\partial^2 \text{SSD}}{\partial x_i \partial x_j} \Big|_{\mathbf{x} = \mathbf{x}_0}, \quad (1.6.1)$$

where i and j are the sequence numbers of the parameters. If the theoretical model (i.e., the fitting function) is correct (i.e., unbiased) and if the differences between the theoretical and actual values are independent and distributed normally, then the distributions of the least squares estimates of the varied parameters are normal, and the estimate of the standard deviation of parameter No. i is

$$s_i = \sqrt{\|G^{-1}\|_{ii} \text{SSD}'} = \sqrt{\|G^{-1}\|_{ii} \text{SSD} / (N_{\text{fit}} - n_{\text{var}})}, \quad (1.6.2a)$$

where N_{fit} is the number of fitted points, n_{var} is the number of varied parameters, and G^{-1} is the inverse of the matrix defined by Eq. (1.6.1) (the matrix G^{-1} is called the variance-covariance matrix). In Eq. (1.6.2a), SSD is the sum of squared deviations corresponding to the optimal parameter values, and SSD' is the reduced SSD (here, the term ‘‘reduced’’ means divided by the number of degrees of freedom $N_{\text{fit}} - n_{\text{var}}$).

In BREMS, Eq. (1.6.2a) is used to estimate the uncertainty (‘‘standard error’’) of the least squares estimate of c in Eq. (1.5.1) or Eq. (1.5.10). In the case of the stretched exponential approximation (1.5.1), the application of expression (1.6.2a) is simplified: it is applied only to the intercept (parameter c) of the linear part of the optimization procedure, using the special case of Eq. (1.6.2a) corresponding to a two-parameter linear model (see Section 1.5.1 for further details).

Eq. (1.6.2a) is based on the assumption that errors of parameter estimates are random. Consequently, this expression of the standard deviation does not take into account a possible bias in parameter estimates. Testing has shown that the bias of the least squares estimate of c in Eq. (1.5.1) or Eq. (1.5.10) tends to increase with the magnitude of the correction of the partial-wave (D)CS due to κ_{\max} -fitting, and this bias typically does not exceed 10% of the mentioned correction. Consequently, the estimate of the standard deviation (uncertainty) of the term c in Eq. (1.5.1) or Eq. (1.5.10) is by default modified in BREMS by adding in quadrature the mentioned correction multiplied by 0.1 to the estimate calculated according to Eq. (1.6.2a):

$$\Delta c = \sqrt{s^2 + 0.01(c - c_0)^2}, \quad (1.6.2b)$$

where s is calculated according to Eq. (1.6.2a), c is the least squares estimate of the first term in Eq. (1.5.1) or Eq. (1.5.10), and c_0 is the partial-wave (D)CS.

Since the fitting function (1.5.1) or (1.5.10) is not perfectly accurate, the mentioned assumptions of independence and normal distribution of the differences between the theoretical and actual values are not satisfied in the case discussed. This makes the estimate of the standard error (1.6.2b) very inaccurate. It may be used only as an indicator of the order of magnitude of the

uncertainty of c at best. However, this estimate has another useful property: it helps to keep the number of varied parameters reasonably small, because otherwise (when the theoretical model is “over-parameterized”) the standard deviations (1.6.2a) become excessively large (sometimes exceeding the least squares estimates of the varied parameters). Consequently, a fitting function that provides a better fit inside the fitting interval (due to a larger number of varied parameters) can sometimes be rejected on the grounds of large standard deviations of varied parameters (because large values of (1.6.2a) usually indicate large differences between the fitting function and the true values *outside* of the fitting interval). If, on the other hand, the inclusion of an additional varied parameter causes a significant decrease of the estimates of the standard deviations (1.6.2a), this can usually be interpreted as an improvement of the fitting function. For this reason, if the stretched exponential approximation (1.5.1) is used and if parameter h in Eq. (1.5.1) is allowed to be non-zero, then the DCS is fitted by the stretched exponential (1.5.1) twice: once with $h = 0$ and once with h varied, and the fitting mode corresponding to the smaller standard error is preferred. CS is also fitted with $h = 0$ and with h varied, but the criterion used for choosing the “optimal” fitting mode is different in this case: if the difference of the two estimates of c obtained in both cases is less than the larger of the two standard errors, then the fitting mode corresponding to the smaller standard error is preferred. Otherwise, the fitting mode with $h > 0$ is preferred.

The availability of two values of the uncertainty (1.6.2b) $\Delta c'$ and $\Delta c''$, corresponding to each of the two fitting intervals (see Eqs. (1.5.11a) and (1.5.11b)), makes it possible to improve the accuracy of the final fitted value of (D)CS by calculating it as an average over two fitting intervals. This average may be either simple or weighted. In the case of a simple average, the uncertainty of the fitted (D)CS is calculated as follows:

$$\Delta c = \frac{1}{2} \sqrt{(\min(\Delta c', |c' - c''|))^2 + (\max(\Delta c'', |c' - c''|))^2}, \quad (1.6.3)$$

where c' and c'' are the least squares estimates of (D)CS corresponding to each of the two values of N_{fit} (the double prime indicates the wider fitting interval). This method of combining the fitting results corresponding to the two fitting intervals is used in BREMS by default. Functions “min” and “max” are used in Eq. (1.6.3), because the uncertainty of c corresponding to the narrower interval ($\Delta c'$) is sometimes overestimated by a large factor, whereas the uncertainty corresponding to the wider interval ($\Delta c''$) is frequently underestimated. The value of (1.6.3) is of the order of $|c' - c''|$ or greater. If the relative range of variation of the unfitted (D)CS inside the narrower interval is less than 0.1 %, then the second term in the square root of (1.6.3) is replaced with $(c' - c'')^2$, because under those conditions $\Delta c''$ is also sometimes overestimated by a large factor. There is also an option to calculate c as a weighed average of c' and c'' , with the weights inversely proportional to the squared uncertainties and normalized to 1:

$$c = f_1 c' + f_2 c'', \quad (1.6.4a)$$

$$f_1 = [1 + (\Delta c' / \Delta c'')^2]^{-1}, \quad f_2 = [1 + (\Delta c'' / \Delta c')^2]^{-1}. \quad (1.6.4b)$$

Assuming that the errors corresponding to each of the two fitting intervals are uncorrelated and sampled from two normal distributions with zero mean and with standard deviations equal to $\Delta c'$ and $\Delta c''$, such calculation provides the maximum-likelihood estimate of the (D)CS. The same assumption leads to the following estimate of the uncertainty of the final fitted (D)CS:

$$\Delta c^{(0)} = \frac{1}{\sqrt{(\Delta c')^{-2} + (\Delta c'')^{-2}}}. \quad (1.6.5a)$$

In order to take into account a possible bias in the estimate of the final fitted (D)CS, and the possible dependence of this bias on the choice of the fitting interval, this estimate of Δc is modified by taking into account two additional measures of the uncertainty of the fitted (D)CS: $c' - c$ and $c'' - c$. The resulting estimate of the uncertainty of the final fitted (D)CS is

$$\Delta c = \sqrt{(\Delta c^{(0)})^2 + f_1^2 (c' - c)^2 + f_2^2 (c'' - c)^2}. \quad (1.6.5b)$$

If the polynomial approximation (1.5.10) has been applied in one or both of the two fitting intervals, then only the result corresponding to the wider interval is used (i.e., Eqs. (1.6.3) – (1.6.5) are not applied in this case).

By default, c is calculated in BREMS using several values of the endpoint of the fitting interval κ_{end} . The default number of values of κ_{end} used is equal to $N_{\text{fit}}/4$, where N_{fit} is the maximum number of points in a fitting interval (N_{fit} is calculated according to Eq. (1.5.11a) or Eq. (1.5.11b)). Thus, κ_{end} is varied inside the interval $K - (N_{\text{fit}}/4) + 1 \leq \kappa_{\text{end}} \leq K$. However, the number of values of κ_{end} is not allowed to become less than 5. I.e., if $N_{\text{fit}}/4 < 5$, then the range of values of κ_{end} is $K - 4 \leq \kappa_{\text{end}} \leq K$. The final estimate of the fitted DCS is the arithmetic average of the least squares estimates corresponding to each value of κ_{end} used. For each value of κ_{end} , the CS is additionally estimated by integrating the fitted DCS with respect to the solid angle Ω . The latter integral will be denoted $\int \text{DCS} d\Omega$. This integral is calculated by numerical quadrature, and it is approximately equal to the least squares estimate of the CS (the difference between the two is caused only by numerical errors, including the possible bias due to inaccuracy of the fitting function (1.5.1) or (1.5.10), because the CS and the values of the DCS for each angle θ are fitted independently). The final estimate of the fitted CS is the arithmetic average of the average of c and the average value of $\int \text{DCS} d\Omega$ (each of the latter two averages is calculated over one or two sets of the fitting intervals, depending on whether one or two values of N_{fit} were used). The estimate of the uncertainty of the fitted (D)CS (i.e., ΔCS or ΔDCS) is equal to the square root of the sum of (a) the average of the values of $(\Delta c)^2$ corresponding to each of the endpoints of the fitting interval (Δc is calculated according to Eq. (1.6.3)), (b) the empirical variance of the fitted (D)CS (the empirical variance is calculated using the same estimates of the (D)CS that are used to calculate the average (D)CS), (c) the squared angular integral of the uncertainty of the fitted DCS, i.e., $(\int |\Delta\text{DCS}| d\Omega)^2$, (d) the squared difference of the mentioned final estimate of the fitted CS and the angular integral of the fitted DCS, i.e., $(c - \int \text{DCS} d\Omega)^2 / 4$. The latter two terms are added only when calculating the uncertainty of the fitted CS, and only when the angular interval is from 0° to 180° , whereas the angular grid is sufficiently dense for accurate estimation of the latter integral (i.e., the maximum angular increment is not greater than 1°). The total uncertainty of the fitted DCS (i.e., the integrand ΔDCS in the definition of the last mentioned term) is additionally modified by adding (in quadrature) up to four other terms to the previously-mentioned estimate:

- the term reflecting the relative change of the unfitted partial-wave DCS due to the replacement of the original S integrals with the “test” values (see also Sections 1.4 and 6.16),
- the term reflecting the relative change of the unfitted partial-wave DCS due to the reduction of l_{max} in comparison with the theoretical maximum of l , which is equal to $\max|\kappa_1| + \max|\kappa_2|$ (see also Sections 1.3.2 and 6.16),
- the standard deviation of the μ -corrected DCS corresponding to the maximum value of κ_{end} (i.e., $\kappa_{\text{end}} = K$) over different polynomial fitting intervals, using the optimal (or user-specified) degree of the fitting polynomial and the optimal (or user-specified) choice of the reference function (see also Section 1.5.4), or the uncertainty of the extrapolated value of the DCS, if the large-angle polynomial extrapolation described in Section 1.7.3 has been applied (this extrapolation is never applied together with the μ -correction),
- the correction of the original κ_{max} -fitted DCS in the transition interval, where the original DCS is joined smoothly with the alternative DCS calculated using a greater value of the ratio $|\kappa_1|_{\text{max}} / |\kappa_2|_{\text{max}}$ (see also Section 1.8).

A similar approach is used to calculate the uncertainty of the fitted shape function (SF). The fitted SF is defined as the ratio of the fitted DCS and the mentioned angular integral of the same DCS (since the latter integral is approximately equal to the fitted CS, the fitted DCS can be calculated by multiplying the values of the fitted CS and the fitted SF). The final estimate of the fitted SF is the average of the values of the mentioned ratio ($\text{DCS} / \int \text{DCS} d\Omega$) corresponding to each

of the endpoints of the fitting interval (κ_{end}). The absolute uncertainty of the SF is calculated as the square root of the sum of two terms: the empirical variance of the ratio $\text{DCS} / \int \text{DCS} d\Omega$, and the average squared value of (1.6.3), divided by the average value of $\int \text{DCS} d\Omega$ squared. The relative uncertainty of the CS, DCS or SF is equal to the ratio of the corresponding absolute uncertainty and the corresponding estimate of the CS, DCS or SF.

When T_1 is sufficiently small or k / T_1 is sufficiently large, the extrapolation described in Section 1.5 becomes unnecessary, because the number of terms in the truncated series for the (D)CS (Eq. (1.1.4) or (1.1.5)) is sufficient to practically reach the saturation value. The minimum relative range of variation of the (D)CS inside the fitting interval, which is needed for the extrapolation to be performed, is 0.1 %. If the relative range is less, then the value of the corresponding relative uncertainty of the (D)CS or the SF is replaced by the relative range of variation with the minus sign.

1.7. Polynomial or spline fitting and extrapolation of the angular dependence of the DCS

1.7.1. Angular spline fitting and extrapolation of the original partial-wave DCS

The distortions of the angular dependence of the original DCS (further called “partial-wave DCS”, or “PW DCS”), which were mentioned at the beginning of Section 1.5.4 and which are illustrated in Fig. 4 and Fig. 8a,b, can be eliminated by angular extrapolation of the PW DCS at each value of κ_{max} (thus extrapolated PW DCS is shown in Fig. 8b by short-dashed lines for five values of κ_{max}). After that, the nonlinear fitting procedure described in Section 1.5 is applied to the set of extrapolated PW DCS corresponding to a set of consecutive values of κ_{max} at each value of the angle θ . This method makes it possible to improve the accuracy of the final DCS at large angles.

The method of angular extrapolation applied in BREMS is based on angular cubic spline fitting: at first the angular dependence of the PW DCS is spline-fitted at intermediate angles, and then it is smoothly continued (extrapolated) to the large-angle interval ending at $\theta = 180^\circ$. In order to calculate the spline coefficients, the following information must be available:

- 1) transformation applied to the original DCS (e.g., logarithm or division by a reference function),
- 2) spline argument (for example, θ , $-\cos \theta$, or $\ln((1 - \cos \theta) / 2)$),
- 3) number and positions of the knots of the spline,
- 4) values of the spline at the knots.

Items No. 1 and No. 2 of the latter list are determined so as to improve the reliability of the large-angle extrapolation. In general, it is improved by reducing the range of variation of the fitted function in the entire angular interval ($0^\circ \leq \theta \leq 180^\circ$) and by making this variation as smooth as possible (i.e., by reducing the number of the lowest-order terms of the Taylor series expansion of the function that are needed to approximate the function with sufficient accuracy). This is achieved by using alternative spline arguments and replacing the original PW DCS with its ratio to a particular reference function. One obvious candidate for the role of a reference function is the DCS obtained from the screened Born approximation (Eq. (1.1.36)). Another candidate is the Sommerfeld-Maue (SM) approximation with the next-to-leading order (NLO) correction and the screening correction (the sum of (1.1.40) and (1.1.44), plus the screening correction calculated in the Born approximation, i.e., the expression in brackets in Eq. (1.1.46) multiplied by k / Z^2). The angular dependences obtained after dividing the PW DCS by each of the two mentioned alternative reference functions are shown in Fig. 8c and Fig. 8d, respectively. In addition to using the angle θ as the spline argument, it is worthwhile to test alternative arguments: $-\cos \theta$ and $\ln((1 - \cos \theta) / 2)$. The angular dependences obtained using the latter two alternative arguments are shown in Fig. 8e and Fig. 8f, respectively. A possible additional transformation is the replacement of the spline-fitted function by its logarithm. As it is evident from Fig. 8e and Fig. 8f, usage of the logarithm in conjunction with the spline arguments $-\cos \theta$ and $\ln((1 - \cos \theta) / 2)$ sometimes makes the angular dependence more linear in shape at large angles (and hence more amenable to large-angle extrapolation). It should be noted that in the case when the spline argument is θ , the angular dependence in the vicinity of $\theta = 0^\circ$ and $\theta = 180^\circ$ is always parabolic (for example, see the short-

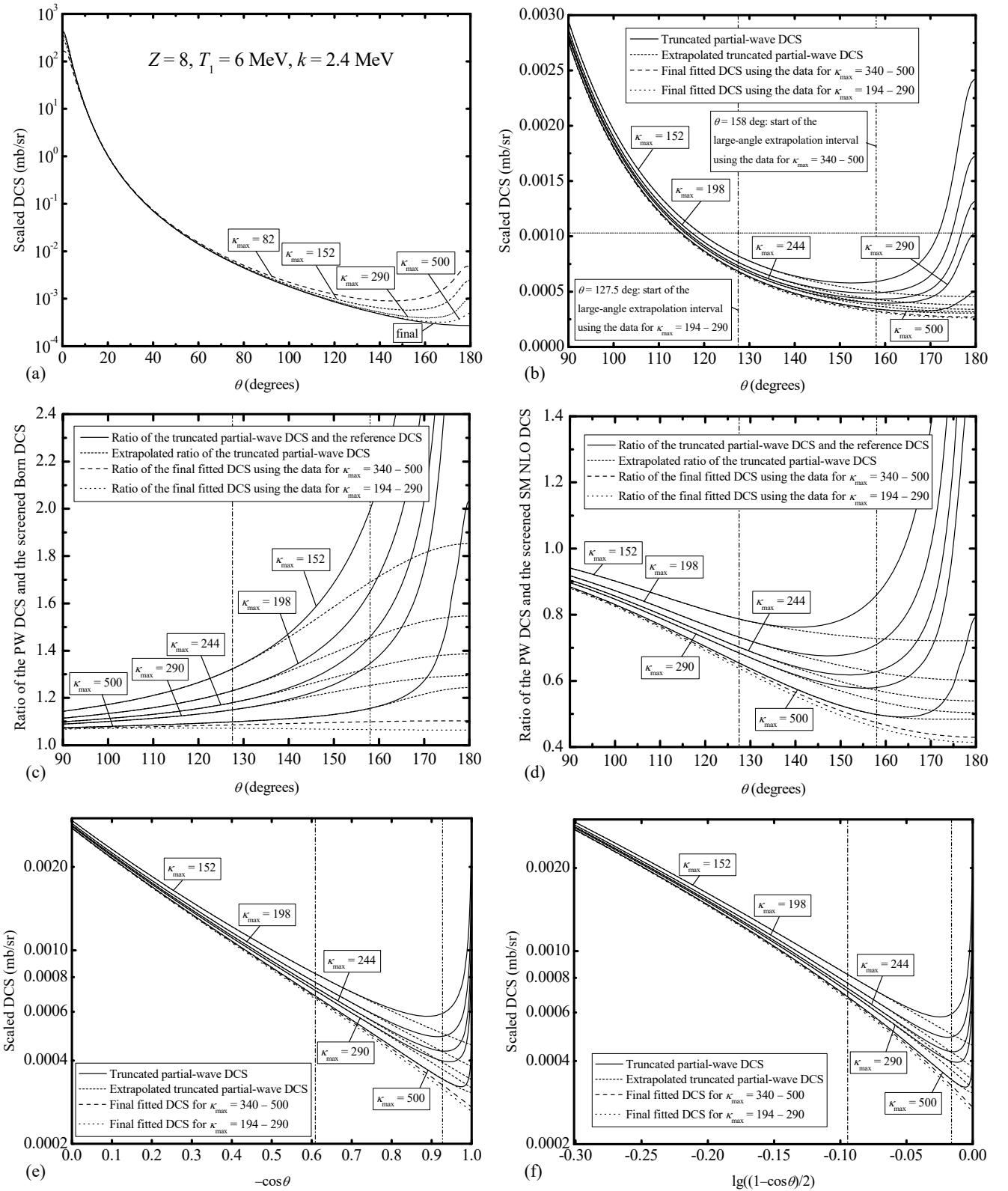


Fig. 8. The calculated angular dependence of the DCS when $Z=8$, $T_1=6$ MeV, $k=2.4$ MeV, and the Kohn-Sham potential is used. **(a)** The DCS obtained by truncating the sum in (1.1.4) (“partial-wave DCS” or “PW DCS”) at four values of κ_{\max} defined by Eq. (1.5.2), and the final fitted DCS from the analysis of the data corresponding to $340 \leq \kappa_{\max} \leq 500$. **(b)** The PW and extrapolated DCS at five values of κ_{\max} , and two final fitted DCS corresponding to intervals $194 \leq \kappa_{\max} \leq 290$ and $340 \leq \kappa_{\max} \leq 500$. The horizontal dotted line indicates the value of the DCS at $\kappa_{\max} = 290$, $\theta = 180^\circ$. **(c)** The same curves as in (b) after division by the approximate DCS calculated using the screened Born approximation. **(d)** The same curves as in (b) after division by the approximate DCS calculated using the Sommerfeld-Maue approximation with the next-to-leading order correction and screening correction. **(e)** The same curves as in (b), plotted logarithmically against $-\cos\theta$. **(f)** The same curves as in (b), plotted logarithmically against $\lg((1-\cos\theta)/2)$. The vertical dash-dotted and dash-dot-dotted lines in (b) – (f) indicate the start of the large-angle extrapolation interval corresponding to the two mentioned ranges of κ_{\max} ($194 \leq \kappa_{\max} \leq 290$ and $340 \leq \kappa_{\max} \leq 500$, respectively).

dashed lines in Fig. 8c), because $d(\text{DCS})/d\theta|_{\theta=0^\circ} = 0$ and $d(\text{DCS})/d\theta|_{\theta=180^\circ} = 0$. The latter two equalities are true regardless of the approximation used when calculating the DCS (in the case of the PW DCS, those equalities follow from the properties of the spherical harmonics in Eq. (1.1.4)).

The extrapolated curves, which are shown by short-dashed lines in Fig. 8b-f, were obtained by cubic spline fitting of the ratio of the original PW DCS and the screened Born DCS (the spline-fitting interval was $10^\circ \leq \theta \leq 127.5^\circ$ when analyzing the data for $194 \leq \kappa_{\max} \leq 290$, and $10^\circ \leq \theta \leq 158^\circ$ when analyzing the data for $340 \leq \kappa_{\max} \leq 500$).

The knots of the spline (item No. 3 of the previous list) are defined in BREMS using a simplified algorithm, which uses up to five parameters in order to define positions of all knots: the starting and ending points of the spline-fitting interval (θ_{\min} and θ_{\max}), the number of knots in the spline-fitting interval (N), and one or two parameters defining the variation of the knot density inside the spline-fitting interval (ε_1 and ε_2 , which are defined below). This simplification (as compared to specification of each knot individually) is justified by a relatively simple shape of the angular dependence of the DCS (for example, see Fig. 8a).

Note: The spline argument cannot be equal to $\ln((1 - \cos \theta) / 2)$ in the angular interval starting at 0° and ending at the first non-zero knot, because $\lim_{\theta \rightarrow 0} [\ln((1 - \cos \theta) / 2)] = -\infty$. Hence, the latter definition of the argument is used only in the angular interval starting at the first non-zero knot, whereas the spline argument in the preceding interval is in such a case equal to θ (the spline function and its first two derivatives are continuous at the first non-zero knot).

In general, the optimal positions of the knots are such that the width of the interval between adjacent knots (the ‘‘inter-knot interval’’) decreases with increasing curvature of the function that is being fitted (in other words, the knot density increases). Hence, it can be expected that the positions of the knots corresponding to the optimal spline approximation of the curve shown by the solid line in Fig. 8a are such that the width of the inter-knot interval is smallest in the vicinity of $\theta = 0^\circ$ and greatest in the vicinity of $\theta = 180^\circ$. Such variation of the knot density can be achieved by requiring that the widths of the inter-knot intervals form a geometric progression:

$$w_i = w_0 \varepsilon^i, \quad i = 1, 2, \dots, N - 2, \quad (1.7.1)$$

where i is the zero-based number of the inter-knot interval, w_i is its width, and ε is the ratio of the widths of adjacent inter-knot intervals (in this example, $\varepsilon > 1$). In the code of BREMS, the parameter ε in Eq. (1.7.1) is defined in terms of the ratio ε_1 of the last and initial inter-knot intervals:

$$\varepsilon = \varepsilon_1^{1/N'}, \quad (1.7.2)$$

where N' is one less than the number of inter-knot intervals:

$$N' = N - 2. \quad (1.7.3)$$

By substituting (1.7.2) into Eq. (1.7.1), the following expression of the logarithm of w_i is obtained:

$$\ln w_i = \ln w_0 + i \frac{\ln \varepsilon_1}{N'}. \quad (1.7.4)$$

For added flexibility, the code of BREMS allows using the second parameter ε_2 , so that the linear dependence (1.7.4) is replaced by a quadratic one:

$$\ln w_i = \ln w_0 + \frac{\ln \varepsilon_1}{N'} i + \frac{\ln(\varepsilon_2 / \varepsilon_1)}{2N'^2} i^2. \quad (1.7.5)$$

In this case, $\ln(\varepsilon_1)/N'$ and $\ln(\varepsilon_2)/N'$ are equal to the values of the first derivative of the function (1.7.5) at the points $i = 0$ and $i = N'$, respectively (see Fig. 9).

After defining the original function, the spline argument and the spline knots (items No. 1 – 3 of the previous list), the values of the optimal spline at the knots (item No. 4) can be uniquely determined by least squares fitting (multiple linear regression). The optimized parameters in this stage of the calculation are the values of the spline at all the knots and the values of its first derivative at $\theta = \theta_{\min}$ and $\theta = \theta_{\max}$, except when the spline argument is θ . In the latter case, the mentioned requirement of zero first derivative at $\theta = 0^\circ$ and $\theta = 180^\circ$ requires modifying the set of

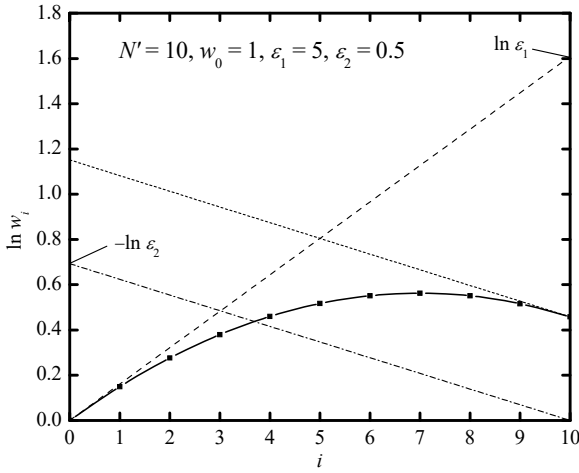


Fig. 9. Values of the natural logarithm of the inter-knot interval (squares connected by the solid line) calculated according to Eq. (1.7.5) using parameter values indicated at the top of the graph (the number of knots is equal to 12). i is the zero-based sequence number of the inter-knot interval. The long- and short-dashed lines are the tangents of the solid curve at the two endpoints. The dash-dotted line is parallel to the short-dashed line and passes through zero at $i = 10$.

the linear regression parameters (which are being optimized) and the set of the basis functions of the linear model. If $\theta_{\min} = 0^\circ$ or $\theta_{\max} = 180^\circ$, then this modification causes a reduction of the number of the linear regression parameters, because they no longer include the corresponding first derivative. If $\theta_{\min} > 0^\circ$ or $\theta_{\max} < 180^\circ$, then the mentioned modification of the set of the linear regression parameters consists in the replacement of the corresponding first derivative by the value of the spline at the additional knot $\theta = 0^\circ$ or $\theta = 180^\circ$, respectively. However, the term “number of knots” and the notation “ N ” will be used to mean only the knots belonging to the spline-fitting interval ($\theta_{\min} \leq \theta \leq \theta_{\max}$). I.e., the mentioned additional knots at $\theta = 0^\circ$ and $\theta = 180^\circ$ will not be included.

Unlike the problem of optimizing the values of the spline at a fixed set of knots, the problem of optimizing the knot positions (i.e., parameters θ_{\min} , θ_{\max} , N , ε_1 , and ε_2) is nonlinear. In the code of BREMS, this problem is formulated as a problem of minimizing an appropriate “objective function” (OF) f , which is defined so as to ensure both a good agreement between the final spline and the original function inside the spline-fitting interval, and a good reliability of the spline extrapolation outside this interval. Both mentioned goals can be achieved by defining the OF as follows:

$$f = \delta_{\text{unc}}^2, \quad (1.7.6)$$

where δ_{unc} is the root-mean-square (rms) value of the relative uncertainty of spline fitting in the angular range $\theta_{\min} \leq \theta \leq 180^\circ$. The uncertainties of the spline values at all the knots are estimated using the general rule of least squares fitting (Eq. (1.6.2a)) during optimization of the spline values at a current set of knots. I.e., the “parameter vector” x in (1.6.1) includes in this case only the values of the spline at N knots, plus the values of the first derivative of the spline at $\theta = \theta_{\min}$ and $\theta = \theta_{\max}$ (unless the spline argument is θ , in which case the mentioned values of the first derivative are either fixed at 0 or replaced by the values of the spline at the additional knots $\theta = 0^\circ$ and $\theta = 180^\circ$, as explained above). The uncertainties of the spline values at the data points are estimated under the assumption that errors of the estimates of the linear regression parameters are uncorrelated and sampled from normal distributions with the standard deviation given by Eq. (1.6.2a). In order to take into account the fact that the original values of the DCS (which are being fitted by a spline function) are themselves obtained by fitting of the type described in Sections 1.5.1, 1.5.2 and 1.5.4 and are consequently inaccurate, the errors of the spline values at the knots are calculated using a modification of the standard expression (1.6.2a), where the sum of squared residuals SSD is increased by adding the sum of squared uncertainties (standard errors) of the original values of the DCS in the spline-fitting interval (if the original (D)CS is the least squares estimate of the term c in Eq. (1.5.1) or Eq. (1.5.10), then those uncertainties are calculated according to Eq. (1.6.2b)).

An increase of the number of adjustable parameters always causes a decrease of the rms value of the residuals inside the fitting interval. However, if this decrease is not substantial, δ_{unc} increases and accuracy of the extrapolation outside of the fitting interval is usually reduced. This property of the OF defined by Eq. (1.7.6) helps to avoid “over-parameterization” of the fitting model (i.e., an excessively large value of N , which would make the angular spline extrapolation less reliable).

The role of parameters θ_{\min} , θ_{\max} and N is different from the role of parameters ε_1 and ε_2 , because $f(1.7.6)$ is a smooth function of the latter two parameters, but it is a discontinuous function of the former three parameters: N is discontinuous itself (an integer number), whereas a change of θ_{\min} , θ_{\max} causes a change of the number of data points inside the spline-fitting interval and a consequent abrupt change of the sum of squared residuals and of the δ_{unc} (see Eq. (1.6.2a)). For this reason, the full optimization of θ_{\min} , θ_{\max} and N is replaced in BREMS by a search among a set of pre-defined values (either the default ones or defined by the user). Parameters ε_1 and ε_2 are optimized by simplex minimization of f as a function of ε_1 and ε_2 at each triplet of values of θ_{\min} , θ_{\max} and N . In order to reduce the probability that the “optimal” values of parameters ε_1 and ε_2 correspond to a local minimum rather than the absolute minimum of f , the initial values of ε_1 and ε_2 are determined before the iterative simplex minimization procedure by a search among a set of pre-defined values (by default, $\lg(\varepsilon_1)$ and $\lg(\varepsilon_2)$ are varied from -10 to $+10$ in steps of 1, for a total of $21^2 = 441$ combinations). During the simplex optimization, the widths of the inter-knot intervals are not allowed to become too small: each such interval is required to contain at least four data points. This constraint is necessary in order to avoid unphysical oscillations (or inflection points) between adjacent knots. Another requirement is that the spline approximation of the DCS must have no more than two extremum points and no more than three inflection points as a function of θ in the angular range $0^\circ < \theta < 180^\circ$ (not counting the extrema at $\theta = 0^\circ$ and $\theta = 180^\circ$). If the spline extrapolation to large angles is performed, then the maximum allowed numbers of extremum points and inflection points are reduced by 1 (to 1 and 2, respectively). This property is tested after the simplex optimization of ε_1 and ε_2 . If the spline approximation of the DCS does not conform to this requirement, then it is rejected (i.e., it is not used for the subsequent comparison between the various combinations of the adjustable parameters).

The choice between the three mentioned alternative reference functions (a constant equal to 1, screened Born DCS, or screened SM NLO DCS), three alternative spline arguments (θ , $-\cos \theta$, or $\ln((1 - \cos \theta) / 2)$ and two options related to the logarithm (either replacing the function by its logarithm or not) is also made on the basis of a comparison of the final value of the objective function $f(1.7.6)$ corresponding to each of those $3 \times 3 \times 2 = 18$ combinations. In order to make this comparison valid, the value of the true DCS is recovered from the value of the transformed DCS by applying the inverse transform (i.e., using it as the argument of an exponential if it has been replaced by its logarithm, and multiplication by the reference function) before calculating the final value of f and making the comparison.

In order to reduce the number of combinations of adjustable parameters that have to be tested and to make the final estimate of the DCS more reliable, there is an option in BREMS to determine the value of θ_{\max} automatically before starting the optimization procedure described above. This determination is based on an empirical observation that the optimal value of θ_{\max} tends to increase (i.e., approaches 180°) with decreasing magnitude of the large-angle distortion of the DCS and with decreasing relative difference between the values of the PW DCS corresponding to different values of κ_{\max} . Consequently, if an extra minimum is detected in the angular dependence of the DCS corresponding to $\kappa_{\max} = K$ (defined by Eq. (1.5.3)) at an angle $\theta' < 180^\circ$ (as in Fig. 8b, solid curves), then the maximum value of θ_{\max} is set to the maximum value of θ satisfying the condition $\theta < \theta'$ and one of these two additional conditions:

- (a) $\text{DCS}(\theta) > \text{DCS}(180^\circ)$, where the DCS corresponds to $\kappa_{\max} = K$,
- (b) the relative variation of the value of DCS corresponding to that angle over the last N_{fit} values of κ_{\max} (i.e., $K - N_{\text{fit}} + 1 \leq \kappa_{\max} \leq K$, where N_{fit} is given by Eq. (1.5.11a)) is less than 10%.

The larger one of the two angles determined from each one of these two conditions is used by default as the largest one in the set of six equidistant values of θ_{\max} to be tested, in increments of 2° . The optimal one among them is chosen on the basis of the requirement of the minimum value of the OF (1.7.6). For example, if $K = 290$, then the first of the two mentioned values of θ corresponds to the first intersection of the dotted horizontal line with the fourth solid curve in Fig. 8b (counting

from the top). This value of θ is equal to 115.5° . The second value of θ corresponds to the rightmost point of the angular interval where the relative difference between the second and fourth solid lines in Fig. 8b is less than 10%. This value of θ is equal to 137.5° . Since the latter value of θ is greater, it is used as the largest one of the six equidistant values of θ_{\max} to be tested in this example. Hence, the mentioned set consists of the six angles from 127.5° to 137.5° , in increments of 2° . The requirement of the minimal value of the objective function (1.7.6) causes the angle 127.5° to be chosen as the optimal one (it is indicated in Fig. 8b–f by the vertical dash-dotted line).

The extrapolated part of the spline approximation corresponds to the interval $\theta_{\max} < \theta \leq 180^\circ$ (see the short-dashed lines in Fig. 8b). This method can be applied for small-angle extrapolation, too (there is such an option in BREMS): in this case, the extrapolated part of the spline function corresponds to the interval $0^\circ \leq \theta < \theta_{\min}$. However, if $\theta_{\min} > 0^\circ$, then the data in the interval $0^\circ \leq \theta < \theta_{\min}$ are not modified by default (unlike in the interval $\theta_{\max} < \theta \leq 180^\circ$).

By default, the angular extrapolation of the PW DCS is not performed, i.e., $\theta_{\min} = 0^\circ$ and $\theta_{\max} = 180^\circ$. In this case, the only effect of the angular spline fitting is smoothing of the angular dependence of the PW DCS. In absence of angular extrapolation, the definition of the objective function (1.7.6) does not have any advantages over the standard definition of the OF used in least squares fitting:

$$f = \delta_{\text{res}}^2, \quad (1.7.7)$$

where δ_{res} is the root-mean-square (rms) value of relative residuals of the spline fitting inside the interval $\theta_{\min} \leq \theta \leq \theta_{\max}$. Eq. (1.7.7) is the default definition of the OF used in the code of BREMS. The knots of the spline and other adjustable parameters are determined from the analysis of the PW DCS corresponding to $\kappa_{\max} = K$. After determining the optimal values of the spline parameters corresponding to $\kappa_{\max} = K$, the same parameters are applied to all smaller values of κ_{\max} , and only the values of the spline function at the knots are calculated for each value of κ_{\max} independently by multiple linear regression. It has also been determined empirically that usage of the analytical Sommerfeld-Maue DCS as one of the reference functions, as well as usage of θ or $\ln((1 - \cos \theta) / 2)$ as the argument of the spline function does not add to the accuracy of the spline-fitted partial-wave DCS. Thus, only two reference functions (the constant equal to 1, and the analytical Born approximation) and only one argument ($-\cos \theta$) are used by default, resulting in the total of $2 \times 1 \times 2 = 4$ minimizations of the OF to be performed at each triplet of values of θ_{\min} , θ_{\max} and N .

Note: In the case of two knots ($N = 2$), the linear and quadratic functions of $-\cos \theta$ are also tested by default (in addition to the cubic polynomial of $-\cos \theta$). In this case, the basis functions of the linear regression are defined so that two of the optimized coefficients are equal to the values of the approximating polynomial at the two endpoints, and the third coefficient (in the case of the quadratic polynomial) is equal to the first derivative at the first endpoint. This makes the uncertainties of values of the approximating polynomial more comparable with those obtained in the case of cubic spline fitting.

1.7.2. Angular spline fitting and extrapolation of the κ_{\max} -fitted DCS

The fitted DCS, which is obtained after the angular spline fitting described above and the subsequent fitting of the data as a function of κ_{\max} by the method described in Section 1.5 (the “ κ_{\max} -fitted DCS”), may be distorted, too, because of the fitting errors. As in the case of the partial-wave DCS (the “PW DCS”), the largest distortions of the κ_{\max} -fitted DCS usually occur at large angles. However, unlike the small- and large-angle distortions of the PW DCS illustrated in Fig. 8a, the mentioned fitting errors are much more difficult to predict. They can be random, or they can include a bias term as well. If the κ_{\max} -fitting errors were purely random, then they could be dealt with by smoothing the κ_{\max} -fitted DCS in the entire angular range $0^\circ \leq \theta \leq 180^\circ$. This smoothing could be implemented, for example, as iterative spline fitting of the kind described above, with $\theta_{\min} = 0$ and $\theta_{\max} = 180^\circ$ and with other adjustable parameters (such as the number of knots N and the knot density parameters ε_1 and ε_2) determined by minimization of the objective function (1.7.6) or (1.7.7). However, if bias is present, then smoothing alone would not suffice. As in the case of the

PW DCS, this problem is solved in BREMS by spline extrapolation. The meanings of the adjustable parameters during the angular spline fitting and extrapolation of the κ_{\max} -fitted DCS are the same as in the case of the angular spline fitting of the PW DCS (see Section 1.7.1). In the case of the κ_{\max} -fitted DCS, the starting angle θ_{\min} of the spline-fitting interval is by default equal to 0, except when T_1 and T_2 are large ($T_1 > 10$ MeV, $T_2 > 3$ MeV, and $T_2 / T_1 > 0.1$ simultaneously) and the PW DCS is a decreasing function of κ_{\max} , and the angular interval characterized by an approximately constant scale factor μ has been found (see Section 1.5.4), in which case θ_{\min} is by default equal to θ_{start} (the starting point of the angular interval corresponding to approximately constant scale factor μ). If the “ μ -correction” described in Section 1.5.4 is not applied, or the PW DCS is an increasing function of κ_{\max} , then the value of θ_{\max} is by default selected from a set of 17 equidistant values from 100° to 180° , with the angular increment equal to 5° . If the “ μ -correction” is applied and the PW DCS is a decreasing function of κ_{\max} , then θ_{\max} is by default equal to θ' (the endpoint of the polynomial fitting interval used for the μ -correction). If either $T_1 \leq 10$ MeV, or $T_2 \leq 3$ MeV, or $T_2 / T_1 \leq 0.1$, then the data in the interval $0^\circ \leq \theta < \theta_{\min}$ are not modified by default. Otherwise, the spline function is extrapolated to the interval $0^\circ \leq \theta < \theta_{\min}$. This may cause large errors at small angles, unless a sufficiently accurate value of the CS (i.e., the integral of the DCS with respect to the solid angle of photon emission) is available, as mentioned further in this section (in the discussion of the objective function, which is minimized during the spline fitting of the κ_{\max} -fitted DCS).

In comparison with the angular spline fitting of the partial-wave DCS (see Section 1.7.1), there is one additional reference DCS available in the case of spline fitting of the κ_{\max} -fitted DCS: the PW DCS corresponding to $\kappa_{\max} = K$, where K is defined by Eq. (1.5.3) (this PW DCS may have been spline-fitted and extrapolated as described in Section 1.7.1).

When the angular extrapolation of the κ_{\max} -fitted DCS is performed, the default minimum value of the average inter-knot interval (which is equal to $(\theta_{\max} - \theta_{\min}) / (N - 1)$) is relatively large (10° , corresponding to 19 knots when $\theta_{\min} = 0^\circ$ and $\theta_{\max} = 180^\circ$). This is justified by the known facts that (a) for sufficiently small Z and large T_2 ($Z < 20$, $T_2 > 500$ keV), the accuracy of the screened Born approximation is usually better than 30 % at all angles, and (b) the convergence of the PW series (1.1.4) and (1.1.5) improves with increasing Z and decreasing T_2 . As a result, the exact DCS is usually close either to the DCS calculated using the screened Born approximation (when $Z < 20$ and $T_2 > 500$ keV), or to the spline-fitted (and possibly extrapolated) PW DCS corresponding to $\kappa_{\max} = K$ (when $Z > 20$, or $T_2 < 500$ keV). Similarity of the κ_{\max} -fitted DCS to a particular reference function means that the ratio of the κ_{\max} -fitted DCS and the reference function is not too different from 1 and varies relatively slowly with θ , which allows using a small number of knots when performing the angular spline extrapolation of that ratio. A smaller number of knots is preferable when performing the angular extrapolation of the κ_{\max} -fitted DCS, because an increase of the number of knots tends to amplify the effects of the random fitting errors on the behavior of the spline in the angular extrapolation range.

As mentioned in Section 1.6, multiple fitting intervals are used during the κ_{\max} -fitting. BREMS can apply the angular spline fitting and extrapolation described above to the average over all κ_{\max} -fitting intervals, or to perform the spline fitting and extrapolation for each κ_{\max} -fitting interval separately, and then to average the spline approximations over all κ_{\max} -fitting intervals. In the latter case, it is possible to use the same set of spline knots and other adjustable parameters for all κ_{\max} -fitting intervals, with only the values of the spline function at the knots calculated for each κ_{\max} -fitting interval independently by multiple linear regression, or to calculate all adjustable parameters of the spline fitting (including the parameters defining the knot positions) independently for each κ_{\max} -fitting interval (the latter approach is the default one). If the values of the spline function are calculated for each κ_{\max} -fitting interval separately, but the other adjustable parameters of the spline fitting (including the set of knots) are the same for all κ_{\max} -fitting intervals, then the rms value δ_{unc} is calculated over all κ_{\max} -fitting intervals. The definition of the objective function,

which is minimized during the angular spline fitting of the κ_{\max} -fitted DCS, includes by default three terms:

$$f = (\delta_{\text{unc}}^2 + \delta_{\text{res}}^2 + \delta_{\text{CS}}^2) / 3, \quad (1.7.8a)$$

where the meaning of the terms δ_{unc}^2 and δ_{res}^2 are the same as in Eqs. (1.7.6) and (1.7.7), and δ_{CS} is the relative difference between the reference CS and the angular integral of the spline-fitted (and possibly extrapolated to small and large angles) κ_{\max} -fitted DCS over the entire solid angle of 4π (as in the case of δ_{unc} , both δ_{res} and δ_{CS} have the meaning of the rms value over all κ_{\max} -fitting intervals, unless the angular spline fitting is performed completely independently for each κ_{\max} -fitting interval). The mentioned ‘‘reference CS’’ can be either obtained by nonlinear fitting of the κ_{\max} -dependence of the partial-wave CS by the fitting function defined by Eq. (1.5.1) or Eq. (1.5.10), or it may be specified by the user. In BREMS, the former approach (based on extrapolation of the partial-wave CS to $\kappa_{\max} \rightarrow \infty$) is by default applied when either $T_1 \leq 10$ MeV, or $T_2 \leq 3$ MeV, or $T_2 / T_1 \leq 0.1$. Otherwise, the mentioned nonlinear fitting of the κ_{\max} -dependence of the partial-wave CS is in general too unreliable (due to a large relative correction of the CS by the κ_{\max} -fitting). Consequently, the reference CS must then be specified by the user explicitly, or obtained by an alternative method, such as cubic spline interpolation between the known values of CS corresponding to the same values of Z and k / T_1 , but different values of T_1 . If neither approach is applicable (due to absence of the required data), then the term δ_{CS} is not included in the definition of the OF, i.e., the OF is defined as follows:

$$f = (\delta_{\text{unc}}^2 + \delta_{\text{res}}^2) / 2. \quad (1.7.8b)$$

However, then large errors of the final κ_{\max} -fitted DCS are possible, especially at small angles and small values of k / T_1 (i.e., near the soft-photon limit). This is because the method of ‘‘ μ -correction’’ (see Section 1.5.4), which is usually required when T_2 is of the order of 1 MeV or greater, is applicable only in a limited angular range $\theta_{\text{start}} \leq \theta \leq \theta_{\text{end}}$, where θ_{start} is typically around 20° and θ_{end} is typically around 170° , if $k > 0$. In the small-angle range $\theta < \theta_{\text{start}}$, the values of DCS obtained by the stretched-exponential or polynomial κ_{\max} -fitting described in Section 1.5.1 and Section 1.5.2 (which are used by default when either $T_1 \leq 10$ MeV, or $T_2 \leq 3$ MeV, or $T_2 / T_1 \leq 0.1$, or the reference CS is not available) or by cubic spline extrapolation of the angular dependence of the fitted DCS to $\theta < \theta_{\text{min}}$ may be subject to large errors if additional information about the small-angle behavior of the DCS is not taken into account. Since the angular distribution of bremsstrahlung is strongly peaked in the forward direction when T_2 is of the order of 1 MeV or greater, the value of the CS (i.e., the integral of the DCS with respect to the solid angle of photon emission) provides the mentioned additional information, thus improving the accuracy of the final κ_{\max} -fitted DCS, if the OF is defined according to Eq. (1.7.8a). In this case, it is advantageous to calculate the values of the DCS at $\theta < \theta_{\text{min}}$ by cubic spline extrapolation rather than by the stretched-exponential or polynomial κ_{\max} -fitting (due to large errors of the latter fitting at small angles when T_2 is of the order of 10 MeV or greater).

After the spline fitting and extrapolation of the κ_{\max} -fitted DCS, the resulting spline function (or its average over all κ_{\max} -fitting intervals) is spline-fitted again in the entire angular interval $0^\circ \leq \theta \leq 180^\circ$, using a relatively large number of knots (up to 61). The adjustable parameters of this spline fitting (excluding the values of θ_{min} and θ_{max} , which are fixed at 0° and 180° , respectively) are optimized by the same method as described above. This spline fitting is performed for the purpose of smoothing out the possible small irregularities (i.e., extra inflection points) that may appear due to the averaging over different κ_{\max} -fitting intervals after the angular spline fitting and extrapolation for each κ_{\max} -fitting interval separately.

1.7.3. Large-angle polynomial extrapolation of the κ_{\max} -fitted DCS in the case of small corrections

If the relative change of the DCS at large angles due to the extrapolation to $\kappa_{\max} \rightarrow \infty$ by the nonlinear fitting described in Sections 1.5.1 and 1.5.2 is relatively small (less than 30 % in absolute

value) in a sufficiently wide angular interval (up to 160°), then the values of the final DCS at greater angles can be calculated by a simpler method than those described in Sections 1.5.1 – 1.5.4. In this case, the large-angle extrapolation can be performed by calculating the optimal coefficients of the extrapolating function, which is defined as a product of a reference function and a polynomial of $\cos \theta$:

$$\text{DCS}_{\text{ext}}(\theta) = \text{DCS}_{\text{ref}}(\theta) \sum_{m=0}^L a_m \cos^m \theta, \quad (1.7.9)$$

where $\text{DCS}_{\text{ref}}(\theta)$ is the mentioned reference function, which is by default equal to the Born-approximation DCS corresponding to the same screening factor that was used for the partial-wave calculations. The degree L of the polynomial in Eq. (1.7.9) is by default determined by testing different values of L starting with $L = 2$. If the rms change of extrapolated large-angle DCS (in the extrapolation range) caused by changing L to $L + 1$ is less than the rms difference between the results corresponding to $L - 1$ and L , and each of the mentioned two rms differences is less than the rms difference between the results corresponding to $L - 1$ and $L + 1$, then L is incremented by 1, and the process is repeated, unless L has reached the maximum allowed value (10 by default), in which case the latter value becomes the final value of L . If the mentioned conditions are not satisfied simultaneously, then the optimal L is set equal to the previous value ($L - 1$). The optimization of the coefficients a_m ($m = 0, 1, \dots, L$) is performed by the method of least squares (i.e., multiple linear regression), using the κ_{max} -fitted DCS as the input data (this κ_{max} -fitted DCS is calculated by the methods described in Sections 1.5.1 and 1.5.2). The starting point of the fitting interval is by default equal to 110° . The endpoint of the fitting interval corresponds to the largest angle where the relative correction is less than 30 % in absolute value. The fitting is by default performed 21 times by successively excluding the last point from the fitting interval (i.e., shifting the endpoint of this interval towards the smaller angles in one-point increments). After that, the values of the extrapolated DCS are calculated as the weighted average over all 21 fitted angular dependences, with the weight factors proportional to the inverse squared uncertainties and normalized to 1. The mentioned uncertainties of the extrapolated values are calculated using the standard methods of nonlinear least squares (this calculation is based on Eq. (1.6.2a)). The final uncertainties of the mentioned weighted average include an additional term, which is added in quadrature: the difference of the estimate of the extrapolated DCS at the current (optimal) value of L and the DCS corresponding to the value of L greater by 1.

BREMS implements a slightly modified version of the method described above, with two threshold values of the relative correction instead of one, as well as two threshold values of the starting angle of the polynomial extrapolation interval. The mentioned two threshold values of the relative correction will be further denoted t_1 and t_2 (their default values are 0.05 and 0.3, respectively) and the two threshold angles will be denoted θ_{e1} and θ_{e2} (their default values are 160° and 170° , respectively). After determining the two largest angles θ_{t1} and θ_{t2} , where the absolute value of the relative correction is less than t_1 and t_2 , respectively, and assuming that $\theta_{t1} \leq \theta_{t2}$ (which is always true in the case of negative corrections, if $t_1 < t_2$), the endpoint θ_p of the polynomial fitting interval (i.e., the starting angle of the polynomial extrapolation interval) is determined as follows:

- if $\theta_{t1} \geq \theta_{e2}$, then $\theta_p = \theta_{t1}$,
- if $\theta_{t1} < \theta_{e2} \leq \theta_{t2}$, then $\theta_p = \theta_{e2}$,
- if $\theta_{e1} \leq \theta_{t2} < \theta_{e2}$, then $\theta_p = \theta_{t2}$,
- if $\theta_{t2} < \theta_{e1}$, then the polynomial extrapolation is not performed.

This modification employs the fact that the extrapolated values are more accurate than the original κ_{max} -fitted values not only when the relative correction is greater than 0.3 in the entire extrapolation interval, but also when it is between 0.05 and 0.3 in the initial part of the extrapolation interval, provided that the starting angle of this interval is sufficiently large (approximately 170° or greater).

Since the method of “ μ -correction” described in Section 1.5.4 is primarily intended to reduce large-angle errors of the final κ_{max} -fitted DCS, the μ -correction becomes unnecessary if the

κ_{\max} -fitted DCS is fitted by the polynomial (1.7.9) at large angles. In addition, the relatively high accuracy of the final DCS obtained by this fitting eliminates the need for testing several endpoints of the spline-fitting interval (θ_{\max}) during the subsequent angular spline fitting (see Section 1.7.2), so that the default value of this endpoint is in this case changed to 180° . Then the only effect of the mentioned angular spline fitting is an additional smoothing of the final angular dependence of the DCS.

In the code of BREMS, the large-angle polynomial extrapolation described above is not applied if both the μ -correction (described in Section 1.5.4) and the alternative method of improving accuracy of the final κ_{\max} -fitted DCS at large angles (described in Section 1.8) are used simultaneously. In such a case, the large-angle polynomial extrapolation will be applied only for fitting the “alternative” DCS, but not for fitting the “original” DCS.

In summary, the order of processing steps after calculating the sets of truncated partial-wave sums (1.1.4) and (1.1.5) for consecutive values of κ_{\max} is the following:

- (1) smoothing of the PW (D)CS with respect to κ_{\max} by replacing it with a moving average (MA),
- (2) angular spline fitting (possibly with extrapolation) of the PW DCS with respect to θ ,
- (3) angular MA smoothing inside the interval of constant scale factor μ (see end of Section 1.5.4),
- (4) extrapolation to $\kappa_{\max} \rightarrow \infty$, i.e., fitting of the dependence of (D)CS on κ_{\max} (see Section 1.5),
- (5) polynomial or spline fitting and extrapolation of the κ_{\max} -fitted DCS with respect to θ .

1.8. Improving large-angle accuracy by using a greater ratio $|\kappa_1|_{\max} / |\kappa_2|_{\max}$ for large angles

As mentioned at the beginning of Section 1.5.1, extrapolation of the truncated partial-wave series (1.1.4) to $|\kappa_1|_{\max} \rightarrow \infty$, $|\kappa_2|_{\max} \rightarrow \infty$ is performed along a straight line in the $(|\kappa_2|_{\max}, |\kappa_1|_{\max})$ plane (see Eq. (1.5.2)), with $|\kappa_2|_{\max}$ acting as the independent variable (it was denoted “ κ_{\max} ” in previous sections). This straight line is defined by Eq. (1.5.2), which can be written as follows:

$$|\kappa_1|_{\max} = n |\kappa_2|_{\max}, \quad (1.8.1)$$

where n is a positive integer number. For small and intermediate angles (less than about 30°), the optimal value of n is close to p_1 / p_2 , where p_1 and p_2 are momenta of the incident and outgoing electron, respectively. For example, if $T_1 = 30$ MeV and $k = 6$ MeV, then $n = 1$. However, as shown in Fig. 10a, a much faster convergence can be obtained at large angles by using a significantly greater value of n . For example, if $n = 30$ (as in Fig. 10a), then the value of the PW DCS corresponding to $\theta = 180^\circ$ is within 1 % of the exact value already at $|\kappa_2|_{\max} = 30$ (see Fig. 10c), whereas in the case $n = 1$ the value of the PW DCS corresponding to $\theta = 180^\circ$ exceeds the exact value by more than two orders of magnitude even when $|\kappa_2|_{\max}$ is as large as 350 (see Fig. 10a). At small angles, the mentioned increase of n has the opposite effect: it causes slowing down of the convergence of the truncated partial-wave series (see Fig. 10b). It is also noteworthy that an increase of the ratio $|\kappa_1|_{\max} / |\kappa_2|_{\max}$ causes reversal of the direction of change of DCS as a function of $|\kappa_2|_{\max}$ at large angles: it is increasing with $|\kappa_2|_{\max}$ (see curves 4 and 5 in Fig. 10c).

The above-mentioned properties suggest the following method of calculating the complete angular dependence of the DCS in cases when the extrapolation methods described in Sections 1.5.1 to 1.5.4 and 1.7.1 to 1.7.3 do not ensure a sufficient accuracy at large angles: the partial-wave DCS (defined by the truncated sum (1.1.4)) should be calculated twice, using both the “original” value of the ratio $n \equiv |\kappa_1|_{\max} / |\kappa_2|_{\max}$ and a much greater value of the mentioned ratio. After extrapolation of each of these two PW DCS to $\kappa_{\max} \rightarrow \infty$, the final DCS is constructed by smoothly joining the small-angle part of the κ_{\max} -fitted DCS corresponding to the smaller n (the “original” DCS) with the large-angle part of the κ_{\max} -fitted DCS corresponding to the larger n (the “alternative” DCS).

Although the methods of fitting and extrapolation described in Sections 1.5.1, 1.5.2, 1.5.4 and 1.7.1 to 1.7.3 are usually sufficient to achieve accuracy of a few percent or better at all angles (see, for example, curve 2 in Fig. 10c), usage of an increased ratio $|\kappa_1|_{\max} / |\kappa_2|_{\max}$ makes it possible to reduce the uncertainties at large angles to values of the order of 0.1 % or less, because the value

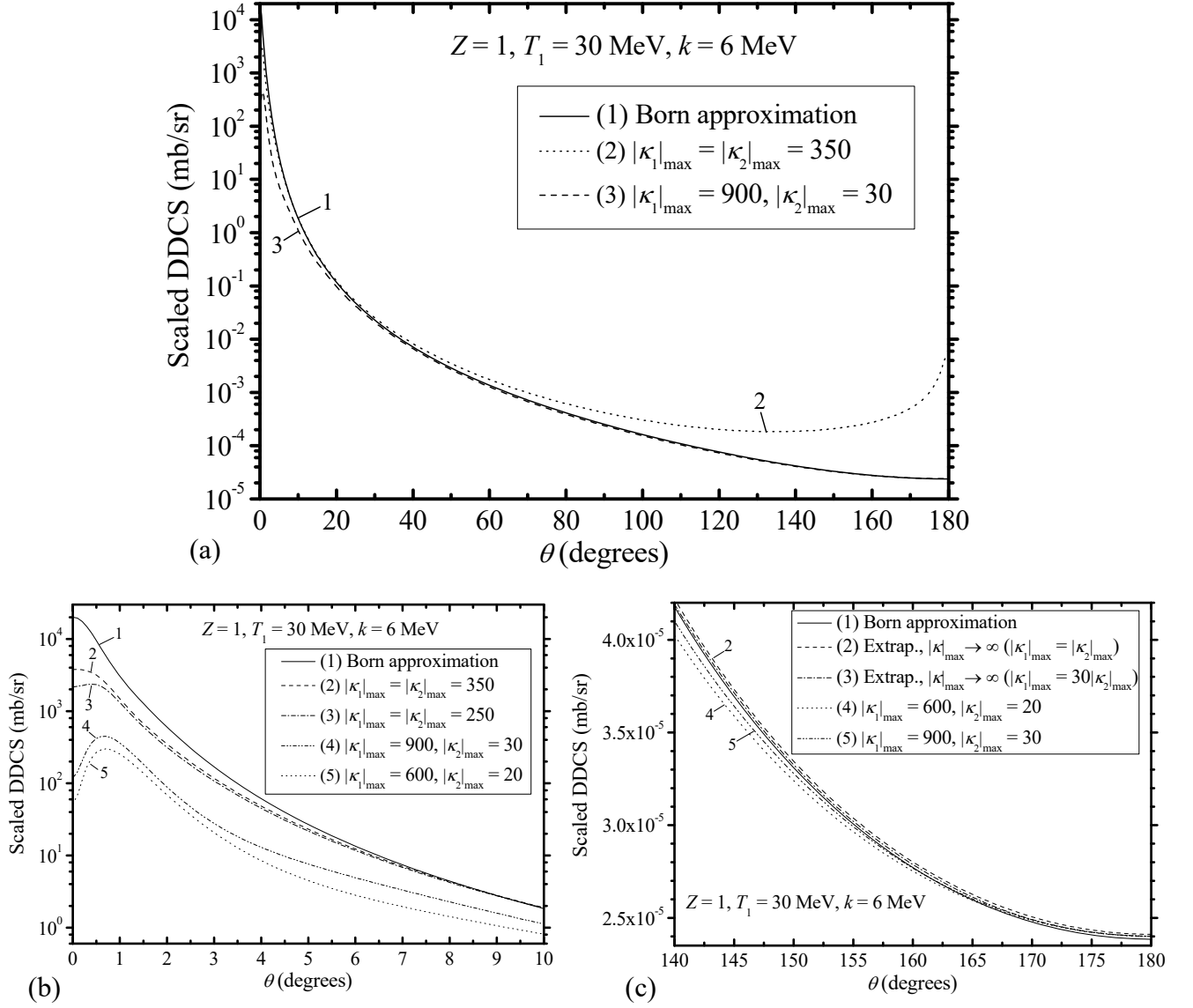


Fig. 10. The calculated angular dependence of the DCS when $Z=1$, $T_1=30$ MeV, $k=6$ MeV, and the Kohn-Sham potential is used. **(a)** The Born-approximation DCS (it is within 1% of the exact DCS), and two partial-wave DCS, obtained by truncating the sum in (1.1.4) at the indicated values of $|\kappa_1|_{\max}$ and $|\kappa_2|_{\max}$. **(b)** The small-angle part of the same three DCS as in “(a)”, and two additional PW DCS corresponding to smaller values of $|\kappa_2|_{\max}$, but the same two values of the ratio $|\kappa_1|_{\max} / |\kappa_2|_{\max}$, i.e., 1 and 30. **(c)** The large-angle part of the Born-approximation DCS of and the two PW DCS corresponding to $|\kappa_1|_{\max} / |\kappa_2|_{\max} = 30$, and two κ_{\max} -fitted DCS obtained by extrapolation of the PW DCS along two straight lines in the $(|\kappa_2|_{\max}, |\kappa_1|_{\max})$ plane: one line is defined by $|\kappa_1|_{\max} = |\kappa_2|_{\max}$ (the extrapolation range is $|\kappa_2|_{\max} > 350$), and another line is defined by $|\kappa_1|_{\max} = 30|\kappa_2|_{\max}$ (the extrapolation range is $|\kappa_2|_{\max} > 30$).

of the alternative PW DCS corresponding to the maximum value of $|\kappa_2|_{\max}$ (i.e., to the start of the κ_{\max} -extrapolation range) is typically within a few percent of the converged value (i.e., the exact value of the DCS) and hence requires minimal additional extrapolation with respect to $|\kappa_2|_{\max}$. In addition, the calculation of the alternative PW DCS (with a greater value of the mentioned ratio) requires a relatively small maximum value of $|\kappa_2|_{\max}$ (in the code of BREMS, it never exceeds 30), whereas the maximum value of $|\kappa_1|_{\max}$ has to be increased over the original one only when $T_1 > 10$ MeV. Thus, the computational cost of this improvement of accuracy is relatively small.

In the code of BREMS, the alternative PW DCS is calculated using approximately the same or greater value of $\max(|\kappa_1|_{\max})$ as the original PW DCS, and a much-reduced value of $\max(|\kappa_2|_{\max})$, which is defined as follows:

$$\max(|\kappa_2|_{\max}) = \min(30, \max(15, \max(|\kappa_2|_{\max})/4)). \quad (1.8.2)$$

This means that the reduced value of $\max(|\kappa_2|_{\max})$ is always inside the interval

$$15 \leq \max(|\kappa'_2|_{\max}) \leq 30. \quad (1.8.3)$$

The value of $\max(|\kappa_1|_{\max})$ used for calculation of the alternative PW DCS (which will be denoted $\max(|\kappa'_1|_{\max})$) is by default calculated as follows:

- (a) if $1 \text{ MeV} < T_1 \leq 10 \text{ MeV}$, then $\max(|\kappa'_1|_{\max})$ is obtained by rounding down the original value of $\max(|\kappa_1|_{\max})$ to the nearest multiple of $\max(|\kappa'_2|_{\max})$,
- (b) if $10 \text{ MeV} < T_1 \leq 85 \text{ MeV}$, then $\max(|\kappa'_1|_{\max})$ is obtained by linear interpolation with respect to T_1 between $\max(|\kappa'_1|_{\max}) = 500$ at $T_1 = 10 \text{ MeV}$ and $\max(|\kappa'_1|_{\max}) = 2000$ at $T_1 = 85 \text{ MeV}$, and then rounding down to the nearest multiple of $\max(|\kappa'_2|_{\max})$,
- (c) if $T_1 > 85 \text{ MeV}$, then $\max(|\kappa'_1|_{\max}) = 2000$ (rounded down to the nearest multiple of $\max(|\kappa'_2|_{\max})$),
- (d) if $T_1 \leq 1 \text{ MeV}$, then the alternative calculation is not performed, because the original calculation ensures a sufficient accuracy of the final DCS at all angles.

For example, if $T_1 = 30 \text{ MeV}$, then $(|\kappa'_1|_{\max})$ is equal to 900, whereas $\max(|\kappa'_2|_{\max})$ is equal to 30 at $k/T_1 \leq 0.8$. Thus, if $T_1 = 30 \text{ MeV}$ and $0 < k \leq 24 \text{ MeV}$, then $n = 900 / 30 = 30$. If $0.9 \leq k/T_1 < 0.9999$, then $\max(|\kappa'_2|_{\max}) < 30$ (accordingly, $n > 30$), and if $k/T_1 \geq 0.9999$, then the alternative calculation is not performed, because the original calculation already uses $\max(|\kappa_2|_{\max}) = 30$ and $n = 30$, which ensures a sufficient accuracy of the final DCS at all angles. The alternative κ_{\max} -fitted DCS is by default calculated in the angular range $30^\circ \leq \theta \leq 180^\circ$.

After the κ_{\max} -fitting, the large-angle part of the original κ_{\max} -fitted DCS is replaced by the mentioned alternative κ_{\max} -fitted DCS. Inside the entire large-angle angular range (up to 180°) where the mentioned replacement is applied, the absolute value of the relative correction of the DCS corresponding to the alternative dataset must not exceed the absolute value of the relative correction corresponding to the original dataset by a factor greater than 10, or at least one of the two mentioned relative corrections must be less than 0.01 in absolute value. In addition, all points that are in the first 3° of this angular range must satisfy the following three requirements: (a) the relative difference of the two κ_{\max} -fitted DCS must be less than 3 % in absolute value, (b) the absolute values of the relative corrections of the PW DCS corresponding to the original and alternative datasets must be less than 99 % and 3 %, respectively, (c) the relative uncertainty (standard deviation) of the alternative κ_{\max} -fitted DCS must be less than 3 % in absolute value. The consecutive points satisfying the latter three constraints correspond to the “transition interval”, where the values of the original κ_{\max} -fitted DCS are replaced by a weighted average of the original and alternative κ_{\max} -fitted DCS. At greater angles, the original κ_{\max} -fitted DCS is replaced by the alternative κ_{\max} -fitted DCS. The weight factor of the mentioned weighted average is a linear function of θ , which is defined so as to smooth out the small discontinuity, which would otherwise exist at the end of the mentioned transition interval after the mentioned replacement. I.e., the final DCS changes smoothly from the original DCS (at the point that immediately precedes the transition interval) to the alternative DCS (at the endpoint of the transition interval). The maximum allowed width of the transition interval is 30° . If the width of the interval satisfying the mentioned three constraints is greater than 30° , then a subinterval with width equal to 30° is selected on the basis of the requirement of the smallest value of the ratio of the maximum relative difference between the two κ_{\max} -fitted DCS to the ratio of the maximum and minimum values of the original κ_{\max} -fitted DCS inside the mentioned subinterval. The uncertainties of the final κ_{\max} -fitted DCS inside the transition interval are calculated by adding up the uncertainties of the original and alternative κ_{\max} -fitted DCS in quadrature, with the same weight factors that are used to calculate the final κ_{\max} -fitted DCS, and the weighted absolute deviations of the same two κ_{\max} -fitted DCS from the final κ_{\max} -fitted DCS. All mentioned numerical values controlling the joining of the two DCS can be modified by the user.

1.9. Approximation of the screening function by a linear combination of exponentials

The expressions of the screened Born-approximation TDCS and DDCS presented in Section 1.1.2 (see Eqs. (1.1.28), (1.1.35), and (1.1.36)) require the point-nucleus screening function $\tilde{V}(r)$ to be expressed as a linear combination of decaying exponential functions (see Eqs. (1.1.34a,b)). Fitting of an arbitrary point-nucleus screening function by such a function without any constraints on the number of exponentials N and the values of the coefficients b_i in Eq. (1.1.34a) is a complicated task. However, if the least-squares requirement of finding the absolute minimum of the sum of squared residuals is replaced by the requirement of finding a set of coefficients ensuring a sufficiently small value of the maximum relative residual (for example, 1 %) in a sufficiently wide interval of the radial coordinate r (for example, at $r < 10^4$ in relativistic units), then the values of N and b_i ($i = 1, 2, \dots, N$) can be selected from a number of fixed pre-defined sets. In such a case, only the preexponential factors a_i in Eq. (1.1.34a) have to be optimized for each set of b_i ($i = 1, 2, \dots, N$). Optimization of a_i at fixed b_i ($i = 1, 2, \dots, N$) can be done by multiple linear regression, hence it is very fast.

In the code of BREMS, the approximation of the point-nucleus screening function by a linear combination of exponentials is implemented as a special mode of operation, which is separate from the calculation of the cross sections. Each set of b_i ($i = 1, 2, \dots, N$) is defined as follows:

$$b_i = 1 / \rho_i, \quad (1.9.1a)$$

where the ‘‘characteristic radii’’ ρ_i are equidistant:

$$\rho_i = i \rho_{\max} / N \quad (i = 1, 2, \dots, N). \quad (1.9.1b)$$

Consequently, the entire set of the b -coefficients can be defined in terms of two parameters: N and ρ_{\max} . The interval of the radial coordinate r , where the maximum residual is minimized, is defined in terms of its endpoint r_{\max} , which is equal to the value of r corresponding to $\tilde{V}(r) = 10^{-6}$ by default. N is varied from 2 to 50 by default (49 values), and ρ_{\max} is varied from $0.02r_{\max}$ to $0.1r_{\max}$ in steps of $0.001r_{\max}$ by default (81 values). Thus, a total of $49 \times 81 = 3969$ sets of the b -coefficients are tested (i.e., the same number of sets of the a -coefficients are calculated by linear regression). All the mentioned parameters may be adjusted by the user. The maximum number of exponential terms (N) allowed in the code of BREMS is 200. The value of r_{\max} should be chosen so as to be greater than the maximum cutoff radius of the interaction potential. The value of 10^4 is sufficiently large for most applications, because the cutoff radius is usually less than 10^4 . The same can be said about the default value of r_{\max} , which corresponds to $\tilde{V}(r) = 10^{-6}$. However, as an additional precaution against unphysical results, some constraints are placed on the behavior of the approximate point-nucleus screening function $\tilde{V}_{\text{appr}}(r)$ in the interval $r_{\max} < r < 10r_{\max}$, too: in this interval, the ratio $\tilde{V}_{\text{appr}}(r) / \tilde{V}(r_{\max})$ is not allowed to become negative or greater than 10 (the latter threshold is also adjustable by the user). If those conditions are not satisfied, then the corresponding set of the a - and b -coefficients is rejected.

The mentioned linear regression is performed without any constraints on the a -coefficients. The condition (1.1.34b) is ensured by ‘‘normalizing’’ the final values of the a -coefficients, i.e., dividing them by their sum Σ_a . The increase of the root-mean-square value of the residuals due to this normalization is insignificant, because $|1 - \Sigma_a|$ is always less than 0.01.

The optimal a -coefficients usually form an alternating sequence, and their absolute values tend to increase rapidly with increasing number of exponentials. Consequently, there is strong cancellation between the exponential terms, and quadruple precision (QP) arithmetic has to be used for the evaluation of $\tilde{V}_{\text{appr}}(r)$ in order to avoid excessive rounding errors. For the same reason, even QP is frequently not sufficient when calculating the analytical expression of the screened Born DDCS (1.1.36). In this case, 200-digit multiple precision (MP) arithmetic is used in BREMS by default. If the DDCS is calculated by numerical angular integration of the screened Born TDCS (1.1.28), the a - and b -coefficients appear only in the expression of the atomic form factor (1.1.35). In this case, QP is usually sufficient for calculation of the AFF, whereas the mentioned TDCS can

be calculated using double precision. As a result, the numerical integration of the TDCS according to Eq. (1.1.31a) by the method of adaptive multidimensional quadrature is usually much faster than calculation of the analytical expression (1.1.36), while ensuring a sufficient accuracy ($\sim 10^{-3}$ % or better).

The distribution package of BREMS contains files with the results of fitting the Kohn-Sham screening function by a linear combination of exponentials using the method described above for $1 \leq Z \leq 100$. For all Z , the maximum relative residual inside the interval $r < 10^4$ is about 1 % or less.

2. Overview of the calculation process and the codes included in BREMS

The process of calculating the CS and DCS for a particular combination of Z , T_1 and k , and for a chosen interaction potential $V(r)$ consists of three stages:

- 1) calculation of the phase shifts and S integrals (1.1.15a,b),
- 2) calculation of the truncated series (1.1.4) and (1.1.5) for a set of values of κ_{\max} in increments of 1,
- 3) improvement of the accuracy of the results by extrapolation and smoothing (see Sections 1.5–1.7).

Each of these stages is performed by a separate subroutine, called from the main program:

Stage 1: S_integrals

Stage 2: Bremsstrahlung

Stage 3: Brems_fit

The main program and all subroutines are written in Fortran-90. The code of the main program is in the file “Brems.f90”. The names of the main source code file for each of the three mentioned subroutines are “S_integrals.f90”, “Bremsstrahlung.f90” and “Brems_fit.f90”, respectively. The subroutine “S_integrals” creates a binary file with the values of phase shifts (denoted $\tilde{\delta}_\kappa$ in Section 1.1.1), normalization factors (denoted A_κ in Eqs. (1.1.18)), S integrals and the system parameters (the S integrals are written to file only when $k \neq 0$). When $\kappa < 0$, the value of $\delta'_\kappa \equiv \tilde{\delta}_\kappa - (\pi/2)$ is stored instead of $\tilde{\delta}_\kappa$, because δ'_κ is used as the primary quantity in the code (i.e., $\tilde{\delta}_\kappa$ is calculated from δ'_κ rather than the other way around). This file is subsequently read by “Bremsstrahlung”, which creates the files with the values of the partial-wave CS, partial-wave DCS and the shape function (defined as the ratio DCS/CS) for each value of κ_{\max} , which is defined as the maximum value of $|\kappa_2|$ in the series (1.1.4) and (1.1.5). Finally, “Brems_fit” reads the values of CS and DCS from the files created by “Bremsstrahlung” and performs the nonlinear fitting described in Section 1.5 and the angular spline fitting or large-angle polynomial extrapolation described in Section 1.7.

If both the original and the alternative datasets are processed (see Section 1.8), then each of the mentioned three stages consists of two consecutive calls to one of the mentioned three subroutines. In stage 1, the second call to subroutine “S_integrals” is used to calculate the part of the alternative set of S integrals that is not contained in the original dataset. This is needed only when $T_1 > 10$ MeV, or when the maximum value l in the original data is less than the theoretical maximum, which is equal to $|\kappa_1|_{\max} + |\kappa_2|_{\max}$ (see also Section 1.3.2). In stages 2 and 3, the additional call is used to process the entire alternative dataset. Specifically, the additional call to subroutine “Bremsstrahlung” (in stage 2) is used to process the entire alternative set of S integrals, yielding the alternative set of partial-wave (PW) DCS, and the additional call to subroutine “Brems_fit” (in stage 3) is used to process the alternative set of PW DCS, yielding the alternative κ_{\max} -fitted DCS. In stages 1 and 2, the two mentioned calls to subroutines “S_integrals” and “Bremsstrahlung” are completely independent. In stage 3, the two calls to subroutine “Brems_fit” are reversed (the alternative dataset is processed first), and they are not completely independent: the second call (corresponding to the original dataset) uses the results of the first call in order to improve the overall accuracy. In particular, if the “ μ -correction” described in Section 1.5.4 is applied during calculation of the original κ_{\max} -fitted DCS, then the scale factor μ is calculated as the

median value of expression (1.5.25) over an appropriate angular interval, where “DCS($\kappa_{\max} \rightarrow \infty, \theta$)” is the κ_{\max} -fitted DCS obtained from analysis of the alternative PW DCS (see also Section 6.18).

In addition, there are three “special” modes of operation of BREMS:

- Calculation of the angular dependence of the approximate DCS according to the Born approximation (see Section 1.1.2) or Sommerfeld-Maue approximations (see Section 1.1.3), and the corresponding CS. All expressions of DCS presented in Sections 1.1.2 and 1.1.3 are implemented. The name of the corresponding subroutine is “Born_SM_appr”. Its source code is in the file “Born_SM_appr.f90”.
- Fitting of a point-nucleus screening function defined in tabular format by a linear combination of exponentials (see Section 1.9). The name of the corresponding subroutine is “FitExp”. Its source code is in the file “FitExp.f90”.
- Cubic spline fitting and interpolation of the logarithm of the scaled single differential cross section (CS) with respect to the logarithm of the kinetic energy of the incident electron (T_1) for a given atomic number Z and for a fixed value of the ratio k/T_1 , where k is the energy of the bremsstrahlung photon, as well as creating the input “grid” data files used for the mentioned spline fitting, which contain values of CS and their relative uncertainties on a two-dimensional grid defined by a set of values of T_1 and k/T_1 . The name of the corresponding subroutine is “Brems_CS_interp”. Its source code is in the file “Brems_CS_interp.f90”.

The source code of several subroutines, which are used in more than one stage or mode of operation of BREMS, is in the file “Brems_common.f90”. The file “File_time.c” contains the source code of a small C program, which is used for determining the time of last modification of a file (Fortran does not have an intrinsic subroutine that could be used for this purpose). In order to eliminate the need for a C compiler, the corresponding object file “File_time.obj” is also included. All nine mentioned files with the source code, and the compiled executable file “Brems.exe” are in the folder “Brems”. In addition, the BREMS distribution package includes a program “Read_S_integrals.f90”, which displays the values of all phase shifts and the S integrals corresponding to the user-specified values of κ_1 and κ_2 . The file “Read_S_integrals.f90” and the compiled executable “Read_S_integrals.exe” are in the subfolder “Read_S_integrals” of the folder “Brems”. Those executables are 64-bit Windows console applications (on Windows 10 and older versions of Windows, the console is opened by running “cmd.exe” or “conhost.exe”, whereas on Windows 11 it is opened by “conhost.exe”). They were compiled using the Intel Fortran compiler (with two non-default compiler options controlling the precision of floating-point operations: “precise” floating point model, and “safe” floating-point speculation). The Linux versions of the files Brems.exe and Read_S_integrals.exe are in the subfolder “Linux_executables”. They were compiled using GNU Fortran on Ubuntu running on the Windows Subsystem for Linux. All executables were compiled with optimization for speed enabled. The folder “Linux_executables” also contains the object module “File_time.o” of the mentioned C program, which was compiled using the GNU C compiler, and the file “Compile.sh” with the complete set of Linux shell (“bash”) commands that must be entered in order to compile both mentioned executables on Linux.

Since the results of the previous stage of a calculation are stored in a file, it is possible to redo only stage 2 or 3 of a calculation, if the data files with the results of the previous stage are available. Examples of such a situation include a resuming of an interrupted calculation process, or a recalculation of the DCS for a different set of values of the angle θ (the values of θ are required only in stages 2 and 3). There is also an option to delete all data files of the previous stage automatically upon a successful completion of the current stage.

Each parameter of the calculation process may be specified either on the command line, or in a file (the “parameter file”), using the format “<parameter_name>=<parameter_value>” (there must be no spaces before or after the equality sign). For example, “IV=1” specifies that the point-Coulomb potential $V(r) = -\alpha Z/r$ (corresponding to the unscreened nucleus) should be used outside the nucleus when solving the system of ODEs (1.1.16a,b). There are 555 user-adjustable parameters

in total (including 82 parameters, which are used only in the mentioned three “special” modes of operation), allowing great flexibility in the process of calculating the CS and DCS and in the number of files created (such as the files with intermediate data). If a parameter value is not specified on the command line or in the parameter file, then a default value will be used. There are only three parameters that do not have default values: the atomic number Z , the incident electron energy T_1 , and the photon energy k . Those parameters must be specified by the user. In the simplest case, the command line of BREMS looks like this:

```
Brems.exe Z=13 T1=0.001 Ep=6e-4
```

In this example, no parameter file would be used, and the program would calculate the CS and DCS for the case when $Z = 13$, $T_1 = 1$ keV, and $k = 600$ eV (the input energy values must be specified in MeV). The values of the control parameters and the scaled CS calculated in stage 2 (before extrapolation of its dependence on κ_{\max}) would be written to the file “CS.txt”, the extrapolated value of the scaled CS would be written to the file “CS_fitted.txt”, and the values of the scaled DCS and the shape function would be written to the two files whose names start with “DCS_fitted_” and “ShapeFn_fitted_”, respectively (the remaining part of the file name indicates the values of Z , T_1 and k). The scaled CS and DCS are defined as the left-hand sides of Eq. (1.1.5) and Eq. (1.1.4), respectively, and their values are expressed in the units indicated after Eq. (1.1.5) and Eq. (1.1.4). If some of the parameters have to be loaded from a parameter file, then its name must be specified on the command line after the keyword “in=”, for example:

```
Brems.exe Z=13 T1=0.001 Ep=6e-4 in=Brems.inp
```

If a parameter value is specified both on the command line and in the parameter file, then the value specified on the command line takes priority (in such a case, a corresponding message is displayed before starting the calculation process). Multiple “in=” directives are allowed, for example: “Brems in=in1.txt in=in2.txt”. If a particular parameter is defined in two or more parameter files, then the program quits with an error message. The parameter names are case-sensitive. There must be no more than one parameter per line in a parameter file. One-line comments (starting with the exclamation mark ‘!’ or the forward slash ‘/’), empty lines, and additional “in=” directives are allowed in a parameter file. If a parameter value is a character string containing ‘/’ or a space, then this string must be enclosed by single quotes (along with the parameter name and the equality sign).

If $T_1 < 1$ MeV, then the values of the DCS and the shape function are calculated for 181 equidistant values of θ from 0° to 180° by default. If $T_1 \geq 1$ MeV, then the entire angular range is split in two subranges $0^\circ \leq \theta \leq 10^\circ$ and $10^\circ < \theta \leq 180^\circ$ with different density of points. In each of those two subranges, the values of θ are equidistant, but the default interval between adjacent values of θ (angular increment) in the second subrange is greater than in the first subrange. The change of point density at $\theta = 10^\circ$ is related to the tendency for the angular distribution of bremsstrahlung photons to become more peaked in the forward direction with increasing T_1 . If $1 \text{ MeV} \leq T_1 \leq 3 \text{ MeV}$, then the angular increment is equal to 0.2° in the first subrange and to 1° in the second subrange (221 points in total). If $3 \text{ MeV} < T_1 \leq 30 \text{ MeV}$, then the angular increment is equal to 0.1° in the first subrange and to 0.5° in the second subrange (441 points). If $T_1 > 30 \text{ MeV}$, then the angular increment in the first subrange is further reduced to 0.02° (841 points in total). All mentioned parameters controlling the angular increment may be modified by the user.

The default values of all parameters for the case when $T_1 = 100$ keV and $k = 10$ keV are given in the BREMS parameter file “Brems_defaults.inp”.

The subfolder “V” contains the subfolder “Kohn-Sham”, which, in turn, contains the text files with the values of the Kohn-Sham potential function in tabular format. There is one file for each value of Z from 1 to 100 (the value of Z is indicated in the name of the corresponding file). Each of those files contains three columns of numbers with the values of the radial coordinate r , the point-nucleus interaction potential $V(r)$ and the point-nucleus screening function $\tilde{V}(r)$. Both r and V are specified in relativistic units (see Section 1.1.1). If the Kohn-Sham potential is required, then the mentioned folder “V” must be either a subfolder of the current folder when starting Brems.exe,

or a subfolder of the folder where Brems.exe is located, or it must be explicitly specified using the parameter “dirV” (see the description of parameter No. 1.1.6 in Section 4.1).

The files with the S integral data contain up to four entries for each S integral: the value of the total integral, the values of the two numerical integrals corresponding to the two sets of numerical tolerances and step sizes (see Section 1.4), and the value of the error caused by the uncertainty of the phase shifts. The latter three entries are needed for estimating the numerical errors (see Section 1.4). After the numerical integration, a temporary file containing only the numerical integrals is created. Further on, this file will be called the “_n” file (because its name ends with the suffix “_n”). If the subsequent analytical integration fails and the final file is not created (for example, due to insufficient maximum precision level requested by the user), then the “_n” file may be reused for another integration attempt (if the “_n” file exists, then it is possible to load the numerical integrals from it). Since the final (complete) file also contains the numerical integral data, it may also be used for skipping the stage of numerical integration and redoing the analytical integration with a different precision level (see also Section 1.3.1).

The subfolder “CS_int” contains 100 ASCII files with the values of the scaled SDCS on a two-dimensional grid defined by a set of fixed values of the incident electron energy (T_1) and of the ratio k / T_1 , where k is the photon energy, for all values of the atomic number Z from 1 to 100. The range of values of T_1 in these files is from 0.1 MeV to 300 MeV, whereas the range of values of k / T_1 is from 0 to 0.95 (see Section 9.6 for additional information about these files).

The subfolder “Test_runs” contains a Windows batch file “Brems_79_100keV_KS.bat”, which performs the entire mentioned set of calculations for the case when the target is gold, incident electron energy is 100 keV and the photon energy is 10 keV or 0. The mentioned file uses the Kohn-Sham (KS) potential. The batch file “Read_S_integrals_79_100keV_10keV_KS.bat” can be used to display some of the data in the binary file with the S integral data created by the mentioned batch file. All ASCII files created by running the Windows batch file “Brems_79_100keV_KS.bat”, as well as the file “Screen_output_Z=79_T1=0.1_Ep=0.01.txt” with the complete text that is displayed on the screen during the first call to Brems.exe in the mentioned batch file, are also in the subfolder “Test_runs” (those files were created by executing the mentioned batch file on a notebook computer with an Intel Core i5-8300H processor and 64-bit Windows 10, without other processor-intensive tasks being run at the same time). The subfolder “Linux_executables” contains two bash scripts for performing the same calculations on Linux (“Brems_79_100keV_KS.sh” and “Read_S_integrals_79_100keV_10keV_KS.sh”, respectively).

The third-party open-source codes, which are needed for compiling Brems.exe and Read_S_integrals.exe, are in the subfolder “AuxiliaryPrograms” of the folder “Brems”. The complete list and descriptions of the third-party Fortran codes are below.

- 1) The routines and data structures of the multiple precision package are in two files “mpfun90.f90” and “mpmod90.f90” [49].
- 2) The routines and data structures of the quadruple precision package are in the file “quad_df_QC.f90” [51].
- 3) Subroutine DHPCG from the IBM System/360 Scientific Subroutine Package (SSP) is used for solving the system of ODEs (1.1.16a,b) by the Hamming’s modified predictor-corrector method (it may be optionally used instead of the default method of the power-series solution). This subroutine is in the file “DHPCG.F”.
- 4) The suite of Runge-Kutta codes RKSUITE (Release 1.0, November 1991), which may also be optionally used for solving the system of ODEs (1.1.16a,b), is in the file “rksuite.f”.
- 5) The codes used to calculate the exponential integral (needed for calculation of the phase correction integrals (1.2.2), (1.2.3), and (1.2.6a,b)) are in the files “de1.f”, “DCSEVL.f”, “INITDS.f”, “D1MACH.f”.
- 6) Subroutine DQAGI and four auxiliary subroutines from the QUADPACK library for calculation of the exponential integral by numerical quadrature at large values of the argument

(when the mentioned function DE1 returns zero). Those codes are in the files “dqagi.f”, “dqagie.f”, “dqelg.f”, “dqk15i.f”, “dqpsrt.f”.

- 7) Subroutine PFQ for calculating the hypergeometric series [57] is in the file “acpa.f”. This subroutine is used for calculating the exact radial wave functions at the stage of initial power-series solution (i.e., at small r) when the point-Coulomb potential is used.
- 8) Subroutines DLOGAM and CLOGAM (in files “DLOGAM.f” and “CLOGAM.f”) are used for calculating the natural logarithm of the absolute value of the gamma function of real and complex arguments, respectively. Subroutine Q_LNGM, which is used for calculating the natural logarithm of the absolute value of the gamma function of real argument at quadruple precision, is in the file “q_lngam.f90”.
- 9) The routines and data for calculating the spherical Bessel functions of the first and second kinds are in the files “SphBes.f90” and “types.f90”. Subroutine SPHJ (or its quadruple-precision version SPHJ_QP) estimates j_l using the Miller’s method (based on the backward recursion), which does not have the stability problems [41, 42]. Subroutine SPHY (or its quadruple-precision version SPHY_QP) estimates y_l using the forward recursion, which is also stable. Calculation of j_l by forward recursion is implemented in subroutines SPHJ2 and SPHJ2_QP. **Note:** The mentioned methods are used for evaluating the asymptotic electron wave functions (1.1.18). However, the values of $j_l(kr)$, which is used in the integrands of the S integrals (1.1.15a,b), are by default calculated by the power-series method, which is more accurate (see also Section 1.2).
- 10) Subroutine F3J and its extended-precision version F3J_QP_MP are used for calculation of the $3j$ coefficients in Eq. (1.1.14). Those subroutines are in the files “F3J.f” and “F3J_QP_MP.f”, respectively. The code of the F3J subroutine has been copied from [58]. As pointed out in the title of [58], F3J is not suitable when at least one of the numbers l_1 , l_2 and l in Eq. (1.1.14) is greater than 80. In the latter case, the subroutine F3J_QP_MP is used and the calculations are performed using either quadruple precision arithmetic (QP, corresponding to approximately 30 significant digits) or multiple precision arithmetic (MP, corresponding to 38 or more significant digits). Subroutine F3J_QP_MP chooses the optimal precision level dynamically: this choice is based on the degree of cancellation of the terms of the Racah formula [48].
- 11) The random number generator RAND from [59] is used for random modification of the S integrals (by randomly adding or subtracting their uncertainties) in order to test sensitivity of the cross sections to the numerical errors of the S integrals. This Fortran subroutine is in the file “RAND.f”.
- 12) Subroutine DSG13 from the IBM System/360 Scientific Subroutine Package (SSP) is used for temporary smoothing of the dependence of (D)CS on κ_{\max} in order to determine if this dependence is significantly different from a linear function. This subroutine is in the file “DSG13.F”.
- 13) Subroutine DMINV from the IBM System/360 Scientific Subroutine Package (SSP), and its quadruple-precision version (“QMINV”), are used for inversion of a matrix of second partial derivatives of the sum of squared deviations for estimation of uncertainties of the parameter values obtained by least squares fitting. Those subroutines are in the files “DMINV.FOR” and “QMINV.f90”, respectively.
- 14) Subroutine DGELS from the IBM System/360 Scientific Subroutine Package (SSP) and subroutine QGELS, which is a quadruple precision version of DGELS, are used for solving a system of linear equations with symmetric coefficient matrix at double precision and quadruple precision, respectively, as a part of the linear regression algorithm. Those subroutines are in files “DGELS.f” and “QGELS.f90”, respectively.
- 15) Subroutine ADAPT by Alan Genz is used for adaptive angular integration of the Born- or SM-approximation TDCS, which is performed in order to calculate the corresponding DDCS or SDCS. This subroutine is in the file “adapt.f”.

The code for calculating the Kohn-Sham potential is not included in the BREMS distribution package, because the Kohn-Sham potential functions for all values of Z from 1 to 100 are stored in tabular format in the folder “V/Kohn-Sham”. Those data were calculated using the Fortran program described in [5]. The source codes of the latter program and of the mentioned subroutines PFQ and CLOGAM were downloaded from the Computer Physics Communications Program Library [60]. In order to improve the accuracy of the Kohn-Sham potential function, the program described in [5] was modified by converting it from single-precision arithmetic to double precision, decreasing the accuracy criteria for convergence and for eigenvalues (variables “DELVR” and “DEL”, respectively) by 3 orders of magnitude in comparison with the original values, and increasing the density of the radial grid.

Although there is no explicit limitation on the value of the incident electron energy T_1 in the code of BREMS, it is currently applicable only at electron energies that are not greater than approximately 30 MeV. This is because an increase of the electron energy requires a larger number of terms in the series (1.1.4) and (1.1.5), accompanied by an increase of the computation time and the memory requirements. If $|\kappa_2|_{\max} > 200$, then the maximum value of $|\kappa_1|$ that is currently allowed is equal to $1000 - |\kappa_2|_{\max}$ (i.e., in this case $|\kappa_1| + |\kappa_2|$ is not allowed to be greater than 1000). If $|\kappa_2|_{\max} \leq 200$, then the maximum value of $|\kappa_1|$ that is currently allowed is 2000. When the kinetic energy of the incident electron is of the order of 1 MeV or greater, the double or quadruple precision is usually sufficient for the analytical integration. This is fortunate, because using multiple precision for the calculation of the entire set of S integrals with large values of $|\kappa_1|_{\max}$, $|\kappa_2|_{\max}$ and l_{\max} , which are needed at the mentioned high energies, would result in prohibitive memory requirements. The amount of memory required by BREMS in MP mode (i.e., at a precision level of 30 or more significant digits) does not depend on the precision level used. For example, if $|\kappa_1|_{\max} = |\kappa_2|_{\max} = l_{\max} = 100$ and the other parameters are equal to the default values, then BREMS would allocate approximately 5 GB of memory for calculating all S integrals using MP, and if $|\kappa_1|_{\max} = |\kappa_2|_{\max} = l_{\max} = 150$, then approximately 15 GB of memory would be needed in MP mode. It should be noted that the minimum precision level, which is sufficient for the analytical integration, decreases with increasing cutoff radius R_a .

At the low-energy end of the spectrum, the single-electron approximation may not be sufficiently accurate due to an increased importance of the many-electron effects at electron energies of the order of 100 eV or lower. It should also be noted that the choice of the self-consistent central potential in the energy range $T_1 < 1$ keV is more important than in the energy range $1 \text{ keV} < T_1 < 30 \text{ MeV}$, where this choice has a relatively weak influence on the angular distribution of bremsstrahlung. The final electron energy T_2 is not allowed to be less than 0.1 eV, which means that the photon energy cannot be greater than $T_1 - 0.1$ eV.

BREMS can be run on modern personal computers, with processing times from several minutes to several hours, depending on the user-specified values of Z , T_1 , and k and on the accuracy requested. BREMS is a single-threaded application. Consequently, in order to use all computing power of a multiprocessor or multicore system, several instances of BREMS should be run simultaneously. This is a natural approach for calculation of the cross sections for different sets of the physical parameters Z , T_1 and k , because the instances of BREMS using different sets of those parameters are completely independent. However, this approach can also be applied in the case of a single set of physical parameters. In the latter case, the computation of the S integrals may be broken into several parts, differing by the range of variation of $\kappa_{1\max}$, or by the type of the integrals computed (numerical or analytical). After the data files with the total S integrals (from 0 to ∞) have been created, the computation should be started from stage 2 (BREMS has the capability to merge the S integral data loaded from multiple files). If the numerical and analytical parts of the S integrals (from 0 to r_0 and from r_0 to ∞ , respectively) have been calculated separately, then the computation should be again started from stage 1, but this time with the input parameters specifying that the numerical and analytical integrals must be loaded from files rather than calculated.

Most of the input parameters of BREMS are used as arguments of the mentioned six subroutines “S_integrals”, “Bremsstrahlung”, “Brems_fit”, “Born_SM_appr”, “FitExp”, and

“Brems_CS_interp”. Some of the parameters (such as the physical parameters Z , T_1 and k) are “shared”, i.e., used in all three stages of the calculation, and the other parameters are used in only one or two stages (for example, the values of the angle θ are used only by Bremsstrahlung, Brems_fit and Born_SM_appr, and the numerical tolerance for nonlinear fitting is used only by Brems_fit). Descriptions of all those parameters will be given in the following sections. There are also several parameters that are used only by the main program in order to determine the default values of some other parameters and the sequence of stages that has to be executed. The names, descriptions and default values of the parameters used only by the main program are given below (the parameter numbers are used only to facilitate references to them in this document, and those numbers are different from the parameter numbers defined in the code of BREMS):

Parameter No. 1 (“**accuracy_level**”) is the number 0, ± 1 , or ± 2 , specifying the “accuracy level” to be used. If this number is 1 or 2, then several other parameters that have the largest effect on the accuracy and the computation time (such as the limits of κ_1 and κ_2) will be set to the default values corresponding to the lower or higher accuracy, respectively, unless those parameters have been explicitly specified by the user. There are 11 such parameters: “tol_A”, “tol_delta”, “Q_last”, “Z_def”, “Kmax1”, “Kmax2”, “lmax”, “lmax_MP”, “lmax_MP_ratio”, “lmax2”, “vary_h_CS”. If the accuracy level is specified with the minus sign, then all those parameters will be assigned the values corresponding to the given accuracy level, even if they have been explicitly set to other values by the user. The default values of parameters “Kmax1” and “Kmax2” depend on the chosen accuracy level only when $T_1 > 0.1$ MeV. Otherwise, the default values of those parameters are the same for both accuracy levels (those values depend on the physical parameters T_1 , k/T_1 , and Z). There are also 15 parameters that are reset to the default values when $\text{accuracy_level} < 0$: “j_QP”, “vary_h_DCS”, “Kmin1”, “Kmin2”, “isAbs_K1”, “isAbs_K2”, “k2_breakpoint1”, “k2_step_first”, “k2_step_last”, “pr_transition2”, “R_atom”, “fitRange_CS”, “fitRange_DCS”, “fitRange2_CS”, “fitRange2_DCS” (the default values of those 15 parameters are the same for both accuracy levels). If the user-specified value of accuracy_level is 0, or if this parameter is not specified by the user, then accuracy_level will be set equal to the default value. When $T_1 \leq 3$ MeV, the default value of accuracy_level is equal to 1. When $T_1 > 3$ MeV, the default value of accuracy_level is equal to 2.

Parameter No. 2 (“**firstStage**”) is the number 1, 2 or 3, indicating the first stage to be executed. The default value of this parameter is 1.

Parameter No. 3 (“**lastStage**”) is the number 1, 2 or 3, indicating the last stage to be executed. The default value of this parameter is 3.

Parameter No. 4 (“**overwrite**”) is a “switch” (1 or 0), indicating whether the existing data files must be overwritten or not. This parameter is used as a substitute for three parameters: parameter “iSkip” of subroutine “S_integrals” (in stage 1), parameter “iCalculate” of subroutine “Bremsstrahlung” (in stage 2), and parameter “iFit” of subroutine “Brems_fit” (in stage 3), which tell each of the mentioned subroutines if the data files of the corresponding stage must be overwritten. If any of the latter three parameters is explicitly specified by the user, then the specification of the parameter “overwrite” will take priority (a corresponding warning will be displayed in such a case). If this parameter is set equal to -1 (the default value), then it will be ignored, i.e., the mentioned individual switches for each of the three stages will be used instead.

Parameters No. 5 (“**Z_max_Born**”) and No. 6 (“**T2_min_Born**”) are the threshold values of the atomic number Z and of the final kinetic energy of the electron T_2 , respectively, which are used when determining whether the analytical Born approximation must be applied by default when parameter No. 1.1.8 (“appr”) is not specified by the user and the option “firstStage=1” is used. If $Z \leq Z_max_Born$ and $T_2 \geq T2_min_Born$ (MeV), then $\text{appr}=0$ by default. This corresponds to the Born approximation (see also the descriptions of parameter No. 1.1.8 in Section 4.1 and parameter No. 4.1.10 in Section 7.1). The default values of parameters “Z_max_Born” and

“T2_min_Born” are equal to 2 and 0.5, respectively (i.e., the Born approximation will be applied by default only when $Z \leq 2$ and $T_2 \geq 0.5$ MeV).

Parameter No. 7 (“**Z_def**”) is the value of the atomic number Z that must be used for calculating the default values of parameters Kmax1 and Kmax2 (as mentioned in the descriptions of parameters No. 1.3.1–6, the default values of Kmax1 and Kmax2 depend on Z when $1 \leq Z \leq 7$). A zero or negative value of this parameter indicates that the current value of Z must be used for this purpose. When $T_1 \leq 3$ MeV or when $Z \geq 7$, the default value of parameter “Z_def” is equal to 0. When $T_1 > 3$ MeV and $Z < 7$, the default value of parameter “Z_def” is equal to 7 (this means that the default values of Kmax1 and Kmax2 do not depend on Z when $T_1 > 3$ MeV).

Parameter No. 8 (“**T1_Kmax_mode_thr**”, alias “**T1_mode_thr**”) is the threshold value of the kinetic energy of the incident electron T_1 (in MeV) that must be exceeded in order to change the method of calculating the default limiting values of $\max|\kappa_1|$, $\max|\kappa_2|$ and $\max(l)$ in the case of non-zero energy of the photon (k). When $T_1 > T1_Kmax_mode_thr$ and $k \neq 0$, the sum (1.1.10) is not truncated by default (see also Section 1.3.2), and the choice of the default values of $\max|\kappa_1|$ and $\max|\kappa_2|$ is based on proximity to the tip of the photon energy spectrum. If $T_1 > T1_Kmax_mode_thr$ and $T_2 / T_1 > 0.1$ (far from the tip), then $\max|\kappa_1|$ and $\max|\kappa_2|$ are by default chosen so that $\max(|\kappa_1|, |\kappa_2|) \leq 500$, $\max|\kappa_2| \geq 50$, and $\max(l)$ is between 500 and 800. If $T_1 > T1_Kmax_mode_thr$ and $T_2 / T_1 \leq 0.1$ (close to the tip), then $\max|\kappa_1|$ and $\max|\kappa_2|$ are by default chosen so that $\max|\kappa_1| \geq 500$, $\max|\kappa_2| \geq 30$, and $\max|\kappa_1| + \max|\kappa_2| \leq 1000$. The default value of parameter “T1_Kmax_mode_thr” is equal to 10. The mentioned threshold value of T_2 / T_1 is specified by parameter No. 9 “tip_thr”.

Parameter No. 9 (“**tip_thr**”) is the threshold value of the ratio T_2 / T_1 that is used to determine if the photon energy is sufficiently close to the tip of the spectrum in order to apply the additional modification of the default values of $\max|\kappa_1|$ and $\max|\kappa_2|$ (see also the description of parameter No. 8 “T1_Kmax_mode_thr”). The default value of parameter “tip_thr” is equal to 0.1.

Note: Parameter “tip_thr” is also used in one of the three conditions for performing the nonlinear fitting of the dependence of partial-wave SDCS on κ_{\max} in stage 3 (as opposed to using the angular integral of the κ_{\max} -fitted partial-wave DDCS as the final estimate of the SDCS). See also the description of parameters No. 3.12.1 (“T1_CS_mode_thr”) and No. 3.12.2 (“T2_CS_mode_thr”) in Section 6.12.

Parameter No. 10 (“**show_CPU_time**”) is a “switch” (1 or 0), indicating whether the displayed execution times must have the meaning of the elapsed CPU time (as opposed to the actual time). The default value of this parameter is equal to 0 (i.e., the actual time is displayed by default). **Note:** If the screen output of the program has been paused (e.g., by pressing the “Pause” key on the keyboard, or by selecting the menu command “Edit/Select” or “Edit/Mark” in the console window on Windows), then the duration of the paused state of the program is not included in the time displayed after resuming execution of the program, regardless of the value of parameter “show_CPU_time”.

Parameters No. 11 “**T2_thr_mu1**” and No. 12 “**T2_thr_mu2**” (alias “T2_thr_mu” for both) are the threshold values of the outgoing electron energy (in MeV), which must be exceeded in order to apply the “ μ -correction” (see Section 1.5.4) by default in stage 3 when T_1 is less than or equal to the value parameter No. 8 (“T1_Kmax_mode_thr”) and when T_1 is greater than T1_Kmax_mode_thr, respectively. The default value of these two parameters are equal to 1 and 0.1, respectively (i.e., the μ -correction will not be applied if $T_2 \leq 0.1$ MeV, unless the user specifically requests it).

Parameter No. 13 “**S_data**” is an integer number 1, 2, or 3 indicating if the alternative dataset (corresponding to an increased ratio $|\kappa_1|_{\max} / |\kappa_2|_{\max}$) must be processed (see also Section 1.8). If S_data = 1, then only the original dataset will be processed (i.e., the program will use only the default value of the mentioned ratio). If S_data = 2, then only the alternative dataset will be

processed. If $S_data = 3$, then both the original and the alternative datasets will be processed, and the final DCS will be constructed by joining smoothly the corresponding two κ_{\max} -fitted DCS calculated in stage 3 (see also the beginning of the current section). The default value of parameter “S_data” is equal to 3. Parameter S_data is automatically reset to 1 when $\max(|\kappa_2|) < 25$, or when $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$, or when $T_1 \leq 1$ MeV (the latter threshold value of T_1 is controlled by parameter No. 1.4.1 “T1_Kmax_mode_thr0+”, which is described in Section 4.4).

In addition to using individual parameter names, BREMS allows using parameter “aliases”, which replace the names of two or more related parameters. For example, the alias “stage” refers to parameters “firstStage” and “lastStage”. Consequently, specifying “stage=2” on the command line or in the parameter file would be equivalent to two directives: “firstStage=2” and “lastStage=2”.

In the next sections, the remaining parameters of BREMS will be described. Those descriptions provide information about some details of the calculation process, too. The names of most parameters either coincide with the names of the corresponding variables in the source code, or they can be transformed into the latter by enclosing the trailing number “1” or “2” with parentheses (this indicates that the variable is an array element).

3. Conventions regarding descriptions of parameters and their numbering in this document

In this document, each parameter of BREMS will be referred to by its name or number. The parameter number has the form “A.B.C”, where “A” is the number of the parameter group, “B” is the number of the parameter subgroup, and “C” is the sequence number of the parameter in the subgroup. The parameter group number identifies the stage or mode of operation of BREMS where the corresponding parameter is used. In other words, it identifies one of the six subroutines mentioned in Section 2, which uses the corresponding parameter. Parameters used by the program “Read_S_integrals” comprise an additional group of parameters. Thus, there are seven groups of parameters:

- 1) stage 1, subroutine “S_integrals”,
- 2) stage 2, subroutine “Bremsstrahlung”,
- 3) stage 3, subroutine “Brems_fit”,
- 4) subroutine “Born_SM_appr”,
- 5) subroutine “FitExp”,
- 6) subroutine “Brems_CS_interp”,
- 7) program “Read_S_integrals”.

The subgroups are defined as groups of parameters having similar purpose, e.g., parameters defining the physical system, parameters controlling the accuracy of the results, parameters defining the set of data files to be created or updated during the calculation, etc.

A range of consecutive parameter numbers will be further specified using the dash in the third component of the parameter number. For example, “1.2.1–3” should be interpreted as three consecutive numbers 1.2.1, 1.2.2, and 1.2.3.

If a parameter name has an alias, then it is also specified in the description of that parameter. In general, more than one alias may be available for a given parameter, depending on the number of properties according to which that parameter can be categorized. For convenience, all aliases together with the corresponding parameter names are listed in Section 10.

4. Calculating the S integrals (stage 1)

Subroutine “S_integrals” is used for stage 1 of the calculation process (see Section 2). The names, descriptions and default values of the parameters of S_integrals that can be modified by the user are given below.

4.1. Physical parameters and parameters defining the point-nucleus screening function

1.1.1. “**Z**” is the atomic number of the target material (Z). Z must be positive. This is the only limitation. In particular, Z is not required to be an integer number, and it may be less than 1.

Note: A negative value of parameter “**Z**” would activate one of the special modes of operation of BREMS: fitting of a tabular screening function by the linear combination of exponentials (1.1.34a) (see Section 1.9 and Section 8).

1.1.2. “**T1**” is the kinetic energy of the incident electron (T_1) in MeV.

1.1.3. “**T2**” is the kinetic energy of the outgoing electron (T_2) in MeV, or the opposite of the ratio T_2 / T_1 . T_2 cannot be less than 0.1 eV. This means that the value of this parameter must be between -1 and T_1 , excluding the range $-0.1 \text{ eV}/T_1 < T_2 < 0.1 \text{ eV}$ (the values -1 and T_1 are allowed). *Note:* this parameter cannot be specified together with parameter No. 1.1.4 (see below).

1.1.4. “**Ep**” is either the energy of the bremsstrahlung photon (k) in MeV, or the opposite of the ratio k / T_1 . The value of this parameter must be between $-(1 - 0.1 \text{ eV}/T_1)$ and $T_1 - 0.1 \text{ eV}$. *Note:* this parameter cannot be specified together with parameter No. 1.1.3 (see above).

1.1.5. “**IV**” is an integer number indicating the type of the point-nucleus interaction potential that must be used. Three types of the point-nucleus interaction potential are currently allowed:

1 – the point-Coulomb potential $-\alpha Z / r$ (the unscreened nucleus),

2 – a linear combination of up to 200 decaying exponentials (possibly including a constant term) divided by r ,

3 – an arbitrary radial potential function $V(r)$ of the form $\bar{V}(r)/r$, where $\bar{V}(r)$ is any smooth negative-valued monotonous function, which is equal to $-\alpha Z$ at $r=0$ and asymptotically proportional to a decaying exponential (or a sum of a decaying exponential and a constant) in the limit $r \rightarrow \infty$. This function must be defined in tabular format. By default, the Kohn-Sham potential is used (see Section 1.1.5). The approximations applied in order to calculate $V(r)$ in the interval $0 < r < r_1$, where r_1 is the first value of r in the $V(r)$ data table, and at the values of r greater than the last value of r in the tabular data, are described in Section 12. In the case “**IV=3**”, the tabulated values of $V(r)$ (or of the screening function $\tilde{V}(r)$) are loaded from a file in the folder specified by parameter “**dirV**” (No. 1.1.6) by default. It is also possible to specify an arbitrary filename (parameter No. 1.1.7 “**fn_V**”). *Note:* in the case “**IV=3**”, the tabulated values of $V(r)$ or $\tilde{V}(r)$ may include the finite-nucleus correction (see Section 1.1.6), in which case the screening function would be equal to zero at $r=0$, and it would not be possible to define the finite-nucleus correction of the screening function separately (see also descriptions of parameters No. 1.1.32 “**V_scr_0**” and No. 1.2.1 “**nuclear_model**”).

The default value of parameter “**IV**” is 3.

1.1.6. “**dirV**” (alias “**dir_V**”) is the name of the folder containing the file with the interaction potential data (when the filename is not specified using parameter “**fn_V**”). Description of the file format is presented in Section 12. If the specified folder name is incomplete, i.e., if it does not start with the forward slash ‘/’ or the backslash ‘\’ and does not contain the colon ‘:’, then it is assumed to be a subfolder either of the BREMS installation folder or of the current folder, depending on whether the path to the BREMS executable file has been specified before its name on the command line or not. If this parameter does not end with the slash ‘/’ or the backslash ‘\’, then its part following the last ‘/’ or ‘\’ is assumed to be an initial part (prefix) of the file name. The default value of this parameter is ‘**V/Kohn-Sham/**’.

1.1.7. “**fn_V**” is the name of the file with the interaction potential data. If this parameter is equal to the empty string, then the mentioned filename is constructed by concatenating the string

specified by parameter “dirV” with the string “⟨Z⟩.txt”, where “⟨Z⟩” is the value of parameter No. 1.1.9 “Z_V”. The default value of this parameter is equal to the empty string.

1.1.8. “**appr**” specifies the method of approximating the analytical point-nucleus screening function during the solution of the coupled radial Dirac equations when IV=2 or IV=1:

“appr=1” indicates that the exact analytical expression of the point-nucleus screening function must be used,

appr = 2 or 3 or 4 indicates that the analytical point-nucleus interaction potential must be transformed into a tabular one. The value of appr indicates the set of radial breakpoints to be used:

“appr=2” indicates that the radial breakpoints must be calculated using parameters “rmin”, “rmax” and “nr” (No. 1.1.12–14),

“appr=3” indicates that the radial breakpoints must be read from the first column in a $V(r)$ data file, whose name is either specified by parameter “fn_V” (No. 1.1.7) or constructed using the values of parameters “Z_V” (No. 1.1.9) and “dirV” (No. 1.1.6),

“appr=4” differs from “appr=3” by up to 100 additional radial breakpoints, which “fill” the “gap” from the last breakpoint to $r = r_{\max}$, where r_{\max} is specified using parameter “rmax” (No. 1.1.13). The start of the mentioned “gap” is the last breakpoint in the “optimal” set of 10 breakpoints, which corresponds to the best exponential fit, exactly as in the case “IV=3” (see Section 12). If $0.99 \cdot r_{\max}$ does not exceed the mentioned breakpoint, then “appr=4” is identical to “appr=3”.

When IV = 1 or 2, “appr” may be zero or negative, which indicates that the differential cross sections must be calculated using the Born approximation or Sommerfeld-Maue approximation, respectively (see Sections 1.1.2 and 1.1.3). However, the case $\text{appr} \leq 0$ does not involve calling the subroutine S integrals, and it is handled by another subroutine (Born_SM_appr). Although the subroutine Born_SM_appr is also called in the case $\text{appr} > 0$, its only role in this case is loading the a - and b -coefficients of the analytical point-nucleus screening function (1.1.34a) when IV=2, or calculating them according to the Thomas-Fermi-Csavinszky approximation (1.1.54). The set of parameters of the subroutine Born_SM_appr pertaining to this role is described further in this section. The other parameters used by the subroutine Born_SM_appr are described in Section 7.

If parameter “appr” is not specified by the user explicitly, then its default value is determined by comparing the values of Z and T_2 with the corresponding threshold values “Z_max_Born” and “T2_min_Born” (parameters No. 5–6 of the main program, described in Section 2). If $Z \leq Z_{\max_Born}$ and $T_2 \geq T2_{\min_Born}$, then $\text{appr}=0$ by default (see also the description of parameter No. 4.1.10 in Section 7.1). If $Z > Z_{\max_Born}$ or $T_2 < T2_{\min_Born}$, then the default value of “appr” depends on the values of parameters “IV” and “nuclear_model”: if IV=1 and nuclear_model=0, then $\text{appr}=1$, if IV=1 and nuclear_model>0, then $\text{appr}=2$; if IV=2, then $\text{appr}=2$; if IV=3, then appr is not used.

1.1.9. “**Z_V**” is an integer number from 0 to 100 indicating the file with the tabular $V(r)$ data, when its name is not specified explicitly (using parameter No. 1.1.7 “fn_V”). The value of 0 is equivalent to setting Z_V equal to the integer part of the current value of Z (specified by parameter “Z”). In the case “IV=3”, this parameter should be used only if it is necessary to use a tabular screening function different from the one specified in the $V(r)$ data file corresponding to the current value of Z . In the case “IV=2”, this parameter should be used only in conjunction with “appr=3” or “appr=4” in order to specify the data file with the values of radial breakpoints (see the description of parameter No. 1.1.8). The default value of this parameter is equal to 0.

1.1.10. “**Zi**” is the ion charge, in units of the elementary charge (this parameter is used only when parameter “**IV**” is not equal to 1). If this parameter is nonzero, then the overall screening function will be defined according to Eq. (1.2.5), where i is the unscreened fraction of the nuclear charge (i.e., the ratio of parameters “**Zi**” and “**Z**”), and $\tilde{V}(r)$ is calculated according to the values of all other parameters controlling the calculation of the screening function (i.e., all other parameters described in the current subsection, and the parameters defining the finite-nucleus correction of the screening function). The default value of this parameter is equal to 0.

1.1.11. “**Zi_V**” is the ion charge corresponding to the tabular point-nucleus interaction potential data, in units of the elementary charge. If this parameter is nonzero, then the input data table will be assumed to correspond to an ion with charge Zi_V (i.e., the program will assume that the input screening function approaches the value of Zi_V / Z_V as r approaches ∞). In such a case, the normalized variable part of the point-nucleus screening function (i.e., the term $\tilde{V}_p(r)$ in Eqs. (1.2.4a–c)) will be calculated by applying the opposite linear transform to the input data, i.e.,

$$\tilde{V}_p(r) = \frac{\tilde{V}_{in}(r) - (Zi_V / Z_V)}{1 - (Zi_V / Z_V)}, \quad (4.1.1)$$

where $\tilde{V}_{in}(r)$ is the input point-nucleus screening function. Thus, the ion charge used for the calculations (parameter “**Zi**”) may be different from the ion charge corresponding to the input data (parameter “**Zi_V**”). The default value of parameter “**Zi_V**” is equal to 0.

1.1.12–14. “**rmin**”, “**rmax**” and “**nr**” are, respectively, the first radial breakpoint, the last radial breakpoint and the number of breakpoints in the radial range $rmin \leq r \leq rmax$ to be used in conjunction with the option “**IV** \leq 2 appr=2” (see above). In addition, the value of $rmax$ is used in conjunction with the option “**IV** \leq 2 appr=4” (see above). The breakpoints are equidistant on the logarithmic scale. The following values are used by default: $rmin = 10$, $rmax = 10000$, $nr = 601$ (i.e., 200 breakpoints per decade).

1.1.15. “**V_parms**” specifies the method of determining the a - and b -coefficients of the analytical point-nucleus screening function (1.1.34a) when **IV**=2:

“**V_parms**=1” indicates that the point-nucleus screening function must be expressed as a linear combination of up to three exponential terms, with the a - and b -coefficients specified by the user on the command line or in the parameter file, using the six parameters “**factor1**”, “**exp1**”, “**factor2**”, “**exp2**”, “**factor3**”, “**exp3**” described below.

“**V_parms**=2” indicates that the a - and b -coefficients must be loaded from the files specified by parameters “**file_parms**” and “**file_parms_lo**”, which are described below. In this case, up to 200 exponential terms are allowed.

“**V_parms**=3” indicates that the a - and b -coefficients must be the same as in the Thomas-Fermi-Csavinsky approximation (1.1.54). In this case, there are three exponential terms in the expression of the point-nucleus screening function.

The default value of parameter “**V_parms**” is 2.

1.1.16–21. “**factor1**”, “**exp1**”, “**factor2**”, “**exp2**”, “**factor3**”, “**exp3**” are the three pairs of the a - and b -coefficients of the analytical point-nucleus screening function (1.1.34a) to be used in the case “**IV**=2 **V_parms**=1” (see above). In this case, it is assumed that the expression of the screening function consists of only three exponential terms. The three parameters “**factor** $\langle n \rangle$ ” are used to specify the values of a_n ($n = 1, 2, 3$), and the three parameters “**exp** $\langle n \rangle$ ” are used to specify the values of b_n ($n = 1, 2, 3$).

Note: In the case of an ion, those six parameters describe only the variable part of the point-nucleus screening function. This part is “normalized to 1”, i.e., it is equal to 1 at $r = 0$ and decays to zero in the limit $r \rightarrow \infty$ (see also Eq. (1.2.4b)).

1.1.22–23. “**file_parms**” and “**file_parms_lo**” are the names of the two files with the “high” and “low” parts of the quadruple-precision (QP) values of the a - and b -coefficients of the analytical point-nucleus screening function (1.1.34a) to be used in the case “IV=2 V_parms=2”. Each QP number is represented in BREMS as a sum two double-precision (DP) numbers – the “high” and “low” parts. The “high” part is equal to the DP approximation of the mentioned QP number, whereas the “low” part is responsible for the additional precision (i.e., additional decimal places). The formats of the two files are identical. The first line of the file contains column headers. The first column contains the values of the atomic number Z , the second column contains the number of the exponential terms (denoted N in Eq. (1.1.34a)), and all remaining columns contain pairs of the corresponding a - and b -coefficients. These two files are assumed to be in the subfolder indicated by parameter No. 1.1.29 (“**dirV_aux**”), which is “V/Kohn-Sham/” by default. The distribution package of BREMS contains the default versions of those two files. They are in the subfolder “V/Kohn-Sham/”, and their names are “FitData.txt” and “FitData_lo.txt” (those are the default values of parameters “**file_parms**” and “**file_parms_lo**”, respectively). These files were generated by the subroutine “FitExp” by fitting the Kohn-Sham screening potential data loaded from the files in the folder “V/Kohn-Sham/” (this mode of operation of BREMS is described in Section 8). The only non-default option used in generating those files was “**R_atom_max=1e4**” (see the description of parameter No. 5.1.10 in Section 8.1).

Note: In the case of an ion, the mentioned coefficients describe only the variable part of the point-nucleus screening function. This part is “normalized to 1”, i.e., it is equal to 1 at $r = 0$ and decays to zero in the limit $r \rightarrow \infty$ (see also Eq. (1.2.4b)).

1.1.24. “**quad**” is a “switch” (1 or 0) indicating if the quadruple-precision (QP) values of the a - and b -coefficients of the analytical point-nucleus screening function (1.1.34a) must be formed by combining the data in the two files specified by parameters No. 1.1.22–23 (“**file_parms**” and “**file_parms_lo**”) in the case “IV=2 V_parms=2”. If **quad** = 1, then both files described above are loaded, and the QP value of each coefficient is obtained by combining the two double-precision “parts” of that coefficient, which are stored in the two files. If **quad** = 0, then only the first one of the two files (specified by parameter “**file_parms**”) is loaded, and the QP values of all coefficients are set equal to the corresponding double-precision values in that file. The default value of parameter “**quad**” is equal to 1 (indicating that QP values of the a - and b -coefficients must be formed by combining the data in the two files).

1.1.25. “**Taylor**” is a “switch” (1 or 0) indicating whether the point-nucleus screening function at $0 < r < r_1$, where r_1 is the first breakpoint in the $V(r)$ data table, must be calculated by the Taylor series expansion at $r = 0$. This parameter is used only in the case of a point-nucleus screening function defined in tabular format, i.e., in the cases “IV=2 appr>1” and “IV=3”. In the case “IV=2 appr>1”, the coefficients of the Taylor series are calculated using the analytical expression of the point-nucleus screening function at quadruple precision. In the case “IV=3”, the Taylor coefficients are read from the file specified by the parameter “**file_Taylor**” (No. 1.1.26). If **Taylor**=0, then in the case “IV=2 appr>1” the point-nucleus screening function at $0 < r < r_1$ is calculated using its analytical expression (1.1.34a) at quadruple precision, and in the case “IV=3” it is calculated by exponential or linear interpolation, depending on the value of parameter “**expInterp**” (No. 1.1.31). In the case “IV=1” or “IV=2 appr<2”, parameter “**Taylor**” is not used. Parameter “**Taylor**” is equal to 1 by default.

Note: In the case of an ion, the mentioned Taylor coefficients describe only the variable part of the point-nucleus screening function. This part is “normalized to 1”, i.e., it is equal to 1 at $r = 0$ and decays to zero in the limit $r \rightarrow \infty$ (see also Eq. (1.2.4b)).

1.1.26. “**file_Taylor**” is the name of the file with the coefficients of the Taylor series expansion of the point-nucleus screening function at $r = 0$, to be used in conjunction with the option “IV=3 Taylor=1” (see the description of parameter No. 1.1.25). By default, the file “TaylorCoefs.txt” created by the subroutine “FitExp” during the fitting of the point-nucleus screening function by a linear combination of exponentials (1.1.34a) is used (the implementation of the mentioned fitting in BREMS is described in Section 8). This file is assumed to be in the subfolder indicated by parameter No. 1.1.29 (“dirV_aux”), which is “V/Kohn-Sham/” by default. The first line of this file contains the column headers. The first column contains the values of the atomic number Z . The second and third columns contain a “reference” value of the radial coordinate r and the exact value of the mentioned linear combination of exponentials at this value of r , respectively. The fourth column contains the highest degree of the terms retained in the truncated Taylor series (i.e., the number of terms, not counting the zero-degree term). The remaining columns contain the values of the coefficients corresponding to each term (starting with the zero-degree coefficient, which is always exactly equal to 1).

Notes:

1. The mentioned “reference” value of r is used as the starting value (r_1) of the $V(r)$ data table in stage 1. It coincides with the starting point of the radial range where the cubic spline interpolation of the point-nucleus screening function is applied. In the case “IV=3 Taylor=0” and in the other cases when the radial breakpoints are loaded from files with the tabular $V(r)$ data, i.e., “IV≤2 appr=3” and “IV≤2 appr=4”, the value of r_1 is also read from the second column of the file specified by “file_Taylor” (in those cases, this is the only value that is read from this file), unless the value of r_1 has been specified using parameter “r_spline” or “file_r_spline” (see also the descriptions of parameters No. 1.1.27–28 below). In all those cases, it must be equal to one of the radial breakpoints specified in the $V(r)$ data file. If this breakpoint is not the first one specified in the $V(r)$ data file, then all smaller breakpoints will be ignored.
 2. In the case “IV=3 Taylor=1”, the “reference” value of the point-nucleus screening function specified in column No. 3 of the file specified by parameter “file_Taylor” (such as the file “V/Kohn-Sham/TaylorCoefs.txt”) is used to eliminate the discontinuity at $r = r_1$ in the radial dependence of the point-nucleus screening function and to provide feedback to the user regarding the accuracy of the approximation of the tabular screening function by the truncated Taylor series in the interval $r < r_1$ (since, as mentioned, the Taylor coefficients correspond to the analytical approximation (1.1.34a) by default, this also provides feedback regarding the accuracy of this approximation). At the start of stage 1, the program calculates the relative deviation of the tabular point-nucleus screening function $\tilde{V}(r_1)$ from its “reference” value $\tilde{V}_{\text{ref}}(r_1)$ and displays it on the screen. Normally, its absolute value should be less than 0.01. In order to eliminate the discontinuity of $\tilde{V}(r)$ at $r = r_1$, the first-degree Taylor coefficient is modified by adding the correction term $(\tilde{V}(r_1) - \tilde{V}_{\text{ref}}(r_1)) / r_1$ to it.
- 1.1.27. “**r_spline**” is the value of the first radial breakpoint (r_1) in the $V(r)$ data table, to be used in conjunction with the options “IV=3 Taylor=0”, “IV≤2 appr=3”, and “IV≤2 appr=4” (i.e., when the radial breakpoints are loaded from the $V(r)$ data file, but the coefficients of the Taylor series are not loaded from a file). It coincides with the starting point of the radial range where the cubic spline interpolation of the screening function is applied. If $r_{\text{spline}} > 0$, then it must coincide with one of the radial breakpoints specified in the $V(r)$ data file. If this breakpoint is not the first one specified in the $V(r)$ data file, then all smaller breakpoints will be ignored. If $r_{\text{spline}} = 0$, then it will be reset to the first breakpoint of the $V(r)$ data table. A negative value of this parameter indicates that r_1 must be read from the file

specified by parameter “file_r_spline” (No. 1.1.28) or by parameter “file_Taylor” (No. 1.1.26). The default value of this parameter is equal to -1 .

- 1.1.28. “**file_r_spline**” is the name of the file with the values of the first radial breakpoint (r_1) in the table with $V(r)$ data for all values of Z , to be used in conjunction with the options “IV=3 Taylor=0”, “IV \leq 2 appr=3” and “IV \leq 2 appr=4” (i.e., when the radial breakpoints are loaded from the $V(r)$ data file, but the coefficients of the Taylor series are not loaded from a file). This file must have two columns of numbers and a line with headers of the two columns. The first column must contain the values of the atomic number Z , and the second column must contain the values of r_1 for each Z . This parameter is used only when parameter No. 1.1.27 “r_spline” is assigned a negative value. If parameter “file_r_spline” is equal to the empty string, then the values of r_1 will be read from the file specified by parameter No. 1.1.26 “file_Taylor”. Otherwise, this file is assumed to be located in the subfolder indicated by parameter No. 1.1.29 (“dirV_aux”), which is “V/Kohn-Sham/” by default. Parameter “file_r_spline” is equal to the empty string by default. **Note:** The distribution package of BREMS includes the file “V/Kohn-Sham/r_spline.txt”, which may be used for this purpose. The values of r_1 in this file are the same as the values of r_1 in the file “V/Kohn-Sham/TaylorCoefs.txt”.
- 1.1.29. “**dirV_aux**” (alias “dir_V”) is the name of the folder containing the files whose names are defined by parameters No. 1.1.22 (“file_parms”), No. 1.1.23 (“file_parms_lo”), No. 1.1.26 (“file_Taylor”) and No. 1.1.28 (“file_r_spline”). If the specified folder name is incomplete, i.e., if it does not start with the forward slash ‘/’ or the backslash ‘\’ and does not contain the colon ‘:’, then it is assumed to be a subfolder either of the BREMS installation folder or of the current folder, depending on whether the path to the BREMS executable file has been specified before its name on the command line or not. If this parameter does not end with the slash ‘/’ or the backslash ‘\’, then its part following the last ‘/’ or ‘\’ is assumed to be the initial part (prefix) of the file name. The default value of this parameter is ‘V/Kohn-Sham/’.
- 1.1.30. “**expExtrap**” is a “switch” (1 or 0) indicating whether the screening function at large values of r in the case “IV=2 appr $>$ 1” must be calculated in the same way as in the case “IV=3”, i.e., by modification of the number of breakpoints on the basis of the optimal exponential fit chosen from 11 tries, and then using the exponent and preexponential factor returned by the fitting routine (see also Section 12). The default value of this parameter is 1, indicating that the exponential fitting must be performed.
- Note:** In the case of an ion, only the variable part of the point-nucleus screening function is fitted as described above. This part is “normalized to 1”, i.e., it is equal to 1 at $r = 0$ and decays to zero in the limit $r \rightarrow \infty$ (see also Eq. (1.2.4b)).
- 1.1.31. “**expInterp**” is a “switch” (1 or 0) indicating whether the point-nucleus screening function at $0 < r < r_1$, where r_1 is the first breakpoint in the $V(r)$ data table, must be calculated by exponential or linear interpolation, respectively, when the Taylor series expansion is not used (see the description of parameter No. 1.1.25 “Taylor”) and the point-nucleus screening function is defined in tabular format, i.e., in the cases “IV=2 appr $>$ 1” or “IV=3”. The default value of this parameter is equal to 1 (i.e., the exponential interpolation is applied).
- 1.1.32. “**V_scr_0**” is the value of the screening function at $r = 0$. This parameter may be specified by the user only in the case “IV=3”, and only when parameter “nuclear_model” (No. 1.2.1) is zero. In such a case, the program will use the value of V_scr_0 to determine if the input screening function data correspond to the point-nucleus screening function, or to the overall screening function (including the finite-nucleus correction). In the former case, V_scr_0 = 1, whereas in the latter case V_scr_0 = 0 (see also Section 1.1.6). Those two values are the only allowed values of parameter “V_scr_0”. By default, this parameter is equal to 1. If the finite-nucleus correction of the screening function is applied (i.e., if parameter “nuclear_model” is non-zero), then this parameter is automatically reset to 0.

Note: In the case “V_scr_0=0 nuclear_model=0”, parameter “IV” (No. 1.1.5) must be equal to 3, parameters “Zi” (No. 1.1.10), “Z_V” (No. 1.1.11), “Taylor” (No. 1.1.25), “expInterp” (No. 1.1.31) must be equal to zero, and parameter “r_spline” (No. 1.1.27) cannot be negative. If the user specifies other values of those parameters, then the program will quit with an error message. If any of these parameters is not specified by the user and its default value does not conform to the mentioned requirement, then it will be automatically reset to the required value (for example, parameter “r_spline” will be reset to zero, which means that cubic spline interpolation of the screening function will be applied starting from the first available radial breakpoint).

4.2. Parameters defining the finite-nucleus correction of the screening function

1.2.1. “**nuclear_model**” indicates the analytical approximation of the radial dependence of the proton density to be used when calculating the finite-nucleus correction of the screening function. Four values from 0 to 3 are allowed, corresponding to the point-nucleus approximation and the three approximations of the nuclear charge distribution mentioned in Section 1.1.6:

0 – the point-nucleus approximation,

1 – the uniform charge distribution defined by Eqs. (1.1.68a–c),

2 – Helm’s uniform-uniform distribution defined by Eqs. (1.1.69a–c),

3 – the Fermi distribution defined by Eqs. (1.1.67a,b).

If the value of parameter “nuclear_model” is specified with the minus sign, then the program will first check if the ratio of the reduced wavelength of the incident electron to the mean nuclear radius (specified by parameter “Rn”) is less than the value of parameter “lred_Rn_thr”. If not, then nuclear_model will be reset to zero (i.e., the point-nucleus approximation will be used). The default value of parameter “nuclear_model” is equal to -3.

1.2.2. “**Rn**” is the mean nuclear radius (in fm), which is denoted “ R_n ” in Eqs. (1.1.67a) – (1.1.68b) and (1.1.69b). If this parameter is zero, then its value will be calculated according to the expression $R_n = 1.07 A^{1/3}$ fm, where A is the mass number (which can be either specified explicitly using parameter No. 1.2.3 “A”, or replaced by the standard atomic weight of the given chemical element). The default value of parameter “Rn” is equal to 0.

1.2.3. “**A**” is the mass number to be used when calculating the mean nuclear radius (see the description of parameter No. 1.2.2 “Rn”). If this parameter is zero, then it will be set equal to the standard atomic weight of the given chemical element (in g/mol). The default value of parameter “A” is equal to 0.

1.2.4. “**lred_Rn_thr**” is the threshold value of the ratio λ_1 / R_n , where λ_1 is the reduced wavelength of the incident electron (equal to $1 / p_1$ in relativistic units), which must be exceeded in order to reset parameter “nuclear_model” to 0 when nuclear_model is initially negative (see the description of parameter 1.2.1 “nuclear_model”). If $\lambda_1 / R_n \leq \text{lred_Rn_thr}$, then nuclear_model will be automatically replaced with $|\text{nuclear_model}|$. Parameter “lred_Rn_thr” is automatically reset to zero if it is not used (i.e., if nuclear_model is initially zero or positive). The default value of this parameter is equal to 40.

1.2.5. “**Rn_max**” is the radial endpoint of the “nuclear grid” (in fm), i.e., the last breakpoint in the set of equidistant breakpoints including the entire nuclear radius and possibly extending to some distance beyond the nucleus. The uniform charge distribution and Helm’s Uu distribution have a “natural” cutoff radius R_c , which is uniquely defined by parameters of the distribution (in the case of the uniform distribution, $R_c = R_U$, which is defined by Eq. (1.1.68a), and in the case of Helm’s Uu distribution, $R_c = R_1 + R_2$, where R_1 and R_2 are defined by Eq. (1.1.69b)). The value of parameter “Rn_max” cannot be less than the mentioned “natural” cutoff radius. The Fermi distribution does not have a “natural” cutoff

radius, because the corresponding proton density $\rho_F(r)$ approaches zero asymptotically (see Eq. (1.1.67a)). In the case of the Fermi distribution, the cutoff radius R_c of the nuclear charge distribution is set equal to the value of parameter “Rn_max”. The latter value must therefore be sufficiently large, so that the value of $\rho_F(r)$ calculated according to Eq. (1.1.67a) is negligibly small at $r > R_c$. The default value of parameter “Rn_max” is equal to 20. This value is sufficiently large, bearing in mind the relatively small value of parameter z (see Eq. (1.1.67b)) and the fact that the mean nuclear radius (given by the value of expression $1.07 A^{1/3}$) is less than 7 fm for all known isotopes of elements with atomic numbers from 1 to 100.

- 1.2.6. “**Rn_grid**” is the number of equidistant radial breakpoints in the “nuclear grid” (see also the description of parameter No. 1.2.5 “Rn_max”), not counting the initial breakpoint at $r = 0$. Consequently, the interval between adjacent breakpoints of the nuclear grid is equal to Rn_max / Rn_grid . The default value of parameter “Rn_grid” is equal to 400. Thus, if Rn_max is equal to the default value (20 fm), then the mentioned interval is equal to 0.05 fm by default.

Note: If the mentioned “nuclear grid” does not overlap with the “electronic grid” (whose breakpoints are either loaded from $V(r)$ data files or calculated as explained in the description of parameter No. 1.1.8 “appr”) and the gap between the last breakpoint of the nuclear grid and the first breakpoint of the electronic grid is sufficiently large, then additional breakpoints will be inserted between them. The intervals between the additional breakpoints form a geometric progression. The number of additional breakpoints is such as to ensure that the values of the interval between adjacent breakpoints of the nuclear grid and the interval between the first two breakpoints of the electronic grid can be approximately obtained by continuing the mentioned geometric progression. If the nuclear grid overlaps with the electronic grid, then the nuclear grid will replace the overlapping part of the electronic grid.

4.3. Parameters defining the sets of S integrals and of terms of the truncated partial-wave series

- 1.3.1–3. “**Kmin1**” (aliases “Kmin”, “K1”, “Km”), “**Kmax1**” (aliases “Kmax”, “K1”, “Km”), and “**isAbs_K1**” (alias “isAbs_K”) are, respectively, the minimum and maximum values of κ_1 , and a “switch” indicating if those values must be interpreted as absolute values. If $isAbs_K1 = 1$, then both $Kmin1$ and $Kmax1$ must be positive, and the program will calculate the S integrals for two ranges of κ_1 : $-Kmax1 \leq \kappa_1 \leq -Kmin1$ and $Kmin1 \leq \kappa_1 \leq Kmax1$. If $isAbs_K1 = 0$, then only the latter range of the values of κ_1 will be used (in this case, $Kmin1$ and $Kmax1$ may be either positive or negative). Normally, $Kmin1 = 1$ and $isAbs_K1 = 1$. This is the recommended (and default) setting if the S integrals are to be used for calculation of bremsstrahlung cross sections. If parameter “Kmax2” (No. 1.3.5) is specified by the user, then the default value of $Kmax1$ is calculated as a product of $Kmax2$ and $k12ratio$ (parameter No. 1.3.7). Otherwise, the default value of $Kmax1$ is calculated by interpolation between 32 tabulated values of $Kmax1$ corresponding to 8 values of T_1 (10 eV, 100 eV, 1 keV, 10 keV, 100 keV, 1 MeV, 3 MeV, 10 MeV) and 4 values of k / T_1 (0, 0.1, 0.4, 0.95). The interpolation with respect to T_1 is linear-log (logarithmic in T_1), and the interpolation with respect to k / T_1 is linear-linear. If $T_1 > 0.1$ MeV, then the interpolated value of $Kmax1$ is rounded to the nearest multiple of 5 (when $k \neq 0$, this rounding is needed to facilitate reusing the values of the integrals S_{11} , S_{12} , S_{21} and S_{22} defined by Eq. (1.2.7) at default values of parameters, when the method of partial-wave interpolation is applied). The mentioned tabulated values corresponding to $T_1 = 1$ MeV, 3 MeV and 10 MeV depend on the chosen accuracy level (1 or 2) defined by parameter No. 1 of the main program (“accuracy_level”), which is described in Section 2. For $Z \leq 7$, those values depend on Z , too (in this interval of values of Z , the default value of $Kmax1$ increases linearly with decreasing Z). If $k = 0$ and $T_1 > 0.1$ MeV, the interpolation with respect to T_1 and Z is performed using a different set of

tabulated values than in the case $k \neq 0$ (the tabulated values of $K_{\max 1}$ corresponding to $k = 0$ are greater than in the case $k \neq 0$). If $IV = 1$ (unscreened point-Coulomb potential) or $Z_i \neq 0$ (an ion), then the default value of $K_{\max 1}$ is additionally increased by a factor that decreases with increasing T_1 , and becomes equal to 1 starting from $T_1 = 100$ keV. The initial (maximum) value of the mentioned factor corresponds to $T_1 \leq 100$ eV and is equal to 3. The mentioned decrease is logarithmic (i.e., the default value of $K_{\max 1}$ is a linear function of $\ln(T_1)$ when $IV=1$ and $100 \text{ eV} \leq T_1 \leq 100 \text{ keV}$).

Note: This description of the method of calculating the default value of $K_{\max 1}$ at $k \neq 0$ is applicable only when $T_1 \leq T1_Kmax_mode_thr$ (the description of parameter No. 8 “ $T1_Kmax_mode_thr$ ” is provided at the end of Section 2).

1.3.4–6. “**Kmin2**” (aliases “**Kmin**”, “**K2**”, “**Km**”), “**Kmax2**” (aliases “**Kmax**”, “**K2**”, “**Km**”), and “**isAbs_K2**” (alias “**isAbs_K**”) are, respectively, the minimum and maximum values of κ_2 , and a “switch” indicating if those values must be interpreted as absolute values. Their interpretation and the limiting values are the same as in the case of parameters No. 1.3.1–3. Normally, $K_{\min 2} = 1$ and $isAbs_K2 = 1$. This is the recommended (and default) setting if the S integrals are to be used for calculation of bremsstrahlung cross sections. If $T_1 \leq 100$ keV, then the default value of $K_{\max 2}$ is equal to the smaller of the following two numbers: the default value of $K_{\max 1}$ corresponding to the current values of T_1 and k / T_1 (see above), and the default value of $K_{\max 1}$ corresponding to $T_1 = T_2$ and $k = 0$. If $T_1 > 100$ keV, then the default value of $K_{\max 2}$ is obtained by additional multiplication of the previously-mentioned value by p_2 / p_1 (i.e., the ratio of the final and initial momenta of the electron), and rounding the result to the nearest integer.

Note: The recommended values of $K_{\min 1}$, $isAbs_K1$, $K_{\min 2}$ and $isAbs_K2$ (i.e., parameters No. 1.3.1, No. 1.3.3, No. 1.3.4, and No. 1.3.6) are the following: $K_{\min 1} = K_{\min 2} = 1$ and $isAbs_K1 = isAbs_K2 = 1$. Although mathematically this set of parameters is equivalent to $K_{\min 1} = -K_{\max 1}$, $K_{\min 2} = -K_{\max 2}$ and $isAbs_K1 = isAbs_K2 = 0$, the former set is the recommended one, because only in that case the program will automatically decrease $K_{\max 1}$ or $K_{\max 2}$ if the user-specified value does not correspond to the available data (when some of the data are loaded from files created previously, rather than calculated in the current run of BREMS). If another set of the mentioned parameters is used and if such an abnormal situation occurs, processing will be terminated immediately with an error message. This remark applies both to `Brems.exe` and to `Read_S_integrals.exe`.

1.3.7. “**k12ratio**” is a positive integer number equal to the ratio of maximum absolute values of κ_1 and κ_2 ($\kappa_{1\max}$ and $\kappa_{2\max}$, respectively), i.e., the value of n in Eq. (1.5.2). If parameter **k12ratio** is not specified by the user, then its default value is calculated by dividing $\kappa_{1\max}$ (which may be either the default value or specified by the user) by $\kappa_{2\max}$ and rounding the result down to an integer (if $\kappa_{1\max} > 2\kappa_{2\max}$), or to the nearest integer (if $\kappa_{2\max} < \kappa_{1\max} \leq 2\kappa_{2\max}$), or it is set to 1 (if $\kappa_{1\max} \leq \kappa_{2\max}$). If parameter $K_{\max 1}$ is not specified by the user, then $\kappa_{1\max}$ is calculated by multiplying $\kappa_{2\max}$ by **k12ratio**.

1.3.8–10. “**k2_breakpoint1**”, “**k2_step_first**” (alias “**k2_step**”), and “**k2_step_last**” (alias “**k2_step**”) control the application of the partial-wave interpolation method described in Section 1.3.4. They are used for defining the set of values of κ_2 that have to be “skipped” in order to reduce the number of the S integrals to be calculated and the number of the systems of ODEs (1.1.16a,b) corresponding to the final electron energy to be solved. If the partial-wave interpolation method is applied, then the subroutine `Bremsstrahlung` (called in stage 2) will subsequently calculate the terms corresponding to the skipped values of κ_2 in the expressions of the cross sections (1.1.4) and (1.1.5) by logarithmic cubic spline interpolation as explained in Section 1.3.4. In stage 1 (subroutine `S_integrals`), this skipping of values of κ_2 is possible only when $isAbs_K2 = 1$ (otherwise, these three parameters are ignored and

no values of κ_2 are skipped). In stage 2 (subroutine Bremsstrahlung), the condition for the partial-wave interpolation is more restrictive: $K_{min1} = K_{min2} = 1$ and $isAbs_K1 = isAbs_K2 = 1$. “k2_breakpoint1” is the initial point of the range of values of $|\kappa_2|$ where the mentioned removal of points must be applied. If $k2_breakpoint1 \geq K_{max2}$ or $k2_breakpoint1 < 1$, then no values of κ_2 will be skipped and parameters No. 1.3.9–10 (“k2_step_first” and “k2_step_last”) will be ignored. “k2_step_first” is the increment to obtain the next value (“breakpoint”) of $|\kappa_2|$ that must be retained (i.e., $k2_breakpoint2$ is equal to $k2_breakpoint1 + k2_step_first$). “k2_step_last” is the approximate interval between the last two breakpoints of $|\kappa_2|$. $k2_step_last$ cannot be less than $k2_step_first$. If $k2_step_last > k2_step_first$, then the intervals between the retained values of $|\kappa_2|$ will approximately form an arithmetic progression. If $k2_step_last = k2_step_first$, then all intervals will be equal to each other, except possibly for the last interval, which in this case may be less than $k2_step_first$ (this happens when $K_{max2} - k2_breakpoint1$ is a not multiple of $k2_step_first$). In any case, the last breakpoint is equal to K_{max2} . For example, if $k2_breakpoint1 = 30$, $k2_step_first = k2_step_last = 5$ and $K_{max2} = 70$, then the set of retained values of $|\kappa_2|$ will be 1–30, 35, 40, 45, 50, 55, 60, 65, 70. If the latter set of parameters is modified by increasing K_{max2} to 72, then the value 72 will be added to the mentioned set of values of $|\kappa_2|$ (i.e., the difference of the last two breakpoints of κ_2 in this case would be 2). Another example with an increasing set of the intervals: $k2_breakpoint1 = 40$, $k2_step_first = 5$, $k2_step_last = 10$ and $K_{max2} = 130$. In this case, the set of retained values of $|\kappa_2|$ would be the following: 1–40, 45, 50, 56, 63, 70, 77, 85, 93, 101, 110, 120, 130. If the photon energy (parameter “Ep”) is non-zero and parameter K_{max2} is greater than or equal to 80, or if $Ep = 0$ and parameter K_{max2} is greater than or equal to 120, then the default values of these three parameters are the following: $k2_breakpoint1 = 30$, $k2_step_first = k2_step_last = 5$ (or 10, if $k12ratio = 1$ and $K_{max2} > 300$, or if $k12ratio \geq 2$ and $K_{max2} \geq 250$). Otherwise, $k2_breakpoint1 = 0$ (i.e., the partial-wave interpolation is not applied).

- 1.3.11. “**lmin**” (alias “l”) is the minimum value of l in Eq. (1.1.10). Normally, $l_{min} = 0$. This is the recommended (and default) minimum value of l if the S integrals are to be used for calculation of bremsstrahlung cross sections.
- 1.3.12–13. “**lmax**” (alias “l”) and “**lmax_MP**” are the two alternative maximum values of l (i.e., l_{max}) in Eq. (1.1.10). If optimization of the precision level is not requested (see the description of parameter No. 1.7.11), then l_{max_MP} will be used if the requested number of significant digits is greater than 21 (i.e. if the quadruple or multiple precision is required), and l_{max} will be used if the requested number of significant digits is less than 22 (i.e., if the double precision is required). The value of l_{max} cannot be less than l_{max_MP} . Two alternative values of l_{max} are used because it is known that the contribution of an S integral to the sum (1.1.10) decreases rapidly with increasing l (especially at low photon energies). However, it is not known beforehand which value of l_{max} is necessary for a sufficiently accurate estimation of cross sections. Since the sensitivity of the cross sections to the value of l_{max} is tested during the next stage (by the subroutine Bremsstrahlung), the user may wish to risk using a smaller value of l_{max} and thus decrease the time of calculating the S integrals. If it later turns out that l_{max} is too small, the S integrals may be recalculated using a larger value of l_{max} . If the interpolation of S integrals with respect to l is not applied (see Section 1.3.3 and descriptions of parameters No. 1.3.15–18) and parameter “del_S_n” (No. 1.8.3) is zero, then an increase of l_{max} would not require recalculating all numerical integrals: the previously-calculated set of numerical integrals may be reused, because the numerical integrals in such a case are calculated for all values of l up to l_{max} (if the total integrals are calculated using a smaller set of the values of l and if $del_S_n = 0$, then the “_n” file is not deleted after the analytical integration). Since the calculations using MP and QP are much slower than the calculations using DP, one should take a greater “risk” in the case of MP or

QP than in the case of DP (hence $l_{\max_MP} \leq l_{\max}$). If optimization of the precision level is requested and $l_{\max_MP} < l_{\max}$, then the value of l_{\max} is also optimized. In such a case, the parameters l_{\max_MP} and l_{\max} are treated as the limits of variation of l_{\max} (for a more detailed explanation, see the description of parameter No. 1.7.11). If one does not wish to truncate the sum in Eq. (1.1.10), then both l_{\max_MP} and l_{\max} should be set equal to $\max(|K_{\min 1}|, |K_{\max 1}|) + \max(|K_{\min 2}|, |K_{\max 2}|) + 1$, or to any larger number. If $K_{\min 1} = K_{\min 2} = 1$, $isAbs_K1 = isAbs_K2 = 1$ and $K_{\max 1} = K_{\max 2}$ (or, equivalently, $K_{\min 1} = -K_{\max 1} = K_{\min 2} = -K_{\max 2}$ and $isAbs_K1 = isAbs_K2 = 0$), then the range of variation of l in Eq. (1.1.10) is from 0 to $2 * K_{\max 1}$. In the case “accuracy_level=1”, the default value of l_{\max} is equal to $\max(|\kappa_1|_{\max}, |\kappa_2|_{\max})$. In the case “accuracy_level=2”, the default value of l_{\max} is equal to $\max(|\kappa_1|_{\max}, |\kappa_2|_{\max}) + (\min(|\kappa_1|_{\max}, |\kappa_2|_{\max}) / 4)$. The default value of l_{\max_MP} is equal to $l_{\min} + (l_{\max} - l_{\min}) * l_{\max_MP_ratio}$, where the parameter “ $l_{\max_MP_ratio}$ ” is described below.

Note: If the interpolation of S integrals with respect to l is applied (see Section 1.3.3 and descriptions of parameters No. 1.3.15–18), then the value of l_{\max} is not optimized, and its default value is automatically reset to the arithmetic average of the original default value (calculated as explained above) and the value of parameter “ l_{\max_MP} ”.

1.3.14. “ **$l_{\max_MP_ratio}$** ” is interpreted as the ratio $(l_{\max_MP} - l_{\min}) / (l_{\max} - l_{\min})$. If l_{\max_MP} is not specified by the user or if $l_{\max_MP_ratio}$ is non-zero, then the value of l_{\max_MP} will be calculated using the values of l_{\max} and $l_{\max_MP_ratio}$ (if l_{\max_MP} is not specified by the user and $l_{\max_MP_ratio}$ is zero, then $l_{\max_MP_ratio}$ will be reset to the default value). If l_{\max_MP} is specified by the user and $l_{\max_MP_ratio}$ is zero, then the user-specified value of l_{\max_MP} will be used. By default, the value of $l_{\max_MP_ratio}$ is linearly interpolated with respect to k / T_1 from a predefined value at $k / T_1 = 0$ to 1 at $k / T_1 \geq 0.95$. This interpolation has been implemented because it was noticed that in the case of a strongly peaked angular distribution of bremsstrahlung photons the values of the DCS corresponding to large angles ($\theta > 150^\circ$) are especially sensitive to the truncation of the sum (1.1.10) with respect to l , and this effect becomes more pronounced with increasing k / T_1 . The mentioned predefined value of $l_{\max_MP_ratio}$ at $k / T_1 = 0$ is equal to $1/3$. If $l_{\max} - l_{\min} < 80$, then a linear interpolation with respect to $l_{\max} - l_{\min}$ is applied in addition to the mentioned interpolation with respect to k / T_1 , with the value obtained by the latter interpolation used as the minimum value of $l_{\max_MP_ratio}$ (it corresponds to $l_{\max} - l_{\min} = 80$), and with the maximum value of $l_{\max_MP_ratio}$ equal to 1 (it corresponds to $l_{\max} = l_{\min}$). Since the default value of l_{\max_MP} is equal to $l_{\min} + (l_{\max} - l_{\min}) * l_{\max_MP_ratio}$, the mentioned linear interpolation of $l_{\max_MP_ratio}$ with respect to $l_{\max} - l_{\min}$ causes a quadratic dependence of the default value of l_{\max_MP} on $l_{\max} - l_{\min}$. If this dependence has a maximum at $l_{\max} - l_{\min} < 80$, then it is additionally “capped” by reducing it to the value corresponding to $l_{\max} - l_{\min} = 80$. This is done in order to prevent the default value of l_{\max_MP} from increasing after l_{\max} is reduced.

Note: In the case of non-zero photon energy (k), this description of the method of calculating the default value of $l_{\max_MP_ratio}$ is applicable only when $T_1 \leq T1_Kmax_mode_thr$ (the description of parameter No. 8 “ $T1_Kmax_mode_thr$ ” is provided at the end of Section 2). When $T_1 > T1_Kmax_mode_thr$ and $k \neq 0$, the default value of parameter $l_{\max_MP_ratio}$ is equal to 1.

1.3.15. “ **$l_interp1$** ” is the starting point of the interpolation range of l (see Section 1.3.3). If the parity of $l_interp1$ is different from the parity of l needed for a particular pair of κ_1 and κ_2 , then the starting point of the interpolation range corresponding to those κ_1 and κ_2 will be increased by 1. If $l_interp1 = -1$ or $l_interp1 \geq l_{\max}$, then the S integrals will not be interpolated with respect to l . If parameter $l_interp1$ is not explicitly specified by the user, then the mentioned interpolation is applied by default, provided that T_1 , $\kappa_{1\max}$, and $\kappa_{2\max}$ are

sufficiently large. In such a case, the starting point of the interpolation range is set equal to 80. In order to apply the mentioned interpolation by default, the following conditions must be satisfied simultaneously: $T_1 > 3$ MeV, $\kappa_{2\max} + \max(|K_{\min 1}|, |K_{\max 1}|) > 400$, parameter No. 1.3.6 (“isAbs_K2”) is equal to 1, and $l_{\max} > 100$ (if “accuracy_level=1”) or $l_{\max} > 125$ (if “accuracy_level=2”).

Note: If the cubic spline interpolation of the S integrals with respect to l is applied, then the S integral data file created in stage 1 contain only the values of the S integrals corresponding to the knots of the cubic spline. At the start of stage 2 (in the subroutine “Bremsstrahlung”), the missing S integrals are calculated by cubic spline interpolation.

- 1.3.16. “**l_step_incr**” is the increment of the interval between the interpolation breakpoints of l inside the interpolation range (see Section 1.3.3). The default value of this parameter is 2.
- 1.3.17. “**l_step_max**” is the maximum interval between the interpolation breakpoints of l inside the interpolation range (see Section 1.3.3). The default value of this parameter is 58.
- 1.3.18. “**l_k2_thr**” is the value of $|\kappa_2|$ that must be exceeded in order to apply the interpolation with respect to l . That is to say, the mentioned interpolation is never applied when $|\kappa_2| \leq l_k2_thr$. The default value of this parameter is equal to 30.

4.4. Using the alternative set of S integrals, and parameters defining it

As mentioned in Section 1.8, when $T_1 > 1$ MeV, accuracy of the DCS at large angles can be improved by increasing the ratio $|\kappa_1|_{\max} / |\kappa_2|_{\max}$. This implies using a value of $\max(|\kappa_2|)$ smaller than the value of parameter No. 1.3.5 (“Kmax2”). In BREMS, the reduced value of Kmax2 is equal to

$$K_{\max 2}^+ = \min(30, \max(15, K_{\max 2}/4)), \quad (4.4.1)$$

where $K_{\max 2}$ is the original value of parameter No. 1.3.5 (“Kmax2”). Thus, $K_{\max 2}^+$ cannot be greater than 30 or less than 15. This reduction of $K_{\max 2}$ alone would not require calculation of additional S integrals, because all S integrals corresponding to $|\kappa_2| \leq 30$ are typically included in the original set of S integrals, according to the default values of parameters No. 1.3.5 (“Kmax2”), No. 1.3.8 (“k2_breakpoint1”), and No. 1.3.18 (“l_k2_thr”), except when the maximum value l in the original data is less than the theoretical maximum, which is equal to $|\kappa_1|_{\max} + |\kappa_2|_{\max}$ (see also Section 1.3.2 and description of parameters 1.3.12–13 “lmax” and “lmax_MP” in Section 4.3). However, when T_1 is of the order of 10 MeV or greater, an increase of the maximum value of $|\kappa_1|$ may be required, too. This means that an additional set of S integrals must be calculated, corresponding to values of $|\kappa_1|$ inside the interval

$$K_{\max 1} + 1 \leq |\kappa_1| \leq K_{\max 1}^+, \quad (4.4.2)$$

where “ $K_{\max 1}$ ” is the value of parameter No. 1.3.2, and $K_{\max 1}^+$ is a greater value of $\max(|\kappa_1|)$.

The set of S integrals corresponding to the increased ratio $|\kappa_1|_{\max} / |\kappa_2|_{\max}$ will be further referred to as the “alternative” dataset. If the original value of $K_{\max 1}$ is less than the value of $K_{\max 1}^+$, and parameter No. 13 (“S_data”) of the main program (see end of Section 2) is equal to 3 (the default value), then stage 1 is split in two parts: calculation of the original dataset (which also contains the part of the alternative dataset corresponding to $|\kappa_1| \leq K_{\max 1}$), and calculation of the remainder of the alternative dataset (with $|\kappa_1|$ inside the interval defined by Eq. (4.4.2)). This remainder of the alternative dataset is written to the file whose name differs from the original filename by the plus sign (“+”) appended to the original name. If an additional suffix defined by parameter 1.9.2 (“suffix”) is used, then the plus sign is placed immediately after this suffix.

In BREMS, the calculation of $K_{\max 1}^+$ is controlled by five parameters, including three breakpoint values of T_1 (further denoted T^+ , T' , and T'') and two breakpoint values of $\max(|\kappa_1|)$ (further denoted $K_{\max 1}'$ and $K_{\max 1}''$), which are the predefined values of $K_{\max 1}^+$ at $T_1 = T'$ and $T_1 = T''$. The following rules are used:

- (a) if $T^+ < T_1 \leq T'$, then $K_{\max 1}^+$ is obtained by rounding down the original value of parameter $K_{\max 1}$ to the nearest multiple of $K_{\max 2}^+$,

- (b) if $T' < T_1 \leq T''$, then $K_{\max 1^+}$ is obtained by linear interpolation with respect to T_1 between $K_{\max 1^+} = K_{\max 1'}$ at $T_1 = T'$ and $K_{\max 1^+} = K_{\max 1''}$ at $T_1 = T''$, and then rounding down to the nearest multiple of $K_{\max 2^+}$,
- (c) if $T_1 > T''$, then $K_{\max 1^+} = K_{\max 1''}$ (rounded down to the nearest multiple of $K_{\max 2^+}$),
- (d) if $T_1 \leq T^+$, then the alternative calculation is not performed, because the original calculation ensures sufficient accuracy of the final DCS at all angles (in this case, parameter S_data is automatically reset to 1).

The names and default values of the mentioned five parameters are given below.

1.4.1–3. “**T1_Kmax_mode_thr0+**”, “**T1_Kmax_mode_thr1+**”, and “**T1_Kmax_mode_thr2+**” are the three breakpoint values of T_1 defined above: T^+ , T' , and T'' , respectively (in MeV). The default values of these three parameters are equal to 1, 10 and 85, respectively.

1.4.4–5. “**Kmax1_min+**” and “**Kmax1_max+**” are the two breakpoint values of $\max(|\kappa_1|)$ defined above: $K_{\max 1'}$ and $K_{\max 1''}$, respectively. The default values of these two parameters are equal to 500 and 2000, respectively.

4.5. Parameters defining the cutoff radius and other threshold values of the radial coordinate

1.5.1. “**nPoints**” is the maximum number of points used for the numerical integration. Normally, the numerical integration should end when all wave functions have attained their asymptotic form (1.1.18) and (for $IV > 1$ and $Z_i = 0$, or $R_atom \neq 0$) the absolute values of both phase correction integrals become less than the user-specified tolerance. This should happen before the maximum number of points is reached, because otherwise the analytical integration will be insufficiently accurate or will not be performed at all. Consequently, **nPoints** should be set to any sufficiently large number (for example, 1 000 000 000, which is the default value).

1.5.2. “**pr_Bessel**” is the value of $p_2 r$ that must be exceeded in order to start checking periodically if the wave functions have attained the asymptotic form (1.1.18). If $p_2 r < pr_Bessel$, then the numerical solution of the differential equations (1.1.16a,b) will continue without calculating the factor A_κ and the phase shift $\tilde{\delta}_\kappa$ (see Eqs. (1.1.18) and (1.2.1)). If $pr_Bessel < 0$, then it is interpreted as the opposite of the value of r that must be exceeded in order to start calculating A_κ and $\tilde{\delta}_\kappa$. Normally, this parameter should be 0 (this is the default value).

1.5.3. “**pr_transition2**” is the minimum value of $p_2 r$ corresponding to transition to analytical integration. If $pr_transition2 < 0$, then it will be interpreted as the opposite of the minimum value of r where the transition occurs (“**r0_min**”). When all wave functions attain their asymptotic form and (for $IV > 1$, $Z_i = 0$ and $R_atom \leq r0_min$) the absolute values of both phase correction integrals decrease below the tolerance defined by parameter No. 1.5.7, the program will end the numerical integration if the current value of $p_2 r$ is greater than $pr_transition2$. Otherwise, the numerical integration will continue up to the point $r = r0_min = pr_transition2 / p_2$. The value of **r0_min** may be optionally “rounded up” as explained in the description of parameter No. 1.7.4. The default value of this parameter depends on whether parameter No. 1.5.4 (“**R_atom**”, indicating the atomic radius) has been explicitly specified by the user and on whether the photon energy is non-zero. If **R_atom** has not been specified and the photon energy is non-zero, then the default value of **pr_transition2** is $-\max(R', 126/p_2)$, where $R' = 800$ when $T_1 \leq 3$ MeV, and $R' = 1200$ when $T_1 > 3$ MeV (i.e., **r0_min** is equal to either R' or twenty wavelengths of the outgoing electron, whichever is greater). Otherwise, the default value of **pr_transition2** is 0. If $R_atom > r0_min$ (i.e., the potential function is truncated, and the cutoff radius is greater than **r0_min**), then the point of transition to analytical integration coincides with **R_atom**. When $IV=1$ (unscreened point-Coulomb potential) or $Z_i \neq 0$ (an ion), the default value of **pr_transition2** is additionally increased by a factor that decreases with increasing T_1 , and becomes equal to 1 starting from $T_1 = 1$ MeV. The initial (maximum) value of the mentioned

factor corresponds to $T_1 \leq 100$ eV and is equal to 10^4 . The default value of `pr_transition2` is inversely proportional to T_1 when $100 \text{ eV} \leq T_1 \leq 1 \text{ MeV}$ and $IV=1$ or $Z_i \neq 0$.

Note: Parameter “`pr_transition2`” is also used when `appr≤0` for specifying the minimum cutoff radius of the interaction potential. When `appr≤0`, the default value of “`pr_transition2`” is 0 (see also the description of parameter No. 4.5.2 in Section 7.5).

1.5.4. “**R_atom**” is the “atomic radius”, defined as the value of the radial coordinate where the interaction potential $V(r)$ becomes zero, i.e., is “truncated”. If this parameter is zero, then the interaction potential will not be truncated. Although the results obtained in the latter case may be more accurate (provided that the absolute value of parameter No. 1.5.7 is small enough), the computation time may become prohibitively long if the electron energy is greater than 1 MeV and the decrease of the screening function is very slow. Besides, it is usually possible to achieve a negligibly small difference between the results obtained with $R_{\text{atom}} = 0$ and with $R_{\text{atom}} \neq 0$ by a judicious choice of the value of R_{atom} . It should be much greater than the typical distance from the nucleus to the point where the interaction event occurs. The latter distance is approximately equal to the inverse of the minimum momentum transfer [12], which is equal to $q_{\min} = p_1 - p_2 - k$ (see also Section 1.3.5). For example, if $1 / q_{\min}$ is of the order of 10, then the value $R_{\text{atom}} = 500$ should be sufficient to achieve acceptable accuracy. If this parameter is negative, then it is interpreted as the opposite of the factor that must be used for multiplying the inverse minimum momentum transfer in order to calculate the value of R_{atom} . In the latter case, the previous parameter (`r0_min`) “doubles up” as the minimum allowed value of R_{atom} (i.e., if the calculated value of R_{atom} is less than `r0_min`, then R_{atom} is set equal to `r0_min`). The default value of this parameter is **(a)** -20 if $T_1 < 1 \text{ MeV}$, **(b)** -13 if $1 \text{ MeV} \leq T_1 < 20 \text{ MeV}$, or if $T_1 \geq 20 \text{ MeV}$ and $T_2 < 10 \text{ MeV}$, **(c)** -7 if $T_1 \geq 20 \text{ MeV}$ and $10 \text{ MeV} \leq T_2 < 20 \text{ MeV}$, **(d)** -4 if $T_2 \geq 20 \text{ MeV}$. When $IV=1$ (unscreened point-Coulomb potential) or $Z_i \neq 0$ (an ion), the default value of R_{atom} is additionally increased by a factor that decreases with increasing T_1 , and becomes equal to 1 starting from $T_1 = 1 \text{ MeV}$. The initial (maximum) value of the mentioned factor corresponds to $T_1 \leq 100$ eV and is equal to 10^4 . The default value of R_{atom} is inversely proportional to T_1 when $100 \text{ eV} \leq T_1 \leq 1 \text{ MeV}$ and $IV=1$ or $Z_i \neq 0$.

Notes: 1) If this parameter is non-zero, then the phase correction integrals will be calculated only for $r < R_{\text{atom}}$ (according to Eq. (1.2.3)).

2) Even if the wave function has not attained the asymptotic form at $r = R_{\text{atom}}$, the numerical solution algorithm is terminated anyway. In such a case, the phase shift and the normalization factor are calculated on the basis of the values of g_κ and f_κ at the first point satisfying the condition $r \geq R_{\text{atom}}$, and the corresponding uncertainties (range widths) are set to zero.

3) If `r0_min` < R_{atom} , then, as mentioned in the description of parameter No. 1.5.3, the point of transition to analytical integration (r_0) is set equal to R_{atom} . Consequently, at electron energies greater than 1 MeV, the judicious choice of R_{atom} (see above) usually results in a significant reduction of r_0 in comparison with the case when the potential function is not truncated ($R_{\text{atom}} = 0$). Since a decrease of r_0 may cause an increase of the precision level needed to compute the analytical integrals to an acceptable accuracy (and hence a significant increase of the time of the analytical integration), it may be advantageous to specify a value of `r0_min` greater than R_{atom} (or to increase R_{atom}) when the electron energy is greater than 1 MeV (see the description of parameter No. 1.5.3).

4) Parameter “`R_atom`” is also used when `appr≤0`. In this case, the default value of “`R_atom`” is equal to 0 (see also the description of parameter No. 4.5.1 in Section 7.5).

- 1.5.5. “**r0_Kmax_p_min**” is the minimum allowed value of the ratio $r_0 / \max(\kappa_{1\max}/p_1, \kappa_{2\max}/p_2)$, where p_1 and p_2 are the initial and final momenta of the electron, and r_0 is the cutoff radius of the potential function. This parameter helps to ensure numerical stability of the forward recursion used for calculating the values of the spherical Bessel functions corresponding to the argument values $p_1 r_0$ and $p_2 r_0$ (because calculation of $j_n(z)$ with $n > 0$ may be subject to numerical instability if $z < n$). If r_0 is not specified explicitly (using parameter “**R_atom**”), but is calculated from other parameters, and if the calculated value of r_0 is less than $r_{0\min} = r0_Kmax_p_min \cdot \max(|\kappa_{2\max}/p_1|, |\kappa_{1\max}/p_2|)$, then the calculated value of r_0 will be replaced with $r_{0\min}$. The default value of this parameter is equal to 1.1.
- 1.5.6. “**tol_V**” is the maximum allowed value of the screening function at the cutoff radius $r = r_0$. The corresponding value of the radial coordinate is the minimum allowed value of the cutoff radius of the potential function ($r_{0\min}$). If r_0 is not specified explicitly (using parameter No. 1.5.4 “**R_atom**”), but is calculated from other parameters, and if the calculated value of r_0 is less than $r_{0\min}$, then the calculated value of r_0 will be replaced with $r_{0\min}$. By default, the parameter is equal to 10^{-10} in the case of zero photon energy, and to 1 in the case of non-zero photon energy (the latter value is equivalent to absence of any constraints, because the corresponding radial coordinate is equal to 0).
- 1.5.7. “**Q_last**” is the value of the phase correction integrals “**Q(1)**” and “**Q(2)**” that must be exceeded for the transition to analytical integration to occur. In the case of screened or truncated potentials ($IV > 1$ and $Z_i = 0$, or $R_atom \neq 0$), Q is negative and approaches zero when r is increased (see Eqs. (1.2.2), (1.2.3), and (1.2.6b)). Consequently, Q_last should be the opposite of the maximum allowed absolute value of $Q(1)$ or $Q(2)$ at the point of transition to analytical integration. In the case of the Coulomb or partially screened potential ($IV = 1$ or $Z_i \neq 0$, and $R_atom = 0$), the values of $Q(1)$ and $Q(2)$ are never used for determining the point of transition to analytical integration, because in this case Q does not have a limiting value. In order to similarly ignore $Q(1)$ and $Q(2)$ when $IV > 1$ and $Z_i = 0$ or $R_atom \neq 0$, Q_last should be set to zero. When $R_atom = 0$ and $Q_last = 0$, the cutoff radius of the potential function is determined “dynamically”, based on the magnitudes of the ranges of variation of the normalization factor “**A**” and the phase shift “**delta**” (given by parameters No. 1.7.6 and No. 1.7.7). In this case, the cutoff radius is equal to the value of the radial coordinate where the mentioned ranges of variation for all values of κ_1 and κ_2 and for both energies of the electron become less than the specified tolerances “**tol_A**” (parameter No. 1.7.6) and “**tol_delta**” (parameter No. 1.7.7), and the asymptotic expressions of the wave functions (in terms of the spherical Bessel functions) are never used for calculating the S integrals before the cutoff radius is reached (even if the ranges of variation of the estimates of the normalization factors and phase shifts for a particular pair of values of E and κ are less than the corresponding tolerances “**tol_A**” and “**tol_delta**”).
- In the case of a non-zero photon energy, the recommended value of Q_last is from -10^{-10} to -10^{-8} . A larger value of Q_last may have to be used if the electron energy is greater than 1 MeV, or if the decay of the screening function $\tilde{V}(r)$ is very slow, in order to reduce the time of numerical integration, especially if the interaction potential is not “truncated” (see the description of parameter No. 1.5.4). In the case of a non-zero photon energy, the default value of this parameter is -10^{-8} or -10^{-10} , depending on the chosen accuracy level (1 or 2, respectively) defined by parameter No. 1 of the main program (“**accuracy_level**”), which is described in Section 2. In the case of zero photon energy, the default value of this parameter is zero.
- 1.5.8. “**R_atom_delta**” (alias “**R_a_delta**”) is the “extended” atomic radius, where the phase shifts are determined. This extension may be needed because the phase shifts are determined by matching the exact expression of the free-field wave function (a superposition of two spherical Bessel functions, Eqs. (1.1.18)) with the solution of the coupled radial Dirac

equations (1.1.16a,b), and because the spherical Bessel functions of the first kind are calculated by forward recursion, which is numerically unstable at small values of the argument. Another possible reason of increasing R_atom_delta over R_atom is a decrease of the minimum precision level needed for the analytical integration from R_atom_delta to $+\infty$ (in this way, the mentioned precision level can be reduced to double precision, causing a reduction of the duration of analytical integration by one or two orders of magnitude). If $R_atom_delta > R_atom$, then the process of numerical solution of the coupled radial Dirac equations will not be terminated at $r = R_atom$. Instead, it will be continued up to $r = R_atom_delta$, using zero interaction potential ($V(r) \equiv 0$). Consequently, the spherical Bessel functions inside the radial interval $R_atom < r < R_atom_delta$ will be calculated by solving the mentioned equations (1.1.16a,b) (where $V(r) \equiv 0$) rather than by forward recursion. If R_atom_delta is equal to zero (the default value), then it will be reset to $r0_Kmax_p_min * \max(\kappa_{1max}/p_1, \kappa_{2max}/p_2)$, where p_1 and p_2 are the initial and final momenta of the electron. If $R_atom_delta < 0$, then it will also be replaced with the mentioned value, but only if the latter is greater than $|R_atom_delta|$. Otherwise, R_atom_delta will be replaced with $|R_atom_delta|$.

- 1.5.9. “**R_atom_delta+**” (alias “**R_a_delta**”) is the value of the extended atomic radius corresponding to the additional set of S integrals (see also Section 1.8, the beginning of Section 2, and the description of parameter No. 1.5.8 “**R_atom_delta**”). The default value of this parameter is equal to 0.

4.6. Parameters controlling the selection of alternative calculation methods

- 1.6.1. “**pr_transition**” is the value of $p_i r$ ($i = 1, 2$) where the transition from the power series solution in the vicinity of $r = 0$ to the solution method specified by parameter No. 1.6.3 (“**method**”) occurs. This transition occurs independently for both i . When negative, this parameter is opposite to the value of r where the transition occurs for the final electron energy (“**r_transition**”). An additional factor that can cause the transition earlier is a failure for the power series to converge. If $IV = 3$ (interaction potential in tabular format) and $pr_transition = 0$, then $r_transition$ is set equal to the first value of r in the $V(r)$ data table (this is the recommended option for the case $IV = 3$). In the case $IV = 1$ or 2 , the recommended value of this parameter is between 5 and 10 (the value of zero is not allowed in this case). If $IV = 3$ and $pr_transition \neq 0$, then $r_transition$ must be less than the first value of r in the $V(r)$ data table. The default value of this parameter is 0 in the case $IV = 3$, and 10 in the case $IV = 2$ or $IV = 1$.

Note: When the final kinetic energy of the electron is of the order of 1 MeV or greater and this parameter is positive, $r_transition$ may become less than $20 \times r_incr_max$, where “**r_incr_max**” is the maximum allowed increment of r for numerical quadrature (parameter No. 1.7.5). Then the mentioned increment would be decreased automatically, making the numerical integration longer (see also the description of parameter No. 1.7.5). In order to avoid this increase of the computation time, $pr_transition$ should be increased, or $r_transition$ should be specified instead.

- 1.6.2. “**iExact**” is an integer number 0, 1 or 2 indicating whether the exact wave function (expressed in terms of the confluent hypergeometric function) must be used at $r < r_transition$ in the case of the point-Coulomb field (this parameter is ignored when $IV > 1$ or $nuclear_model > 0$). If $IV = 1$ and $iExact = 0$, then in the range of values of r corresponding to $r < r_transition$ the wave function will be expressed in terms of the power series with the coefficients calculated using the recurrence relations derived from Eqs. (1.1.16a,b) (this approach is always applied for $IV > 1$). If $IV = 1$ and $iExact \neq 0$, then the wave function at $r < r_transition$ will be calculated using its exact expression (see [6, Eq. (5.76) and Eq. (5.77)]). [The exact expression of the wave function is not used for greater values of r , because the evaluation of the confluent hypergeometric function is

sufficiently fast and accurate only for relatively small argument values.] If $IV = 1$ and $iExact = 2$, then, in addition to the above, the exact phase shift (1.1.23) will be used in the asymptotic expression of the wave function (1.1.18). [The value of $\tilde{\delta}_\kappa$ calculated according to Eq. (1.1.23) is adjusted by adding $2\pi n$, where n is an integer number, so that the final value of $\tilde{\delta}_\kappa$ is between $-\pi$ and π .] Since the values of the phase shifts are sufficient to calculate $\lim_{k \rightarrow 0}(kS_1)$ and $\lim_{k \rightarrow 0}(kS_2)$ (see the end of Section 1.2), the availability of the simple analytical expression of the exact phase shifts means that it is not necessary to solve the system of ODEs (1.1.16a,b) numerically in the case $k = 0$, $IV = 1$, $iExact = 2$. In the case $k \neq 0$, $IV = 1$, $iExact = 2$, the mentioned system is solved (because the functional form of the wave functions is needed in the entire integration range of the numerical integrals), and the exact value of the phase shift is used as an additional “test” point for evaluating the range of phase shifts (see also Section 1.2 and Section 1.4). This causes an increase of the effective range if the exact phase shift is outside of the true range of the values of $\tilde{\delta}_\kappa$ obtained from the analysis of the wave functions. The default value of parameter “iExact” is 0.

- 1.6.3. “**method**” controls the method of the numerical solution of the system of ODEs (1.1.16a,b). In the case “method=1”, the Hamming’s modified predictor-corrector method is used. In the case “method=2”, the Runge-Kutta formula pair (7,8) is used. In the case “method=3”, the power-series solution method is used. The default value of this parameter is 3. **Note:** All these methods are essentially equivalent in terms of the accuracy. The power-series solution method is usually the fastest, and the Runge-Kutta method is the slowest. The Runge-Kutta and the power-series solution methods are less likely to cause a premature termination of the solution routine due to a numerical error when κ_1 and κ_2 is too large. Sometimes, this is a disadvantage, because such an error condition may be used as an indicator that the maximum value of κ_1 or κ_2 should be reduced, causing a reduction of the total calculation time (due to a reduction of the number of S integrals and of the number of terms in the truncated series (1.1.4) and (1.1.5)). In the case “method=1”, such an error occurs when the number of bisections of the initial increment becomes greater than 10.
- 1.6.4–5. “**Jtest_interval**” and “**Jtest_period**” are used to specify the interval (in integration steps) of measuring the speed of calculation of the set of spherical Bessel functions $j_l(kr)$ used as a factor in the integrands of the S integrals (see Eqs. (1.1.15a,b)), and the period of this test (in units of $Jtest_interval$ integration steps). This test is performed for the purpose of choosing one of the two possible calculation algorithms: either the method of backward or forward recursion, or the power-series method (see Section 1.2). If $Jtest_interval$ is positive, then the method corresponding to the smallest time of $Jtest_interval$ consecutive integration steps will be chosen, and this comparison will be repeated after $Jtest_period * Jtest_interval$ integration steps. If $Jtest_interval = 0$, then only the recursion method will be used. If $Jtest_interval$ is equal to -1 or to a very large positive number, then only the power-series method will be used. In any case, the power-series method will be applied only after the initial part of the solution of the coupled radial Dirac equations (i.e., after termination of the special case of the power-series algorithm applied to the electron wave functions at small values of the radial coordinate), and only after the estimates of all required spherical Bessel functions calculated by recursion become non-zero. The default value of parameter “ $Jtest_interval$ ” is -1 (i.e., the Bessel function $j_l(kr)$ is calculated using the power-series method by default, except at the smallest values of r , where the recursion algorithm is always used). The default value of parameter “ $Jtest_period$ ” is 20.
- 1.6.6–7. “**nmult_ratio**” and “**nterms3_max**” control application of an alternative method of numerical quadrature (described in the next paragraph) during calculation of the initial part of S integrals (from 0 to the cutoff radius r_0). Parameter “ $nmult_ratio$ ” is the maximum allowed ratio of the total number of multiplications using the alternative method and using

the original method (the value of `nmult_ratio` should be less than 1, because the aim is to *reduce* the number of multiplications in comparison with the original method). Parameter “`nterms3_max`” is the maximum allowed degree of the power-series expansion of spherical Bessel functions $j_l(kr)$, which are used in the integrands of S integrals (1.1.15a,b). If a sufficient accuracy of the power-series expansion of $j_l(kr)$ cannot be achieved with the specified maximum degree inside the current radial interval of 20 breakpoints, then the original method will be applied in this interval. If either `nmult_ratio` or `nterms3_max` is equal to 0, then the alternative method will never be applied. The default value of `nmult_ratio` is equal to 0 (i.e., the alternative method is not applied by default). The default value of `nterms3_max` is equal to 20.

The original method requires calculating the value of the spherical Bessel function $j_l(kr)$ in the integrands of the integrals defined by Eqs. (1.1.15a,b) for each breakpoint of the numerical integration grid, and then multiplying the calculated value of $j_l(kr)$ with the corresponding values of $g_{\kappa_1}(r)$ and $f_{\kappa_2}(r)$ (in the case of S_1 integrals), or $g_{\kappa_2}(r)$ and $f_{\kappa_1}(r)$ (in the case of S_2 integrals). Afterwards, those products are combined according to the 10th order Newton-Cotes formula, and the result is added to the current value of each S integral. The alternative method is based on determining the coefficients of the power-series expansion of $j_l(kr)$ with a relatively small value of the maximum degree (n_{\max}) inside a radial interval spanning a sequence of 20 breakpoints, then calculating the auxiliary integrals over the same interval with $j_l(kr)$ in Eqs. (1.1.15a,b) replaced by x^n , where x is the offset from the start of the mentioned radial interval and n varies from 0 to n_{\max} , then linearly combining those auxiliary integrals using the mentioned coefficients, and finally adding the result to the stored intermediate values of the S integrals. The mentioned auxiliary integrals are calculated using the 10th order Newton-Cotes formula (which is also used in the case of the original method). In the case of a large value of l_{\max} (much greater than 100), the alternative method may cause a significant reduction of the total number of multiplication operations that have to be performed during the numerical quadrature, because the value of n_{\max} is typically between 10 and 20, i.e., much less than l_{\max} . Although the alternative method involves additional multiplications due to the mentioned additional step of linear combination of the auxiliary integrals at the end of each cycle of 20 breakpoints, the total number of multiplications may still be reduced, because n_{\max} is typically less than 20 (n_{\max} may even be less than 10, if the photon energy k is small enough). However, at the time of this writing, testing has not shown any improvement in performance when the alternative method is applied (even when the total number of multiplications is reduced by half, the duration of numerical quadrature using the alternative method is greater than in the case of the original method). This lack of improvement may be caused by alternating accesses to multiple large double-precision data arrays when computing the mentioned linear combination of the auxiliary integrals, whereas the original method always involves sequential access to only one large double-precision data array at a time, with the array index changing in increments of 1 (thus, the alternative method may be more impacted by the memory latency of the computer).

4.7. Parameters controlling the accuracy of intermediate calculations

- 1.7.1. “`nterms_max`” (alias “`n_terms_max`”) is the maximum degree of the power-series expansion of the wave function, i.e., the maximum number of terms in that expansion, excluding the term of degree 0. The default value of this parameter is 100.
- 1.7.2. “`nterms_max_J`” (alias “`n_terms_max`”) is the maximum degree of the power-series expansion of the spherical Bessel function $j_l(kr)$, which is used in the integrand of S integrals (see Eqs. (1.1.15a,b)). This parameter is used only when the mentioned spherical Bessel function is calculated by the power-series method, rather than by recursion (see the description of parameters No. 1.6.4–5). The default value of this parameter is 150.
- 1.7.3. “`step1`” is the increment of p_1r for solution of the differential equations using the Hamming’s modified predictor-corrector algorithm (i.e., when the option “`method=1`” is used). The recommended value of this parameter is $\leq 10^{-3}$, and the default value is 10^{-3} .
- 1.7.4. “`pr_incr`” is the increment of p_1r for numerical quadrature using the 10th order Newton-Cotes formula. `pr_incr` should exceed `step1` at least by a factor of 2. The recommended value

is ≤ 0.1 . If this parameter is specified with the minus sign, then the value of r_0 (the point of transition from the numerical integration to the analytical integration) will be “rounded up” i.e., the region of the numerical integration will be extended up to the value of the radial coordinate equal to 10^n , $2 \cdot 10^n$ or $5 \cdot 10^n$ in relativistic units, where n is an integer number. This option is useful for creating a library of cross sections for multiple chemical elements, because the integral from r_0 to ∞ (the “analytical” integral) is expressed as a linear combination of the four integrals (1.2.7), and each of the latter four integrals depends only on r_0 , T_1 and k (but not on the atomic number Z). Thus, if the values of r_0 , T_1 and k are exactly the same for different Z , then it will be possible to reuse the values of the mentioned four integrals and thus to skip the stage of the analytical integration for some combinations of Z , T_1 and k (in such a case, a change of Z would require only to recalculate the coefficients of the mentioned linear combination, which depend on the phase shifts). The default value or parameter “pr_incr” is 0.1.

1.7.5. “r_incr_max” is used to define the maximum allowed increment of r for numerical quadrature. This increment may be either specified explicitly or calculated from the rate of change of the screening function (1.1.17) near $r = 0$:

- (a) If r_incr_max is positive, then it is interpreted as the mentioned maximum allowed increment of r . r_incr_max must be chosen so that the relative change of the interaction potential over this distance is much less than 1 (otherwise the numerical quadrature may be insufficiently accurate). An additional requirement is that r_incr_max cannot be greater than $0.05 \times r_{\text{transition}}$, where “r_transition” is the mentioned point of transition from the power-series solution in the vicinity of $r = 0$ to the algorithm specified by parameter No. 1.6.3 (“method”) for the final electron energy (see the description of parameter No. 1.6.1). If r_incr_max does not conform to this requirement, then it is decreased to $0.05 \times r_{\text{transition}}$, and pr_incr is decreased proportionally (if pr_incr becomes less than $2 \times \text{step1}$, then step1 is set equal to $0.5 \times \text{pr_incr}$). The actual increment of r is subsequently set equal to $r_{\text{incr}} = \min(\text{pr_incr}/p_1, r_{\text{incr_max}})$. If r_incr is decreased in comparison with pr_incr/ p_1 (i.e., if r_incr_max is less than pr_incr/ p_1), then both pr_incr and step1 are decreased proportionally. The recommended initial value of this parameter is ≤ 0.1 .
- (b) A negative value of parameter “r_incr_max” is interpreted as the opposite of the maximum allowed absolute change of the screening function (delta_V_series_max) near $r = 0$, which must be used for calculating the initial value of the integration step size and also for its automatic adjustment inside the interval of power-series solution in the vicinity of $r = 0$, i.e., at $r < r_{\text{transition}}$, where “r_transition” is the value of the radial coordinate corresponding to the transition from the power-series solution in the vicinity of $r = 0$ to the algorithm specified by parameter No. 1.6.3 (“method”). In this case, the maximum allowed initial value of the integration step (r_incr_max) is initially set to pr_incr_init/ p_1 , where “pr_incr_init” is the initial value of parameter No. 1.7.4 (“pr_incr”), and then r_incr_max is doubled or halved iteratively until the optimum value is found. This value of r_incr_max is subsequently used to set the initial value of the integration step size “r_incr”: if r_incr (which is initially set to pr_incr_init/ p_1) is greater than r_incr_max, then the initial value of r_incr will be set equal to r_incr_max. Afterwards, the value of r_incr may be increased automatically, because this increase is capped only by the value of pr_incr_init* $i\text{Run}/p_1$ and (at $r < r_{\text{transition}}$) by the value of $0.05 \times r_{\text{transition}} \times i\text{Run}$, where “iRun” is equal 1 or 2 for the initial or “test” numerical integration, respectively. The mentioned automatic increase of r_incr is controlled by parameter No. 1.7.8 (“delta_V_max”) at $r > r_{\text{transition}}$, or by the value of delta_V_series_max at $r < r_{\text{transition}}$ (in the latter case, the function whose rate of change is being checked is the screening function rather than the interaction potential).

The default value of parameter “r_incr_max” is -0.01 .

1.7.6–7. “**tol_A**” and “**tol_delta**” are, respectively, the maximum allowed relative range of the last 10 calculated values of the normalization factor A_κ and the phase shift $\tilde{\delta}_\kappa$ needed to switch from the numerical solution using the algorithm specified by parameter No. 1.6.3 (“method”) to the approximate phase-shifted free-space solution (1.1.18), respectively. When $\kappa < 0$, the relative change of the phase shift is based on the value of $\tilde{\delta}_\kappa - (\pi/2)$ instead of $\tilde{\delta}_\kappa$, because $\tilde{\delta}_\kappa$ approaches $\pi/2$ at large negative values of κ if the screening function approaches zero at $r \rightarrow \infty$. The parameter **tol_delta** may be negative. Then it will be interpreted as the opposite of the maximum allowed *absolute* range of $\tilde{\delta}_\kappa$ (in radians). If parameter No. 1.5.4 (“**R_atom**”) is zero, then the recommended value of **tol_A** is from $2 \cdot 10^{-9}$ to 10^{-7} , and the recommended value of **tol_delta** is from $-2 \cdot 10^{-9}$ to -10^{-7} (a smaller value of **tol_A** or **tol_delta** may cause numerical difficulties, resulting in a failure to attain the asymptotic form (1.1.18)). If parameter “**R_atom**” is non-zero and parameter No. 1.6.3 (“method”) is equal to 3, then both **tol_A** and **tol_delta** are equal to zero by default. If **R_atom** is zero, or if “method” is not equal to 3, and the photon energy (“**Ep**”) is non-zero, then the default value of **tol_A** is 10^{-7} or $2 \cdot 10^{-9}$, depending on the chosen accuracy level (1 or 2, respectively) defined by parameter No. 1 of the main program (“**accuracy_level**”), which is described in Section 2. The corresponding default value of **tol_delta** is -10^{-7} or $-2 \cdot 10^{-9}$, respectively. If **R_atom** is zero, or if “method” is not equal to 3, and the photon energy (“**Ep**”) is zero, then the default values of parameters **tol_A** and **tol_delta** do not depend on the accuracy level and are equal to $2 \cdot 10^{-9}$ and $-2 \cdot 10^{-9}$, respectively. In the case of an ion (i.e., when parameter “**Zi**” is non-zero, or when parameter “**IV**” is equal to 1), the mentioned default values of parameters **tol_A** and **tol_delta** are additionally increased by a factor equal to $\max(5000 \cdot |\text{Zi}|/Z, 1)$, where “**Zi**” is the ion charge in units of the elementary charge, and Z is the atomic number. In the case “**IV=1**”, the mentioned factor is the same as with $\text{Zi} = Z$.

Note: The number of roughly equidistant values of r where A_κ and $\tilde{\delta}_\kappa$ are calculated is stored in the integer variable “**ntest**”, and the approximate interval between the adjacent values of $p_1 r$ corresponding to the mentioned “test” values of r (i.e., the period of updating A_κ and $\tilde{\delta}_\kappa$) is stored in the integer variable “**d_pr_test0**” (at the time of this writing, **ntest** = 10 and **d_pr_test0** = 50). These “test” values of r are the same for all wave functions. The updates of the average values of the normalization factors A_κ and the phase shifts $\tilde{\delta}_\kappa$ and the calculation of their ranges of variation are done at two alternating intervals of the radial coordinate r : each odd-numbered update is done after an interval of $(n_1 + 0.5)\pi/p_1$, and each even-numbered update is done after an interval of $(n_2 + 0.5)\pi/p_2$, where n_1 and n_2 are integers, which are chosen so that both those intervals are approximately equal to $\text{d_pr_test0} / p_1 = 50 / p_1$. Those values of the update periods have been chosen in order to maximize the cancellation of the oscillating term in the normalization factors and the phase shifts (see Section 1.2), and thus to improve the accuracy of the mentioned average values (the radial period of the mentioned oscillations is equal to π / p).

1.7.8. “**delta_V_max**” controls the option of doubling the size of the integration step automatically if it is less than $0.5 \cdot \text{pr_incr_init} \cdot i\text{Run} / p_1$, where “**pr_incr_init**” is the initial value of parameter No. 1.7.4 (“**pr_incr**”) and “**iRun**” is equal 1 or 2 for the initial or “test” numerical integration, respectively, and also less than half of the distance corresponding to a predefined value of the relative decrease of the interaction potential $V(r)$. Enabling this option causes a reduction of the time of numerical integration at low energies (especially in the case of the point-Coulomb potential). The value of parameter “**delta_V_max**” is interpreted as the mentioned maximum relative decrease of $V(r)$. This parameter is used only

outside of the interval of the initial power-series solution, i.e., in the range of values of r where the wave functions corresponding to all values of κ_1 and κ_2 are calculated either by iterative solution of the coupled radial Dirac equations (using the method specified by parameter No. 1.6.3) or by evaluating the asymptotic expressions (1.1.18). If `delta_V_max` is zero, then the integration step will be fixed outside of the interval of the initial power-series solution. Inside the interval of the initial power-series solution, the size of the integration step is controlled by parameter No. 1.7.5 “`r_incr_max`” (see above). The default value of parameter “`delta_V_max`” is 0.01.

- 1.7.9. “**acc_fact**” is the modification factor to be applied to the four parameters controlling the accuracy of the numerical solution of the coupled radial Dirac equations (`pr_incr`, `r_incr_max`, `step1` and `delta_V_max`). I.e., the default or user-specified values of the mentioned four parameters are additionally multiplied by the mentioned factor, yielding the final values of those four parameters. The default value of parameter “`acc_fact`” is 1 (i.e., no additional modification is applied).
- 1.7.10. “**j_QP**” is an integer number 0, 1, or 2, which defines the way the quadruple-precision (QP) arithmetic must be used during the numerical quadrature when calculating the spherical Bessel function of the first kind $j_l(kr)$, which is used as a factor in the integrands of the S integrals (1.1.15a,b), by the method of backward or forward recursion. If `j_QP`=0, then QP will not be used. If `j_QP`=1, then QP will be used for calculating $j_l(kr)$ at $kr \leq l_{\max}$ (where $j_l(kr)$ is calculated by backward recursion), but not at $kr > l_{\max}$ (where $j_l(kr)$ is calculated by forward recursion). If `j_QP`=2, then QP will always be used for calculating $j_l(kr)$ by recursion. The default value of parameter “`j_QP`” is 2. **Note:** This parameter has no effect when the default method of calculating $j_l(kr)$ (the power-series method) is applied (see also the description of parameters No. 1.6.4–5).
- 1.7.11. “**ndp**” is the approximate number of significant digits used for calculation of the analytical integrals (the “precision level”). Double precision is indicated by `ndp` = 15 – 21, quadruple precision is indicated by `ndp` = 22 – 36, multiple precision is indicated by `ndp` ≥ 37. When `ndp` < 0, it is the opposite of the initial number of digits, and the program will attempt to “optimize” the precision level as explained in Section 1.3.1. I.e., if it is determined that the current precision level is not sufficient to ensure the precision of at least 6 significant digits in the final values of the four integrals (1.2.7) corresponding to the largest value of the sum $N_1 + N_2 + l$, then the program will attempt to reduce the precision level until the accuracy of the first six significant digits is ensured (the latter number of digits can be changed by changing parameter No. 1.7.12 “`tol_test_a`”). In addition, if `lmax_MP` < `lmax` and the interpolation of S integrals with respect to l is not applied (see Section 1.3.3 and descriptions of parameters No. 1.3.15–18), then the value of l_{\max} will be optimized, too, i.e., it will be decreased in steps of $\max(0.1(l_{\max} - l_{\min}), 5)$ starting with “`lmax`” until double precision becomes sufficient, or until a user-specified minimum value of l_{\max} (“`lmax_MP`”) is reached (the previously mentioned optimization of the precision level will be performed for each value of l_{\max}). If `ndp` = 0, then the analytical integration will not be performed, and only the file with the numerical integrals (file name suffix “_n”) will be created. In order to extract the numerical integral data from an existing complete file and to create the corresponding “_n” file, the options `ndp` = 0 and `iSkip` = -2 must be used (see the description of parameter No. 1.9.8 “`iSkip`” in Section 4.9). If `ndp` > 0, then the specified precision level will be used. When `ndp` is positive, it cannot be less than 15 or greater than 1000. When `ndp` is negative, it cannot be greater than -22 or less than -1000. When $\min(T_2, k) \leq 100$ keV, the default value of this parameter is -300. Otherwise, the default value of this parameter is -100.

Note: In the case of large values of $|K_{\max 1}|$, $|K_{\max 2}|$ and `lmax`, multiprecision calculations may require a prohibitive amount of memory (this amount does not depend on the precision level used, as long as the latter corresponds to the MP mode, i.e., more than 29 significant digits). For example, if $|K_{\max 1}| = |K_{\max 2}| = l_{\max} = 100$ and the other

parameters are equal to the default values, then approximately 5 GB will be needed for calculating all S integrals using MP, and if $|K_{\max 1}| = |K_{\max 2}| = l_{\max} = 150$, then approximately 15 GB of memory would be needed in MP mode. The smallest absolute value of ndp corresponding to the MP mode is 37. Consequently, in order to ensure that the program never attempts to allocate such amount of memory and quits with an error message after determining that quadruple precision is not sufficient, ndp must be set equal to -37 .

- 1.7.12. “**tol_test_a**” indicates the relative error tolerance for analytical integration (from the cutoff radius r_0 to $+\infty$) at the largest values of $|k_1|$, $|k_2|$ and l , when optimization of the precision level is performed (i. e., when $ndp < 0$). The default value of this parameter is equal to 10^{-6} . *Note:* All versions of BREMS prior to v1.5.8.0 used multiple precision arithmetic with precision of 22–23 significant digits as a substitute for double precision (15–16 significant digits) during optimization of the precision level (i.e., when $ndp < 0$). Consequently, the mentioned default value of **tol_test_a** is approximately equivalent to the error tolerance of 10^{-13} used in BREMS prior to v1.5.8.0 when optimization of precision level was performed (the current version of BREMS does not substitute MP for DP during the mentioned optimization).

4.8. Parameters controlling the type and number of datasets to be created

- 1.8.1. “**iTestRun**” indicates if the test numerical integration mentioned in Section 1.4 (with all tolerances and step sizes increased by a factor of 2) must be performed. If this parameter is positive, then the test integration will be performed, and if it is 0 or negative, then the test integration will not be performed (see also Section 1.4). In addition, this parameter is used for creating a file with the integrals of the products of three spherical Bessel functions and r^2 from r_0 to ∞ (the integrals S_{11} , S_{12} , S_{21} and S_{22} , defined by Eqs. (1.2.7)), and for loading the values of those integrals from an existing file. Unless changed by the user, the name of this file is formed by combining the prefix “**S_integrals_**” and the values of the incident electron energy (T_1), bremsstrahlung photon energy (k), the lower bound of the integrals (r_0), and the suffix “**_a**”. Consequently, this file will be called the “**_a**” file. In order to skip the numerical integration and create the “**_a**” file, this parameter must be set equal to -2 . In order to calculate the second part of the S_1 and S_2 integrals by combining the values of the S_{ij} integrals ($i, j = 1, 2$) loaded from an existing “**_a**” file, this parameter must be set equal to 2 or -1 (in the first case, the test numerical integration will be performed, and in the second case it will not be performed). The name of an existing “**_a**” file is defined using parameters No. 1.9.4–6. If there are several “**_a**” files with names differing from the specified name only by the suffix “**_1**”, “**_2**”, ..., “**_999**” at the end, then the data will be read from all those files, too (if there is some overlap between the data stored in different files, then the newly loaded data replace the data that were loaded previously).

In the case $k = 0$, only the options “**iTestRun=0**” and “**iTestRun=1**” are allowed. Since the S integrals are not calculated numerically in the case $k = 0$ (see the end of Section 1.2), the option “**iTestRun=1**” is applied in this case only to the process of solving the coupled radial Dirac equations (1.1.16a,b). I.e., when **iTestRun=1**, the system of ODEs is solved using two sets of computational tolerances and step sizes. Thus, two sets of phase shifts and normalization factors are obtained. The differences of the corresponding phase shifts and normalization factors in the mentioned two sets are used for estimating their uncertainties.

The default value of parameter “**iTestRun**” is 1.

- 1.8.2. “**j_file**” controls an option to create or use the binary “**_j**” file with the values of the spherical Bessel function of the first kind $j_l(kr)$, which is used as one of the factors in the integrand of the S integrals (1.1.15a) and (1.1.15b). Loading values of $j_l(kr)$ from this file (instead of calculating them at each step of the numerical integration) may improve the

performance when the S integrals are calculated for different intervals of $|\kappa_1|$ before merging them into a single dataset (see Section 4.10). This improvement is achieved by eliminating the overhead caused by redundant recalculations of $j_l(kr)$. The name of the “_j” file is constructed as the name of the “_n” file, with the only difference in the last character (“j” instead of “n”) and absence of the additional numerical suffix. The allowed values of parameter “j_file” are the following:

- 0 – do not use the “_j” file,
- 1 – only create the “_j” file,
- 2 – load values from the “_j” file created previously.

The default value of parameter “j_file” is equal to 0 (i.e., the “_j” file is not created or used by default).

- 1.8.3. “del_S_n” is a “switch” (1 or 0) indicating if the file with the numerical integration data (the “_n” file) must be deleted after a successful calculation of the total S integrals (from 0 to ∞). The default value of this parameter is 1, indicating deletion of the “_n” file.

4.9. Parameters defining the names of input and output files, and the conditions for overwriting

- 1.9.1–2. “prefix” and “suffix” are, respectively, the character strings that must be inserted at the beginning and at the end of the name of the file with the S integral data. The file name suffix does not include the extension (the file name extension is always “.dat”). The file name prefix may include the folder name (folder names must be terminated with the slash ‘/’). If parameter No. 1.9.1 is the empty string (specified by writing a space after “prefix=”), then no prefix will be used, and the file with the S integral data will be created in the current folder. If parameter No. 1.9.2 is the empty string, then no suffix will be used. In order to specify an arbitrary name, parameter No. 1.9.1 must be the period ‘.’, and parameter No. 1.9.2 must be the name of the file (possibly with the folder name, and without the extension “.dat”). If parameter No. 1.9.1 is not the period ‘.’, then the default name (with the specified prefix and suffix) will be used. In absence of the prefix or the suffix, the default name has the following format: “S_integrals_Z_T.TE±XX_k.kkkE±YY.dat”, where “Z” is the atomic number consisting of 1, 2 or 3 digits, “T.TE±XX” is the kinetic energy of the incident electron (MeV) rounded to 2 significant digits in scientific notation, and “k.kkkE±YY” is the energy of the bremsstrahlung photon (MeV) rounded to 4 significant digits in scientific notation (“E±XX” and “E±YY” are the respective decimal exponents). If parameter No. 1.8.1 (“iTestRun”) is equal to -2 , then the default name format is “S_integrals_T.TE±XX_k.kkkE±YY_r.rE±PP_a.dat”, where “r.rE±PP” is the lower bound of the integrals (1.2.7) rounded to 2 significant digits in scientific notation (“E±PP” is the decimal exponent). By default, parameters “prefix” and “suffix” are equal to the empty string.

- 1.9.3–6. “Ep00”, “r_fileName”, “prefix0”, and “suffix0” (respectively) are needed only in the case of zero photon energy, when the phase shifts have to be loaded from a data file corresponding to an earlier calculation rather than calculated by solving the system of ODEs (1.1.16a,b), or when the integrals from r_0 to ∞ must be calculated by combining the values of the S_{ij} integrals ($i, j = 1, 2$) defined by Eq. (1.2.7), which are stored in an existing “_a” file. These four parameters define the name of the phase shift data file or the “_a” file. In the case of zero photon energy, parameter No. 1.9.3 is the photon energy (MeV) used for creating the phase shift data file, or the opposite of its ratio to the incident electron energy. If $k = 0$ and parameter No. 1.9.3 has not been explicitly specified, then the program will calculate the phase shifts by solving the system of ODEs (1.1.16a,b) instead of loading the phase shifts from file. Otherwise, it will be assumed that the atomic number, incident electron energy and the type of the interaction potential used for creating the phase shift data file are the same as specified by parameters No. 1.1.1, No. 1.1.2, and No. 1.1.5. In the case

of non-zero photon energy and $iTestRun = 2$ or -1 (i.e., when these parameters define the name of an existing “_a” file), parameter No. 1.9.4 is the value of the lower integration bound (r_0) that must be used to form the names of the “_a” files (assuming that they are formed in the default manner). If this parameter is zero, then the file names will be formed using the actual value of r_0 , which may be calculated by the program or specified by parameter No. 1.5.3. If the names of the phase shift data file or the “_a” files have been formed in the default manner (see the description of parameters No. 1.9.1 and No. 1.9.2), then parameters No. 1.9.5 and No. 1.9.6 are used to specify those prefix and suffix, respectively. They are interpreted in the same way as parameters No. 1.9.1 and No. 1.9.2 described above. In particular, if parameter No. 1.9.5 is the period ‘.’, then parameter No. 1.9.6 must specify the full name of the phase shift data file or the “_a” file (parameter No. 1.9.3 or No. 1.9.4 is ignored in this case). There is only one difference in treatment of parameters No. 1.9.5 and No. 1.9.6 in comparison with treatment of parameters No. 1.9.1 and No. 1.9.2: if the name of the output file is formed in the default manner, then the default values of parameters No. 1.9.5 and No. 1.9.6 are equal to the specified values of parameters No. 1.9.1 and No. 1.9.2, respectively (rather than to the empty string). Otherwise, the default values of parameters No. 1.9.5 and No. 1.9.6 are equal to the empty string. The default value of parameter `r_fileName` is 0.

- 1.9.7. “**start_suffix**” is an integer number from 0 to 999 indicating the starting value of the additional suffix “_<number>” that is automatically appended to the name of the output file (a value of 0 means that there will be no additional suffix; see also the description of parameter No. 1.9.8). The default value of this parameter is 0.
- 1.9.8. “**iSkip**” defines the actions that must be taken when a data file with the current name already exists. The allowed values of this parameter are 0, ± 1 , ± 2 , and -3 . If this parameter is equal to 0 and a file with the current name already exists, then the output file name will be modified by appending a suffix “_1”, or “_2”, ..., or “_999”. A value of 1 indicates that processing must be skipped after determining that a data file with the original name already exists (this applies both to the complete file and to the file with the numerical integrals, i.e., the “_n” file). A value of 1 is useful for resuming an interrupted batch run. A value of -1 indicates that the data file must be overwritten if it exists. A value of 2 indicates that the numerical integral data must be loaded from the existing “_n” files if there are no existing complete files (otherwise it is equivalent to 1, i.e., no processing). A value of -2 is equivalent to $+2$ if there is no existing complete file, otherwise it indicates that the complete file must be overwritten after extracting the numerical integrals from the existing “_n” file or from the complete file if there is no “_n” file. In order to extract the numerical integral data from an existing complete file and to create the corresponding “_n” file, the options `ndp = 0` and `iSkip = -2` must be used (“ndp” is set by parameter No. 1.7.11). The option “`iSkip=-3`” differs from “`iSkip=-2`” in that an existing complete file is not overwritten. Instead, a new file with an additional suffix “_1”, “_2”, etc is created (as in the case “`iSkip=0`”). If there is no complete file, then the option “`iSkip=-3`” is equivalent to “`iSkip=-2`” or “`iSkip=2`”. If `iSkip` is equal to -3 , then, in order to load the numerical integrals from files, the “_n” file or the complete file without the subscript (“_1”, “_2”, etc.) in the file name must exist (otherwise, the numerical integrals will be calculated instead of being loaded from files, even when the “_n” files or the complete files with subscripts “_1”, “_2”, etc. are available). In the case of zero photon energy, `iSkip` cannot be equal to ± 2 or -3 (in this case, the name of the file with the phase shift data must be specified using parameters No. 1.9.3 and No. 1.9.5–6). If the numerical S integral data have to be loaded from existing files and there are several files with names differing from the specified name only by the suffix “_1”, “_2”, ..., “_999” at the end, then the data will be read from all those files, too (if there is some overlap between the data stored in different files, then the newly

loaded data replace the data that were loaded previously). The default value of this parameter is -1 .

1.9.9–10. “**update_n**” and “**prefix_suffix_n**” control an alternative method of processing the available “_n” data files (see also the description of parameter No. 1.9.8 “iSkip”). If parameter “update” is equal to 1 or 2 and there is no request to read the numerical S integral data from pre-existing “_n” or complete files (i.e., if parameter “iSkip” is not equal to ± 2 or -3), or if there are no “_n” or complete files at the indicated location, then the program will attempt to load the numerical integrals from the data files with the names defined by prefix-suffix pairs listed in the file whose name is given by parameter “prefix_suffix_n”. The mentioned data files may be either “_n” files or complete files. If some of the required numerical integrals are missing, then only those integrals will be calculated (unlike in the case “iSkip= ± 2 ” or “iSkip= -3 ”, when the data files must contain *all* needed numerical integrals), and the final “_n” and complete files will contain both the loaded numerical integrals and the calculated numerical integrals. If there are no missing numerical integrals, then the numerical integration will not be performed (only the coupled radial Dirac equations will be solved), and the final “_n” and complete files will contain the same numerical integrals that were loaded at the start of the current run. The first non-empty line of the file whose name is indicated by parameter “prefix_suffix_n” must contain the number of prefix-suffix pairs. The second non-empty line must contain the first prefix, the third non-empty line must contain the first suffix, the fourth non-empty line must contain the second prefix, etc. (i.e., even-numbered non-empty lines contain prefixes, and the odd-numbered non-empty lines contain suffixes). If a prefix or suffix is absent, then it must be indicated by two single quotes ". If a prefix or suffix contains spaces, then it must be enclosed by single quotes. Empty lines are ignored. The prefix may include the folder name, and the suffix may end with “_n”, which indicates that the data file is an “_n” file (containing the results of integration from 0 to r_0). If there are several files with names differing from the specified name only by the additional suffix “_1”, “_2”, ..., “_999” at the end, then the data will be read from all those files, too (if there is some overlap between the data stored in different files, then the newly loaded data replace the data that were loaded previously). In the case “update_n=2”, absence of a file corresponding to a particular prefix-suffix pair is not treated as a terminal error (only a warning is displayed). If parameter “update_n” is equal to 1 and a required file is not found or is empty, then the program will quit with an error message. If the value of parameter “update_n” is specified with the minus sign, then the original file will be deleted after a successful update. The default value of parameter “update_n” is 0 (i.e., the program does not attempt to load the data files listed in the file indicated by parameter “prefix_suffix_n”, and the latter parameter is ignored by default). The default value of parameter “prefix_suffix_n” is the empty string, which means that it must be specified by the user if parameter “update_n” is assigned a non-zero value.

4.10. Parameters controlling the splitting of S integral data into several subsets

Since BREMS has the capability to load the S integral data from several files (see the descriptions of parameters No. 1.9.8 “iSkip” and No. 1.8.1 “iTestRun”), it may be advantageous to break the computation of the numerical and analytical parts of the S integrals (from 0 to r_0 and from r_0 to ∞ , respectively) into several parts, differing by the range of variation of κ_1 (its endpoints are defined by parameters No. 1.3.1–2, i.e., “Kmin1” and “Kmax1”). All “partial” numerical and analytical S integral data files may subsequently be merged into a single data file with the complete S integrals using the option “iSkip=2 iTestRun=2”. If the partial data files are created by running several instances of BREMS simultaneously, then the utilization of the computing power of a multiprocessor or multicore system is improved. This method of improving the performance is especially effective in the case of large values of Kmax1 and Kmax2, when calculation of the entire set of S integrals in a single run of BREMS may be prohibitively long. The maximum gain in performance is achieved when the total number of the simultaneous “partial” runs of BREMS is

equal to the total number of logical processors available, and when their durations are approximately equal to each other. In the case of “_n” files (with the values of the integrals from 0 to r_0), this means that the numbers of numerical integrals calculated by each instance of BREMS must be approximately equal to each other. In the case of “_a” files (with the values of the integrals from r_0 to ∞), this means that numbers of terms of the form (1.2.10a,b) calculated by each instance of BREMS must be approximately equal to each other. In order to ensure this equality, BREMS includes a special mode of operation, where the only output is the set of ranges of values of κ_1 according to the values of parameters No. 1.3.1–12 and No. 1.3.15–18 and the parameters defining the method of splitting the entire set of S integrals into smaller subsets. This mode of operation is implemented in the subroutine “S_integrals”, which performs “stage 1” of the calculation (see Section 2), hence it can be activated only when parameter “firstStage” is equal to 1 (the default value). However, unlike the normal operation, this mode does not involve calculation of the S integrals or the continuum wave functions, and it is terminated immediately after determining the optimal endpoints of each partial range of κ_1 . Afterwards, the values of those endpoints may be specified after “Kmin1=” and “Kmax1=” on the command line used to start BREMS. The numerical suffixes may be appended to the names of the “partial” “_n” and “_a” files using parameter “start_suffix” (No. 1.9.7). It should be noted that there are three parameters whose default values may be affected by the user-specified values of parameters “Kmin1” and “Kmax1”. Those parameters are “Kmax2”, “lmax”, “l_interp1”. In order to avoid automatic modification of those three parameters caused by a change of “Kmin1” and “Kmax1”, their values must be specified explicitly. Those values can be determined by starting BREMS with the maximum (or default) value of “Kmax1”, and then interrupting the current run by pressing “Ctrl+C” after the corresponding default values of the mentioned three parameters are displayed on the screen (if there is a warning that “lmax” and “lmax_MP” have been reset to their arithmetic average, then one should use the final value of parameter “lmax”, which is displayed immediately after the mentioned warning). The value of parameter “lmax_MP” must be set equal to the value of parameter “lmax” (this can be achieved using the alias “lm”, which makes it possible to set both those parameters simultaneously).

The parameters specific to this mode of operation are described below.

- 1.10.1. “**split_n**” indicates if the program must calculate the set of intervals of κ_1 such that the numbers of S integrals corresponding to all such intervals are approximately equal. If this parameter is equal to 0, then this mode of operation will not be used. If this parameter is equal to 1, then the endpoints of all mentioned intervals will be written to the text (ASCII) file with the name “k1minmax_n_Z_T.TE±XX_k.kkkE±YY.txt”, where “Z” is the atomic number consisting of 1, 2 or 3 digits, “T.TE±XX” is the kinetic energy of the incident electron (MeV) rounded to 2 significant digits in scientific notation, and “k.kkkE±YY” is the energy of the bremsstrahlung photon (MeV) rounded to 4 significant digits in scientific notation (“E±XX” and “E±YY” are the respective decimal exponents). In the mentioned file, each pair of endpoints is placed on a separate line (two numbers in each line). If this file already exists, then it will be overwritten. If split_n is equal to a negative integer number, then the output format will be different: each pair of endpoints will be appended to a file with the name “k1minmax_n_⟨threadNum⟩.txt”, where “⟨threadNum⟩” is the thread number (zero-based), i.e., the sequence number of the corresponding instance of BREMS. The number of the first thread (i.e., the offset) is equal to -split_n-1. The values of Kmin1 and Kmax1 in each line are preceded by the values of Z, T_1 , k, l_interp1, lmax, and Kmax2 (the latter three parameters are included because their default values depend on Kmax1 and Kmin1). The first line of this file contains column headers (“Z”, “T1(MeV)”, “Ep(MeV)”, “l_int”, “lmax”, “Kmax2”, “Kmin1”, “Kmax1”). The default value of parameter “split_n” is equal to 0 (i.e., this mode of operation is not activated by default).
- 1.10.2. “**split_a**” indicates if the program must calculate the set of intervals of κ_1 such that the numbers of terms of the form (1.2.10a,b) corresponding to all such intervals are approximately equal. The interpretation of values of this parameter and the format of the

output data files are the same as in the case of parameter “split_n” described above. The only difference is in the output file names: the characters “_n” are replaced with “_a”. The default value of parameter “split_a” is equal to 0 (i.e., this mode of operation is not activated by default).

Note: Since the expression of the free-field continuum wave function (1.1.18) corresponding to a particular value of κ includes spherical Bessel functions of orders κ and $\kappa - 1$, there is some overlap in the data calculated by the instances of BREMS corresponding to adjacent intervals of κ_1 . This overlap of the data in the partial “_a” files does not cause any problems when merging them into the complete S integral data file; its only drawback is a computational “overhead”, i.e., redundant recalculation of some integrals from r_0 to ∞ . This overhead increases with decreasing widths of the partial intervals of κ_1 .

1.10.3. “**splitInfo**” is the name of a text (ASCII) file with the number of threads. Since two or more different computers with different capabilities may be used simultaneously, the number of threads and the corresponding “weight factors” must be specified for each computer separately. The ratio of the weight factors corresponding to different computers should be approximately equal to the ratio of their speeds, i.e., to the reciprocal ratio of the processing times when performing the same calculation (this would ensure approximate equality of the processing time on different computers). The weight factors must be specified separately for the two mentioned types of partial S integrals – the “numerical” integrals (from 0 to r_0) and the “analytical” integrals (from r_0 to ∞). Only the *ratios* of the weight factors corresponding to different computers are important (i.e., an increase or decrease of all weight factors by the same multiplier would not have any effect). In the case of a single computer, the weight factors are not used. The first line of the “splitInfo” file must contain the number of computers. There must be one additional line for each computer. This line must have three entries: the number of threads, the weight factor corresponding to calculation of the numerical integrals, and the weight factor corresponding to calculation of the analytical integrals. The default value of parameter “splitInfo” is “SplitInfo.txt”. There is a file with such a name in the distribution package of BREMS, and it corresponds to the case when there are 10 threads and a single computer.

1.10.4–5. “**piece_n**” and “**piece_a**” control an alternative splitting method: split the total number of S integrals or terms into roughly equal “pieces”. The average size of a single piece (i.e., the average number of S integrals or terms in it) is specified by the value of parameter “piece_n(a)”. In such a case, the file specified by parameter “splitInfo” is not used. If piece_n(a) is zero, then the default method (using the “split info” file specified by parameter “splitInfo”) will be used. If piece_n(a) is greater than or equal to the total number of integrals (terms), then the output data will correspond to a single “piece” (i.e., no splitting). The default value of these two parameters is equal to 0 (i.e., the program calculates the size of one “piece” from the number of threads, rather than the other way around).

4.11. Information displayed on the screen during calculation of the S integrals

During execution of stage 1, the subroutine S_integrals displays some real-time information about the calculation process. To avoid text wrapping (which would reduce readability of the output data on the screen), the screen buffer width must be at least 235 (in Windows this can be achieved, e.g., by entering “mode 235” at the command prompt in the console window before starting the calculation). At the start of the calculation, the total number of S integrals is displayed. Since the analytical integration is performed by calculating the integrals of products of three spherical Bessel functions and r^2 (see Eqs. (1.2.7)) and then combining them according to Eqs. (1.1.15) and (1.1.18), the number of the latter integrals is displayed, too. In addition, the total number of terms of the form (1.2.13) that have to be added up during calculation of the coefficients of the linear combinations of the integrals (1.2.14a,b) is shown (it is denoted “nterms_tot”). The total time of the analytical

integration is roughly proportional to the latter number (another factor that strongly affects the time of the analytical integration is the precision level used). After this preliminary information, the process of the numerical integration begins. During this process, a line with the current values of several variables is printed on the screen every 5 seconds. This line contains the following information:

- the current time of the numerical integration (in seconds),
- the sequence number of the last step of the numerical quadrature (“i”),
- the current value of the radial coordinate r (“r”),
- the percentage done, i.e., the ratio of the current value of r and the limiting radius (this entry is present only if the limiting radius has been defined, i.e., when the interaction potential is “truncated”, i.e., when $R_{\text{atom}} \neq 0$, or during the “test” numerical integration, or when $pr_{\text{transition2}} \neq 0$ and $r < pr_{\text{transition2}} / p_2$),
- the current values of $p_1 r$ and $p_2 r$ (“p(1)*r” and “p(2)*r”, respectively),
- the number of wave functions that have not attained the asymptotic form yet (“Nasymp”),
- the current values of the S integrals (“S1” and “S2”) corresponding to the largest absolute values of κ_1 , κ_2 and l (with an additional condition that $\kappa_2 \neq \kappa_1$),
- the maximum ranges of variation of A_κ and $\tilde{\delta}_\kappa$ over the last 10 “test” points (“A_range” and “delta_range”).

If the photon energy is zero, then the values of the S integrals are not displayed, because the numerical integration in this case involves only the solution of the coupled radial Dirac equations (1.1.16a,b) (for the same reason, the numerical integration is much faster in the case $k = 0$ than in the case $k \neq 0$). If A_range and delta_range have not been calculated yet, then they are not displayed. A_range is the maximum relative range of A_κ , i.e., $\max((A_{\text{max}} - A_{\text{min}}) / \langle A \rangle)$, where A_{max} and A_{min} are the maximum and minimum values of A_κ over the last set of “test” points for a given value of κ and a given electron energy, $\langle A \rangle$ is the average value of A_κ over the same set of points, and the overall maximum is calculated over both energies and all values of κ_1 and κ_2 . The variable delta_range may be either the maximum relative range of $\tilde{\delta}_\kappa$ or the maximum absolute range depending on the sign of parameter No. 1.7.7 (see Section 4.7), and it is defined similarly to A_range (just replace “A” with “ $\tilde{\delta}$ ” in the previous sentence). When “Nasymp” is non-zero, the values of the numerical integrals that are displayed during the numerical integration may have been calculated using unnormalized wave functions and may therefore differ from the final values by an order of magnitude or more. If all wave functions have attained the asymptotic form (1.1.18), i.e., if “Nasymp” is zero, but the other conditions for terminating the numerical integration are not satisfied yet, then the last two entries of the output line change: “A_range” and “delta_range” are replaced by the values of the two phase correction integrals (“Q(1)” and “Q(2)”).

The indices of the displayed S integrals are indicated in parentheses after “S1” or “S2” in this order: κ_1 , κ_2 , l .

During the analytical integration, feedback is provided to the user every 10 seconds in the form of messages indicating the percentage of the terms of the type (1.2.13) calculated.

The information that is displayed after terminating the numerical and analytical integration is mostly self-explanatory. It includes the values of the S integrals and their uncertainties corresponding to the largest absolute values of κ_1 , κ_2 and l (with the additional condition that $\kappa_2 \neq \kappa_1$), and the corresponding values of the factors A_{κ_1} and A_{κ_2} in Eqs. (1.1.18) and the phase shifts $\tilde{\delta}_{\kappa_1}$ and $\tilde{\delta}_{\kappa_2}$ (the values of $\tilde{\delta}_{\kappa_1}$ and $\tilde{\delta}_{\kappa_2}$ are adjusted by adding $2\pi n$, where n is an integer number, so that the final values of the phase shifts are between $-\pi$ and π), as well as some overall statistics, such as the maximum change of the numerical S_1 and S_2 integrals after increasing the computational tolerances and step sizes by a factor of 2 (the maximum absolute change is denoted “S1_num_maxDiff_abs” and “S2_num_maxDiff_abs”, and the maximum relative change is denoted “S1_num_maxDiff_rel” and “S2_num_maxDiff_rel”), and the maximum change of the

total S_1 and S_2 integrals after changing the phase shift by the value of the corresponding range (the maximum absolute change is denoted “S1_maxDiff_abs” and “S2_maxDiff_abs”, and the maximum relative change is denoted “S1_maxDiff_rel” and “S2_maxDiff_rel”). In the case $IV = 1$ (unscreened point-Coulomb potential) and $iExact = 0$ or 1 , when the exact values of A_κ and $\tilde{\delta}_\kappa$ are known ($A_\kappa = 1$, and $\tilde{\delta}_\kappa$ are given by Eqs. (1.1.23)–(1.1.25)) but not used, the exact values of $\tilde{\delta}_\kappa$ are displayed along with the values estimated numerically, so that the accuracy of the numerical solution of the system of differential equations (1.1.16a,b) can be evaluated if the point-Coulomb field has not been truncated ($R_atom = 0$). If the point-Coulomb field has been truncated ($R_atom \neq 0$), then the empirical values of $\tilde{\delta}_\kappa$ should not be expected to be close to the values given by Eq. (1.1.23), but this difference should be approximately the same for all κ if R_atom is sufficiently large (see the remark after Eq. (1.2.3) in Section 1.2). The difference between the value of $\tilde{\delta}_\kappa$ calculated numerically and the exact value given by Eq. (1.1.23) is also displayed (it is denoted “difference”, and the difference obtained after the additional subtraction of the term $\nu \ln(2pR_a)$ is denoted “difference2”).

If $\kappa_1 < 0$ or $\kappa_2 < 0$, then the value of

$$\delta'_\kappa = \begin{cases} \bar{\delta}_\kappa & \text{if } \kappa > 0, \\ \bar{\delta}_\kappa - \frac{1}{2}\pi & \text{if } \kappa < 0 \end{cases} = \begin{cases} \delta_\kappa & \text{if } \kappa > 0 \text{ or } \text{mod}(\kappa, 2) = 0, \\ \delta_\kappa + \pi & \text{if } \kappa < 0 \text{ and } \text{mod}(\kappa, 2) = 1 \end{cases} \quad (4.11.1)$$

is displayed before the value of $\bar{\delta}_\kappa$ (the value of δ'_κ is denoted “delta'”). The second equality of Eq. (4.11.1) follows from Eq. (1.1.19). If the screening function approaches zero at $r \rightarrow \infty$, then the value of $\bar{\delta}_\kappa$ approaches $\pi/2$ at large negative values of κ , whereas the value of δ'_κ approaches zero (see Eq. (4.11.1)). However, the estimate of the latter value is not affected by cancellation errors caused by calculating the difference of two very similar numbers, because δ'_κ is used as the primary quantity in the code, i.e., the program calculates $\bar{\delta}_\kappa$ from δ'_κ rather than the other way around.

If the photon energy is zero, then there are some differences between the format of the data that are displayed during the execution of subroutine `S_integrals` and the data that are described above due to significant differences of the calculation procedure.

5. Calculating the cross sections as the truncated partial-wave series (stage 2)

Subroutine “Bremsstrahlung” is used for stage 2 of the calculation process (see Section 2). The names, descriptions and default values of the parameters of Bremsstrahlung that can be modified by the user are given below.

5.1. Physical parameters

2.1.1–4. These four parameters are the same as parameters No. 1.1.1–4 of `S_integrals` (see Section 4.1), i.e., they specify the atomic number, initial electron energy, final electron energy, and photon energy, respectively.

5.2. Parameters defining the sets of S integrals and of terms of the truncated partial-wave series

2.2.1–12. These twelve parameters are the same as parameters No. 1.3.1–12 of `S_integrals` (see Section 4.3). However, if the calculation starts from stage 2, then these parameters are not required to be exactly equal to the corresponding parameters of the subroutine `S_integrals` used in stage 1. In such a case, the set of values of κ_1 , κ_2 and l defined on the command line or in the parameter file is required only to be contained inside the set of values of κ_1 , κ_2 and l corresponding to the specified files with the S integral data. If it is not so and if $Kmin1 = Kmin2 = 1$ and $isAbs_K1 = isAbs_K2 = 1$, then $Kmax1$, $Kmax2$ or $lmax$ will be reduced automatically to make them equal to the corresponding values of the S integral data.

- 2.2.13. “**lmax2**” is the upper limit of summation with respect to l when calculating the R factors (1.1.10). The default value of parameter “lmax2” is equal to the value of parameter “lmax” (No. 1.3.12). *Note*: If interpolation with respect to l is not applied, then setting lmax2 to a value less than lmax is equivalent to decreasing lmax to lmax2. If interpolation with respect to l applied, then there is no longer such equivalence, because parameter “lmax” defines not only the limits of l , but also the knots of the cubic spline interpolation (see Section 1.3.3). Hence, if lmax is decreased to lmax2 without recalculating the S integrals, then the program will attempt to apply the mentioned interpolation at the start of stage 2 using the values of the mentioned knots that are different from those in the S integral data file (created using a larger value of lmax), and this would cause termination of the program with an error message about missing S integral data (see also the note after the description of parameter No. 1.3.15 of $S_integrals$ in Section 4.3).
- 2.2.14–17. These four parameters are the same as parameters No. 1.3.15–18 of $S_integrals$ (see Section 4.3).
- 2.2.18. “**k2_excl_last**” is a “switch” (0 or 1) indicating whether the last value of $|\kappa_2|$ must be excluded from the set of the breakpoints used to calculate the cubic spline coefficients for the partial-wave interpolation (see Section 1.3.4). In the case “k2_excl_last=1”, the interpolated values between the last two breakpoints of $|\kappa_2|$ are calculated using the same spline coefficients as between the previous two breakpoints. This parameter was added after noticing that in the case “IV=1” and at low electron energies (of the order of 10 eV or lower) there is a discontinuity at the last value of $|\kappa_2|$ in the dependences of the terms of the CS and DCS on $|\kappa_2|$ (the last term is much less than the smoothly extrapolated value). Consequently, if the last value of $|\kappa_2|$ is not excluded from the calculation of the spline coefficients, the interpolating curve has an oscillatory character between the last several pairs of breakpoints of $|\kappa_2|$, causing large errors in the cross sections. The default value of this parameter is 1 in the case “IV=1” or when parameter “Zi” is non-zero, and 0 otherwise.
- 2.2.19. “**lmax_decr**” is a non-positive increment of lmax that must be applied for testing the sensitivity of the cross sections to the value of l_{max} and to the uncertainties of the S integrals (see also the description of the output files of stage 2 in Section 5.8). If lmax_decr < 0, then both mentioned error tests will be performed. If lmax_decr = 0, then only the sensitivity to the uncertainties of the S integrals will be tested. If lmax_decr > 0, then there will be no error testing of any kind. Regardless of the value of lmax_decr, the error testing will be performed only if $Kmin1 = Kmin2 = 1$ and $isAbs_K1 = isAbs_K2 = 1$. The default value of this parameter is $-\max(1, \min(10, lmax/10))$.

5.3. Parameters defining the set of angles

- 2.3.1–3. “**theta_min**” (alias “theta0”), “**theta_max1**” (alias “theta_max”), and “**np1**” (alias “np”) define the set of equidistant values of the photon emission angle θ that must be used for calculating the differential cross section (DCS). theta_min and theta_max1 are the minimum and maximum angles, respectively (in degrees), and np1 is the number of values of θ . Normally, theta_min = 0 and theta_max1 = 180, unless two values of the angular increment are used (see below). By default, theta_min=0. The default values of parameters theta_max1 and np1 depend on T_1 :
- if $T_1 < 1$ MeV, then theta_max1 = 180 and np1 = 181;
 - if $1 \text{ MeV} \leq T_1 \leq 3$ MeV, then theta_max1 = 10 and np1 = 51;
 - if $3 \text{ MeV} < T_1 \leq 30$ MeV, then theta_max1 = 10 and np1 = 101;
 - if $T_1 > 30$ MeV, then theta_max1 = 10 and np1 = 501.
- 2.3.4–5. “**theta_max2**” (alias “theta_max”) and “**np2**” (alias “np”) define the second set of equidistant values of the photon emission angle θ that must be used for calculating the DCS. It is assumed that the starting angle of this set is equal to the upper bound of the first angular

range “theta_max1” (parameter No. 2.3.2). “theta_max2” is the overall maximum value of θ , and “np2” is the number of values of θ in the second set, excluding the mentioned starting value (“theta_max1”). If $np2 \leq 0$, then the second angular range will not be used. By default, $theta_max2 = 180$. The default value of parameter np2 depends on T_1 :

- if $T_1 < 1$ MeV, then $np2 = 0$ (i.e., the second angular range is not used);
- if $1 \text{ MeV} \leq T_1 \leq 3 \text{ MeV}$, then $np2 = 170$;
- if $T_1 > 3 \text{ MeV}$, then $np2 = 340$.

Notes: 1. The integration of the DCS is done in the two angular ranges defined by parameters No. 2.3.1–5 independently, using the 10th-order Newton-Cotes formula. Consequently, it is recommended to set the number of angular integration steps in each of those two ranges (i.e., $np1 - 1$ and $np2$) equal to a multiple of 10.

2. If $np1 = np2 = 0$, then only the CS data will be calculated (but not the DCS data).

5.4. Parameters controlling calculation of the Wigner 3j coefficients

- 2.4.1. “**dir_3j**” is the name of the folder where the binary files with the Wigner 3j coefficient data are located. If the specified folder name is incomplete, i.e., if it does not start with the slash ‘/’ or ‘\’ and does not contain the colon ‘:’, then it is assumed to be a subfolder either of the BREMS installation folder or of the current folder, depending on whether the path to the BREMS executable file has been specified before its name on the command line or not. If the specified folder does not exist, then it will be created. If the folder name has a non-trailing slash, then one should keep in mind that Windows uses backslashes ‘\’ for file paths, whereas Linux uses forward slashes ‘/’. If the folder name contains a forward slash and no backslash, then on Windows the attempt to create this folder will fail (however, if the folder already exists, then the attempt to open a 3j data file will succeed). The default value of this parameter is ‘3j’.
- 2.4.2. “**lock_3j**” is a “switch” (0 or 1) indicating if access to the 3j data folder must be blocked until all R factors (1.1.10) are calculated. If $lock_3j = 1$, then a temporary read-only file (with the name “read”) will be opened in the 3j data folder during the calculation of the R factors. If another instance of the program (with $lock_3j$ set to 1) accesses the 3j data folder, it will first check for existence of the mentioned file, and then attempt to delete it if it exists. If the file exists and the delete attempt is not successful, then the program will wait until the mentioned file is deleted by the instance that created it. This may help to avoid an excessively high HDD usage (and a consequent slowdown of execution), which could happen if multiple instances of the program attempt to read a large amount of 3j data from the same HDD simultaneously. The default value of this parameter is equal to 0 (i.e., access to the 3j data folder is not blocked by default).
- 2.4.3–4. “**update_3j_start**” and “**update_3j_end**” control an option to update the Wigner 3j coefficients stored in old data files (created by a version of BREMS older than v1.5.6.0). If the program detects an old format of the files with the 3j coefficients corresponding to values of $\max(l_1, l_2)$ in the range $update_3j_start \leq \max(l_1, l_2) \leq update_3j_end$, then those 3j coefficients will be recalculated, and the corresponding data files will be recreated. The remaining 3j coefficients will not be recalculated, whereas the corresponding files may be modified or not, depending on parameter No. 2.4.5 “update_3j_format” (see below). Default values: $update_3j_start=81$, $update_3j_end=160$.
- 2.4.5. “**update_3j_format**” is a “switch” (0 or 1) indicating that the format of the Wigner 3j data files corresponding to the values of $\max(l_1, l_2)$ that are either less than $update_3j_start$ or greater than $update_3j_end$ files must be updated, i.e., the redundant 3j coefficients (which are not needed for the calculation of the bremsstrahlung cross sections) must be removed (causing a decrease of the file size approximately by half). The default value of this parameter is equal to zero (i.e., the 3j data files created by a version of BREMS older than

v1.5.6.0 are not modified by default, if the value of $\max(l_1, l_2)$ does not belong to the interval $\text{update_3j_start} \leq \max(l_1, l_2) \leq \text{update_3j_end}$.

- 2.4.6. “**only_3j**” is a “switch” (0 or 1) indicating that only the files with values of the Wigner 3j coefficients must be created or updated to the latest format (by removing the redundant 3j coefficients). When $\text{only_3j} = 1$, the program creates the 3j data files corresponding to the range of $\max(l_1, l_2)$ defined by parameters “start_3j” and “end_3j” (No. 2.4.7–8), and then exits immediately. The only parameters used in this mode are those that are relevant to calculation of the Wigner 3j coefficients (those are the parameters whose names contain characters “3j”). The default value of parameter “only_3j” is equal to zero.
- 2.4.7–8. “**start_3j**” and “**end_3j**” define the endpoints of the range of $\max(l_1, l_2)$ corresponding to the 3j data files that must be modified when the option “only_3j=1” is used (see the description of parameter No. 2.4.6). The default values of these two parameters are equal to 81 and 2000, respectively.

5.5. Parameters defining the names of input and output files, and the conditions for overwriting

- 2.5.1–2. These two parameters are the same as parameters No. 1.9.1–2 of S_integrals (see Section 4.9), i.e., they define the names of the input files with the S integral data.
- 2.5.3–4. “**suffix2_CS**” and “**suffix2_DCS**” (alias “suffix2” for both) are the additional suffixes to be inserted at the end of the names of some output files. The sequence of characters specified by parameter “suffix2_CS” will be inserted in the three names starting with “_CS_”, and the sequence of characters specified by parameter “suffix2_DCS” will be inserted in the five names starting with “DCS_” or “ShapeFn_” files (see the description of the output files of stage 2 in Section 5.8). If this parameter is the empty string (specified by writing a space after “suffix2_(D)CS=”), then no additional suffix will be used. By default, these two parameters are equal to the empty string.
- 2.5.5. “**iCalculate**” indicates whether the cross section files with the data for different κ_{\max} must be regenerated. If $\text{iCalculate} = 0$, then the cross sections will be calculated only when the output data files do not exist, or when the parameters $\text{Kmin}(1,2)$ or $\text{isAbs_K}(1,2)$ do not satisfy the mentioned requirement $\text{Kmin1} = \text{Kmin2} = 1$, $\text{isAbs_K1} = \text{isAbs_K2} = 1$. If $\text{iCalculate} = 1$, then the cross sections will always be calculated, and the output data files will be overwritten if they exist. If $\text{iCalculate} = -1$ and the output files with the cross section data already exist, then Bremsstrahlung will not calculate the cross sections and will regenerate only the files with the shape function data (the required the CS and DCS data will be loaded from the existing files). In the latter case, if neither of parameters No. 2.3.1–5 is explicitly specified by the user, then all angles will be read from the first column of the existing file with the DCS data (or from the first line of this file, if it was created using a version of BREMS older than 1.5.0.0). If $\text{iCalculate} = -1$ and at least one of parameters No. 2.3.1–5 is specified explicitly, then the set of angles will be constructed as explained in the descriptions of parameters No. 2.3.1–5, and the program will attempt to locate the corresponding lines (or columns, if the file was created using the version of BREMS older than 1.5.0.0) in the existing file with the DCS data. If the data for at least one of the angles is not available, then the program will quit with an error message. The numerical integration of the angular dependence of the DCS (which is needed for calculating the CS and the shape functions) is performed using the final set of angles (i.e., if some of the angles, for which the DCS data are available, have been skipped due to the user-specified values of parameters No. 2.3.1–5, then the skipped DCS data will not be used for the mentioned integration). The default value of parameter “iCalculate” is 1.

5.6. Other parameters

- 2.6.1–2. “**del_S_int**” and “**del_S_int+**” (alias “**del_S**” for both) is a “switch” (1 or 0) indicating if the S integral data files created in the previous stage (by the subroutine `S_integrals`) must be deleted after a successful calculation of the cross sections. If the alternative set of S integrals is used (see Section 4.4) and if it is not completely contained inside the original dataset, then parameter “**del_S_int+**” is used to indicate if the remainder of the alternative dataset (stored in the data files with ‘+’ at the end of the filename) must be deleted. Parameter “**del_S_int**” applies only to the files without the additional plus sign in the filename. The value “1” of these two parameters (indicating deletion of the S integral data files) will have an effect only if `firstStage = 1`. The default value of parameters “**del_S_int**” and “**del_S_int+**” is 0.
- 2.6.3. “**checkTabPos**” is a “switch” (1 or 0) indicating if the format of files “`CS.txt`” and “`CS_2.txt`”, which form the third group of files described in Section 5.8, must be checked for consistency. If this parameter is equal to 1, then the program will compare tab positions and length of the first and last lines of the file (this check is performed after appending the line with the results of the current run). If a discrepancy is found, then a warning will be displayed (however, execution of the program will not be stopped). If this parameter is equal to 0, then the mentioned check will not be performed. The default value of this parameter is equal to 1.

Note: Parameter “**checkTabPos**” is also used in stage 3 by subroutine “`Brems_fit`” (for checking the file “`CS_fitted.txt`”), and by subroutine “`Born_SM_appr`” (for checking the file “`CS_Born_SM.txt`”). In the case “**checkTabPos=1**”, a similar check of input files is also performed when generating the grid data for the cubic-spline fitting and interpolation of the logarithm of the scaled SDCS with respect to the logarithm of the incident electron energy (see Section 9). However, in the latter case, *all* lines are checked, and a change of tab positions is treated as a terminal error (i.e., the program then exits with an error message).

5.7. Usage of the Wigner 3j coefficients

The calculation process in Bremsstrahlung starts with creation of the array of the Wigner 3j coefficients, which are used in Eq. (1.1.14). The 3j coefficients may be calculated or loaded from binary files, depending on the maximum absolute value of κ_1 and κ_2 used in the calculation:

$$\kappa_{12\max} \equiv \max(|\kappa_1|, |\kappa_2|). \quad (5.1)$$

The 3j coefficients are loaded from files (rather than calculated) only when $\kappa_{12\max}$ belongs to the interval $80 < \kappa_{12\max} \leq 2000$. The two endpoints of this interval are defined by two internal variables, which are named “`kmax_3j`” and “`kmax_3j_2`”, respectively (at the time of this writing, `kmax_3j = 80` and `kmax_3j_2 = 2000`). Only the values of the 3j coefficients corresponding to $l_1 \leq l_2$ are stored (the values corresponding to $l_1 > l_2$ are calculated using the symmetry properties of the 3j coefficients). A separate file is used for each value of $l_2 > 80$. Those files are loaded (or created) during the calculation of the R factors (1.1.10) when a given value of l_2 becomes needed for the first time. All 3j files are in a separate folder, whose name is specified using parameter No. 2.4.1 (“`dir_3j`”); file names have the format “`3j_⟨l₂⟩.dat`”. If the mentioned folder does not exist, or if there is no required file in it, then the coefficients will be calculated and the file will be created. The maximum number of the 3j coefficients that may be calculated or loaded from files during a single run of BREMS is equal to

$$\text{nCoefs} = \frac{\kappa_{12\max}^4}{12} + \frac{2\kappa_{12\max}^3}{3} + \frac{23\kappa_{12\max}^2}{12} + \frac{7\kappa_{12\max}}{3} + 1. \quad (5.2)$$

All these coefficients would be needed only when both κ_1 and κ_2 vary from $-\kappa_{12\max}$ to $\kappa_{12\max}$, and l varies from 0 to $2\kappa_{12\max}$. If the range of variation of κ_1 , κ_2 or l is narrower, or if the partial-wave interpolation method described in Section 1.3.4 is applied, then some of those coefficients will not be used during the calculation of the cross sections. If $l_2 \leq 500$, then the maximum value of l_1 is

equal to l_2 . If $500 < l_2 \leq 800$, then the maximum value of l_1 is equal to $1000 - l_2$. If $800 < l_2 \leq 2000$, then the maximum value of l_1 is equal to 200. The number of 3j coefficients stored in a data file corresponding to a particular value of l_2 is equal to

$$\text{nCoefs}(l_2) = \frac{l_m^3}{3} + \frac{3l_m^2}{2} + \frac{13l_m}{6} + 1, \quad (5.3a)$$

where

$$l_m \equiv \begin{cases} \min(l_2, 1000 - l_2) & \text{when } l_2 \leq 800, \\ 200 & \text{when } 800 < l_2 \leq 2000. \end{cases} \quad (5.3b)$$

5.8. Output data of stage 2 (subroutine “Bremsstrahlung”)

Subroutine Bremsstrahlung creates or updates up to 11 human-readable ASCII files. Their names end with extension “.txt”. If both the original and alternative sets of S integrals are processed (see Section 1.8 and the beginning of Section 2), then two sets of files, each one consisting of up to 11 files, will be created. The names of the files corresponding to the alternative dataset differ from the names of the corresponding files of the original dataset by the plus sign ‘+’ at the end (if an additional suffix defined by parameters No. 2.5.3–4 is used, then the mentioned plus sign appears immediately before this suffix). The most complete set of files is created when $K_{\min 1} = K_{\min 2} = 1$ and $\text{isAbs_K1} = \text{isAbs_K2} = 1$ and $\text{lmax_decr} < 0$. The description of the output data that is presented below pertains only to the latter case.

It is convenient to define the following three groups of files according to their purpose:

- I. Seven files with the dependences of the CS, DCS and shape function on κ_{\max} . The names of those files include the name of the input file with the S integral data. If those files already exist, then they may be overwritten or not, depending on the value of parameter No. 2.5.5.
- II. Two files with the DCS and shape function for the last (greatest) value of κ_{\max} . I.e., those files contain a subset of the data contained in the files of I group. Their format (two columns of numbers, with values of θ in column 1) is convenient for plotting the angular dependence of the DCS or the shape function. The names of those files are formed by appending the two suffixes defined by parameters No. 2.5.2 and No. 2.5.4 (“suffix” and “suffix2_DCS”) to a fixed sequence of characters. These files are overwritten during each run of Bremsstrahlung, except when parameter No. 2.5.5 is equal to 0 and the files with the CS and DCS data already exist.
- III. Two files with the values of the physical and control parameters, as well as the value of the SDCS obtained by evaluating the truncated partial-wave series (1.1.5), and values of several statistics indicating the accuracy of the calculations. The names of these two files are fixed. A line of text is appended to these files after each calculation of cross sections, i.e., after creating the files with the CS and DCS data.

In the case “S_data=2” or “S_data=2” (see the description of parameter No. 13 of the main program at the end of Section 2), the names of all mentioned files corresponding to the alternative dataset (with an increased ratio $|\kappa_1|_{\max} / |\kappa_2|_{\max}$) will have the plus sign ‘+’ inserted at the end of the file name. In the names of the files that are re-created in each run of BREMS (rather than updated by adding a line), the plus sign is inserted immediately before the suffix defined by parameter 2.5.3 (“suffix2_CS”) or No. 2.5.4 (“suffix2_DCS”), or immediately after the suffix defined by parameter No. 1.9.2 (“suffix”). In the names of the files that are updated in each run of BREMS by adding a line, the plus sign is inserted immediately before the extension “.txt”.

In order to avoid a crash when two or more instances of BREMS attempt to update the same file simultaneously, a temporary read-only file with the name “write_lock2” is opened in the current folder just before updating the mentioned files (the number “2” in the mentioned file name indicates that this file was created in stage 2 of the current run of BREMS). If another instance of the program attempts to update the same files, it will first check for existence of the mentioned temporary file, and then attempt to delete it if it exists. If the file exists and the delete attempt is not

successful, then the program will wait until the mentioned file is deleted by the instance that created it.

All files created in stage 2 contain two or more columns of numbers with fixed width and with a header above each column. The values of the CS and DCS in the output data are defined as the left-hand sides of Eqs. (1.1.5) and (1.1.4), respectively, i.e., they are equal to the true cross sections multiplied by k / Z^2 (the units are indicated after Eqs. (1.1.5) and (1.1.4)). Further on, when referring to numerical values of the cross sections, the scaled CS and DCS (with the scaling factor k / Z^2 and with units indicated after Eqs. (1.1.5) and (1.1.4)) will always be implied. This note also applies to the output of the subroutines `Brems_fit` and `Born_SM_appr`.

The names of the files of the first group are formed by adding the prefix “_CS_”, “DCS_” or “ShapeFn_” and the suffix defined by “suffix2_(D)CS” to the S integral data file name. The mentioned prefixes replace the prefix defined by parameter No. 2.5.1, which is used for forming the name of the files with the S integral data, whereas “suffix2_(D)CS” is appended to the suffix defined by parameter No. 2.5.2. In addition, if the full error testing has been requested (i.e., if parameter No. 2.2.19 “lmax_decr” is negative), two files with an additional suffix “_test” and two files with an additional suffix “_test2” are created. The names of the latter four files also start with the prefix “_CS_” and “DCS_”. The two files whose names end with “_test” contain the values of CS and DCS calculated using a set of modified S integrals and the same range of values of l in Eq. (1.1.10) as the two “_CS_” and “DCS_” files whose names do not end with “_test” or “_test2” (the values of S integrals are modified by randomly adding or subtracting their uncertainties). The two files whose names end with “_test2” contain the values of CS and DCS calculated using a reduced value of l_{\max} and the same set of unmodified S integrals as the two “_CS_” and “DCS_” files whose names do not end with “_test” or “_test2” (if `lmax_decr` = 0, then l_{\max} is not reduced and those two files are not created). Starting with BREMS v1.5.6.7, the file “DCS_..._test2.txt” has four additional lines at the beginning, indicating the maximum values of $|\kappa_1|$, $|\kappa_2|$ and l_{\max} , and the mentioned reduced value of l_{\max} (those four values are preceded by “Kmax1=”, “Kmax2=”, “lmax2=”, and “l_test=”, respectively). The three files whose names start with “_CS_” contain four columns of numbers. The first column in those three files contains the values of κ_{\max} (column header “kmax”). The second, third and fourth columns of the three “_CS_” files contain the values of the CS (“CS”), the angular integral of the DCS (“DCS_integral”), and the relative difference of the previous two values (“rel_diff”). The number of columns in the three “DCS_” files and the “ShapeFn_” file is greater than the maximum value of κ_{\max} by 1. The first column in all four files of this group contains the values of θ (column header “theta”). All columns starting from the second one in the “DCS_” and “ShapeFn_” files contain the values of the DCS or the shape function corresponding to a given value of κ_{\max} (the latter value is indicated in the header of the column).

Note: The “DCS_” and “ShapeFn_” files created in stage 2 by versions of BREMS older than v1.5.0.0 have the data transposed in comparison with the above description (i.e., different columns correspond to different values of θ , and different lines correspond to different values of κ_{\max}). Those files may also be used as input for stage 3 (they are interpreted correctly by BREMS). The files “DCS_..._test2.txt” created by versions of BREMS older than v1.5.6.7, which do not have the mentioned additional four lines inserted at the beginning, are also interpreted correctly by BREMS.

Two files “DCS1(suffix)\(suffix2_DCS).txt” and “ShapeFn1(suffix)\(suffix2_DCS).txt” make up the second group of the output files of stage 2. Each of them contains two columns of numbers. The first column contains the values of θ (in degrees). The second column contains the values of the DCS or the shape function, respectively.

The name of the main file of the third group is “CS.txt”. Every calculation of bremsstrahlung cross sections ends by appending a line of text to this file. The mentioned line contains several physical and control parameters, as well as the values of the CS, angular integral of the DCS, their relative difference, the maximum relative differences between the data corresponding to the two sets of S integrals (original and modified) and the two values of l_{\max}

(original and reduced), and the processing time. The entries in each line of this file have the following meaning:

- (1) the atomic number of the target material (column header “**Z**”),
- (2) the kinetic energy of the incident electron in MeV (“**T1(MeV)**”),
- (3) the energy of the bremsstrahlung photon in MeV (“**Ep(MeV)**”),
- (4) the cutoff radius of the interaction potential in relativistic units, or the number 0 if the interaction potential has not been truncated (“**R_atom**”),
- (5) the type of the interaction potential (“**IV**”),
- (6) the ion charge, in units of the elementary charge (“**Zi**”),
- (7) the type of the nuclear charge distribution, which is specified by parameter No. 1.2.1 (“**nuclear_model**”),
- (8) the mean nuclear radius in fm (“**Rn(fm)**”),
- (9) the number of exponential terms in the expression of of the interaction potential (“**nexp**”), if it is approximated by a linear combination of exponentials (this number is non-zero only in the case “**IV=2**”),
- (10) the number of cycles (“**nCyc**”). If the dependence of the CS and DCS on κ_{\max} has not been calculated (i.e., the condition $K_{\min 1} = K_{\min 2} = 1$ and $\text{isAbs_K1} = \text{isAbs_K2} = 1$ is not satisfied), then $\text{nCyc} = 1$. Otherwise, it is equal to K defined by Eq. (1.5.3),
- (11) the minimum value of κ_1 (“**kmin1**”),
- (12) the maximum value of κ_1 (“**kmax1**”),
- (13) the number 1 or 0 indicating whether the limits of variation of κ_1 are defined in terms of its absolute value (“**k1abs**”),
- (14) the minimum value of κ_2 (“**kmin2**”),
- (15) the maximum value of κ_2 (“**kmax2**”),
- (16) the number 1 or 0 indicating whether the limits of variation of κ_2 are defined in terms of its absolute value (“**k2abs**”),
- (17) the value of the first breakpoint of κ_2 (“**k2_bp1**”),
- (18) the interval between the first two breakpoints of κ_2 (“**dk2_1**”),
- (19) the interval between the last two breakpoints of κ_2 (“**dk2_n**”),
- (20) the value of parameter No. 2.2.18 “**k2_excl_last**” (“**k2excl**”),
- (21) the minimum value of l (“**lmin**”),
- (22) the maximum value of l (“**lmax**”),
- (23) the upper limit of summation with respect to l when calculating the R factors (1.1.10) (“**lmax2**”),
- (24) the reduced value of l_{\max} , which has been used for calculating one of the two “test” sets of the CS and DCS, which is stored in the files whose names include the suffix “_test2” (see also Section 1.3.2 and Section 5.8), or the number “-1” if $\text{lmax_decr} \geq 0$ (“**test**”),
- (25) the starting point of the interpolation range of l , or the number “-1” if the interpolation with respect to l has not been applied (“**l_int1**”),
- (26) the increment of the interval between the interpolation breakpoints of l inside the interpolation range, or the number 0 if the interpolation with respect to l has not been applied (“**d_lstep**”),
- (27) the maximum interval between the interpolation breakpoints of l inside the interpolation range, or the number 0 if the interpolation with respect to l has not been applied (“**stepMax**”),
- (28) the threshold value of $|\kappa_2|$, which must be exceeded in to apply to the interpolation with respect to l , or the number 0 if the interpolation with respect to l has not been applied (“**l_k2_thr**”),
- (29) the value of the CS corresponding to the maximum value of κ_{\max} (“**CS**”),
- (30) the value of the angular integral of the DCS calculated using the 10th-order Newton-Cotes formula (“**DCS_integral**”),

- (31) the relative difference of the previous two values (“**rel_diff**”),
- (32) the maximum “scaled” absolute difference between the original set of values of the CS (obtained with the original l_{\max} and unmodified S integrals) and the “test” set of values of the CS, which is obtained with the original l_{\max} and with the S integrals randomly incremented or decremented by the magnitude of the corresponding uncertainty, and which is stored in the files whose names include the suffix “_test” (see also Section 1.4 and Section 5.8). It is defined as the maximum absolute difference of the original and “test” cross sections divided by the maximum value of the original cross section. The maximum is calculated over the entire set of used values of κ_{\max} (i.e., $\kappa_{\max} = 1, 2, \dots, K$, where K is defined by Eq. (1.5.3)). If $l_{\max_decr} > 0$, then this entry is replaced by a single zero “0”. The header of this column is “**max|relDiff_CS|**”,
- (33) the maximum “scaled” absolute difference between the original set of values of the DCS and the “test” set of values of the DCS (obtained with the original l_{\max} and with the S integrals randomly incremented or decremented by the magnitude of the corresponding uncertainty). It is defined in the same way as the maximum scaled absolute difference of the CS (see above). The maximum is calculated over all values of κ_{\max} and θ . If $l_{\max_decr} > 0$, then this entry is replaced by a single zero “0”. The header of this column is “**max|relDiff_DCS|**”,
- (34) the definition of the number in column “**max|relDiff2_CS|**” differs from the definition of the number in column “**max|relDiff_CS|**” only in the “test” set of cross sections used (in this case, the “test” cross sections are calculated using the reduced l_{\max} and the original S integrals). If $l_{\max_decr} \geq 0$, then this entry is replaced by a single zero “0”,
- (35) the definition of the number in column “**max|relDiff2_DCS|**” differs from the definition of the number in column “**max|relDiff_DCS|**” only in the “test” set of cross sections used (in this case, the “test” cross sections are calculated using the reduced l_{\max} and the original S integrals). If $l_{\max_decr} \geq 0$, then this entry is replaced by a single zero “0”,
- (36) the time of calculating the numerical integrals with the bounds of integration equal to 0 and r_0 in stage 1 (this time is expressed in seconds, the column header is “**t[0_to_r0]**”),
- (37) the time of calculating the analytical integrals with the bounds of integration equal to r_0 and ∞ in stage 1 (this time is expressed in seconds, the column header is “**t[r0_to_Inf]**”),
- (38) the total duration of stage 2 in seconds (“**t[CS_DCS]**”),
- (39) the total duration of the current run of BREMS in seconds (“**total_time**”),
- (40) the version number of the program used for the calculations (“**BREMS_ver**”). The version number is written as an integer number obtained by concatenating all four components of the version number, with the last three components having two digits each (the first of these two digits may be zero). For example, BREMS v1.5.7.0 would be indicated by “1050700”,
- (41) the timestamp (i.e., last modification time) of the executable file used for the calculations (“**exe_timestamp**”). The timestamp is written as a 14-digit integer number, whose first eight digits indicate the date using the format YYYYMMDD, and the last six digits indicate the time using the format HHMMSS. For example, the timestamp “20230527132051” indicates the time 13:20:51 on May 27, 2023,
- (42) the timestamp of the S integrals data file used for the calculations (“**S_int_timestamp**”),
- (43) the timestamp of one of the files belonging to the first group of files created in the current run. This is the file whose name starts with “_CS_” and does not include the suffix “_test” or “_test2” (see the beginning of the current section). The header of this column is “**_CS_timestamp**”.

If $\text{firstStage} = 2$, or if stage 1 is skipped due to availability of the files with the S integral data, then the times of the numerical and analytical integration (in columns “**t[0_to_r0]**” and “**t[r0_to_Inf]**”) are copied from the last loaded binary file with the S integral data, which contains at least some of S integrals needed for the current run. If the numerical or analytical integrals were loaded from files in stage 1, then the corresponding time of the numerical or analytical integration, which is written to

the output file with the S integral data in stage 1, is copied from the last loaded binary file with the corresponding data, which contains at least some of S integrals needed for the current run.

In the case “IV=2” (indicating the approximation of the point-nucleus screening function by a superposition of decaying exponentials), a line is also appended to another file of the third group, which is named “CS_2.txt”. This line contains the same entries as the line appended to the file “CS.txt” (excluding the column “IV”), and eleven additional entries, which provide additional information specific to the option “IV=2”. The common entries are in the same order as in the file “CS.txt”, except for the number of exponential terms in the expression of the interaction potential (column “nexp”), which is placed after the column “_CS_timestamp” in the file “CS_2.txt”. The additional entries are the following:

- “V_parms”, “appr”, “nbp”, “rMin”, “rMax”, which indicate the values of parameters No. 1.1.15 (“V_parms”), No. 1.1.8 (“appr”), the number of radial breakpoints (in the case “appr=2”, this number coincides with the value of parameter No. 1.1.14 “nr”), and the values of parameters No. 1.1.12–13 (“rmin” and “rmax”), respectively. Those five entries are inserted after the column “Rn(fm)”.
- “factor1”, “exp1”, “factor2”, “exp2”, “factor3”, “exp3” with the values of the preexponential factors and exponents of the first three terms of the mentioned linear combination of decaying exponentials. Those six entries are appended to the end of the line (after the column “nexp”).

During the calculation of the scaled CS and DCS (Eq. (1.1.5) and Eq. (1.1.4), respectively), Bremsstrahlung displays the same data that are included in the “_CS_” file (see the description of the files of the first group above). The intermediate values of the scaled CS and DCS are written every 5 seconds to the temporary files (their names are formed by appending the suffix “_tmp” to the original filenames). At the end of the calculation, Bremsstrahlung displays the value of the scaled CS (1.1.5) corresponding to the last (greatest) value of κ_{\max} (i.e., to $\kappa_{\max} = K$).

If the dependence of the CS and DCS on κ_{\max} is not calculated (i.e., if the condition $K_{\min 1} = K_{\min 2} = 1$ and $isAbs_K1 = isAbs_K2 = 1$ is not satisfied), then only 5 files are updated in stage 2: the file “CS.txt”, the two files of the second group (whose names start with “DCS1” and “ShapeFn1”), and the files “DCS.txt” and “ShapeFn.txt”. After the cross sections are calculated, a line with the physical and control parameters and the values of the DCS and the shape function is appended to each of the latter two files. The first 23 columns in the latter two files contain the same data as columns No. 1 – 5, No. 9 – 23, and No. 25 – 27 in the file “CS.txt” (see above).

6. Extrapolating the cross sections as a function of κ_{\max} , and angular spline extrapolation (stage 3)

Subroutine “Brems_fit” is used for stage 3 of the calculation process (see Section 2). The names, descriptions and default values of the parameters of Brems_fit that can be modified by the user are given below.

6.1. Physical parameters

3.1.1–5. These five parameters are the same as parameters No. 1.1.1–5 of S integrals (see Section 4.1), i.e., they specify the atomic number, initial electron energy, final electron energy, photon energy, and the type of the interaction potential, respectively.

6.2. Parameters defining the subset of data to analyze

3.2.1. “kmax_fit” is the upper limit on the value of κ_{\max} in the input files with the cross section data. If this parameter is equal to -1 , then all available cross section data will be used. If this parameter is equal to -2 , then the upper limit of κ_{\max} will be equal to $\min(\kappa_{1\max}, \kappa_{2\max})$, where $\kappa_{1\max}$ and $\kappa_{2\max}$ are either specified explicitly using parameters No. 1.3.1–6 (see Section 4.3), or equal to the default values corresponding to the current values of Z , T_1 and k . The default value of this parameter is -1 .

- 3.2.2. “**kmin_fit**” is used when the value of κ_{\max} is reduced in Brems_fit due to large differences between the original and test cross sections (see the descriptions of parameters No. 3.14.1–2). If the reduced value of κ_{\max} is less than kmin_fit, this is treated as a terminal error. If there is no additional reduction of κ_{\max} in Brems_fit, then this test is not performed. If the user-specified value of kmin_fit is non-positive, then kmin_fit is reset automatically to $\max(\kappa_{\max})/2$ before starting stage 3. The default value of parameter “kmin_fit” is 1 (i.e., any reduction of κ_{\max} is allowed in stage 3).
- 3.2.3–4. “**fitRange_CS**” and “**fitRange_DCS**” (alias “fitRange” for both) control the width of the fitting interval when fitting the function $\text{CS}(\kappa_{\max})$ or $\text{DCS}(\kappa_{\max})$, respectively. By default, the number of points (i.e., values of κ_{\max}) in the fitting interval (N_{fit}) is calculated according to Eq. (1.5.11a) when fitRange_(D)CS is equal to 2, or according to Eq. (1.5.11b) when fitRange_(D)CS is equal to 1. The calculated value of N_{fit} is rounded to the nearest integer. It is also possible to specify the value of N_{fit} using parameter “Nfit_CS” or “Nfit_DCS” (see the description of parameters No. 3.2.5–6). If fitRange_(D)CS is equal to 3, then both values of N_{fit} will be tried, and the fitted (D)CS will be calculated as the average of the least squares estimates corresponding to each of the two fitting intervals. The default values of parameters fitRange_CS and fitRange_DCS are equal to 3 and 2, respectively. If $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$, then a different default value of fitRange_(D)CS is used: in this case, both fitRange_CS and fitRange_DCS are equal to 1 by default.
- 3.2.5–6. “**Nfit_CS**” and “**Nfit_DCS**” (alias “Nfit” for both) specify the number of values of κ_{\max} inside the κ_{\max} -fitting interval when fitting the dependence $\text{CS}(\kappa_{\max})$ or $\text{DCS}(\kappa_{\max})$, respectively. This number corresponds to fitRange_(D)CS=2 (the number corresponding to fitRange_(D)CS=1 will be less by half). If Nfit_(D)CS<0, then this parameter will be interpreted as the opposite of the value of K that must be used for calculating the value of N_{fit} corresponding to fitRange_(D)CS=2 according to Eq. (1.5.11a). If Nfit_(D)CS=0, then this number will be calculated automatically from the values of parameters fitRange_(D)CS, shift_k_mode_(D)CS and kmax_fit using Eq. (1.5.11a). In the case shift_k_mode_(D)CS=3, the value of Nfit_(D)CS (in conjunction with fitRange_(D)CS) defines the minimum width of the fitting interval (corresponding to shift 0). The default value of parameters “Nfit_CS” and “Nfit_DCS” is equal to 0.
- 3.2.7–8. “**shift_k_max_CS**” and “**shift_k_max_DCS**” (alias “shift_k_max” for both) are equal to the maximum shift of the endpoint of the fitting interval during the nonlinear fitting of the functions $\text{CS}(\kappa_{\max})$ and $\text{DCS}(\kappa_{\max})$, respectively (see Section 1.5 and Section 1.6). The endpoint of the fitting interval is changed in increments of 1 for shift_k_max_(D)CS+1 fitting cycles. In each case, the starting point of the interval is recalculated (see the description of parameters No. 3.2.3–4), so that the entire interval is shifted in the direction of the decreasing κ_{\max} relative to the original interval. The fitting is performed starting with maximum negative shift (-shift_k_max_(D)CS) and ending with zero shift (i.e., the original fitting interval). In the case “fitRange_(D)CS=3”, each “shift” corresponds to two fitting cycles differing by the width of the fitting interval but having the same endpoint. In this case, the fitted (D)CS corresponding to each shift is calculated as the arithmetic average of the two least squares estimates corresponding to each of the two widths of the fitting interval. After performing the fitting for all shift_k_max_(D)CS + 1 shifts, the arithmetic average of the optimal values of (D)CS corresponding to all shifts is used as the optimal κ_{\max} -fitted (D)CS. The standard deviation of the average fitted (D)CS over all shifts contributes to the estimate of the overall uncertainty of the κ_{\max} -fitted (D)CS, except when the relative range of variation of the (D)CS in the fitting interval corresponding to “shift 0” is less than 0.001 (i.e., 0.1 %), in which case the fitting is not performed (i.e., the final (D)CS is set equal to the unfitted (D)CS corresponding to the largest value of κ_{\max}), and the standard deviation is set equal to the range of variation of the (D)CS corresponding to shift

0. When the angular integral of the κ_{\max} -fitted DCS can be estimated with sufficient accuracy, i.e., when $\text{fitMode} \neq 0$ and the limiting values of θ are 0 and 180° and the maximum angular increment is less than or equal to 1° , then the average value of the κ_{\max} -fitted DCS integral (over all shifts of DCS) is used, too, when calculating the final fitted CS and its standard deviation. The final fitted CS is equal in this case to the arithmetic average of the original κ_{\max} -fitted CS (averaged over all shifts of the CS) and the average fitted DCS integral (averaged over all shifts of the DCS). Parameter “ $\text{shift_k_max_ (D)CS}$ ” is one of two alternative parameters used to specify the maximum shift. Another one is parameter No. 3.2.9 “ shift_k_max_ratio ”. The final value of the maximum shift is equal to the smaller of the two values corresponding to each of the two parameters. Parameter “ $\text{shift_k_mode_ (D)CS}$ ” is used only when parameter “ $\text{shift_k_mode_ (D)CS}$ ” is equal to 1 (see the description of parameters No. 3.2.14–15). When parameter “ $\text{shift_k_mode_ (D)CS}$ ” is equal to 1 (the default value of the latter parameter), then the default value of parameter “ $\text{shift_k_max_ (D)CS}$ ” is very large (1000). Consequently, the maximum shift is in this case determined using only the value of parameter “ shift_k_max_ratio ” by default. When parameter “ $\text{shift_k_mode_ (D)CS}$ ” is greater than 1, then the default value of parameter “ $\text{shift_k_max_ (D)CS}$ ” is equal to 19, which indicates 20 equidistant fitting intervals (see also the description of parameters No. 3.2.14–15).

- 3.2.9. “**shift_k_max_ratio**” is used for an alternative estimation of the maximum shift of the endpoint of the fitting interval (see also the description of parameters No. 3.2.3–4). It is equal to the ratio of the maximum shift and N_{fit} (the meaning of N_{fit} is explained in Section 1.5.1). The actual value of the maximum shift is equal to the smaller of two values: $\text{shift_k_max_ (D)CS}$ (described above) and $\text{shift_k_max_ratio} * N_{\text{fit}}$. This parameter is used only when parameter “ shift_k_mode_CS ” or “ shift_k_mode_DCS ” is equal to 1 (see the description of parameters No. 3.2.14–15). The default (and maximum allowed) value of this parameter is 0.25.
- 3.2.10. “**range_ratio_max**” is the maximum allowed ratio of the values of the range of variation of the CS in any two “shifts” (see the description of parameters No. 3.2.7–8). All shifts where the absolute range of variation of the CS exceed the minimum observed range of variation of the CS by a factor greater than “ range_ratio_max ” are excluded. The default value of this parameter is equal to 10.
- 3.2.11. “**fit_SF_DCS**” is the number 1, 2 or ± 3 , specifying the type of PW data that must be used for κ_{\max} -fitting by the function (1.5.1) or (1.5.10) when $\text{fitMode} \neq 0$: the shape function (SF) data or the DCS data. “ $\text{fit_SF_DCS}=1$ ” indicates the SF data, and “ $\text{fit_SF_DCS}=2$ ” indicates the DCS data (the other type of the κ_{\max} -fitted data are obtained by multiplication or division of the specified κ_{\max} -fitted data by the κ_{\max} -fitted CS, respectively). If $|\text{fit_SF_DCS}|=3$ and the scaling factor μ in Eq. (1.5.12a) is approximately constant in a sufficiently wide angular range where the partial-wave DCS is an increasing function of κ_{\max} , then the program will switch from fitting the DCS to fitting the SF after the maximum angle of the mentioned angular range (this endpoint is always close to the angle where the dependence $\text{DCS}(\kappa_{\max})$ reverses the direction of change). The difference between $\text{fit_SF_DCS}=+3$ and $\text{fit_SF_DCS}=-3$ is that in the former case the μ -correction of the DCS will be applied (in addition to the mentioned switch from fitting the DCS to fitting SF), whereas in the latter case the μ -correction will not be applied. See also the descriptions of parameters “ $\text{thr_range_mu}[1,2]$ ” (No. 3.6.12–13) and “ $\text{tol_mu}[1,2]$ ” (No. 3.6.14–15). The default value of parameter “ fit_SF_DCS ” is equal to 2.
- 3.2.12. “**tol_err_test**” is the maximum allowed relative difference of the original (unfitted) PW CS and the κ_{\max} -fitted CS for performing the error test. If the absolute value of the mentioned difference is less than tol_err_test , then the error test will be performed, otherwise it will not be performed. The error test is performed by redoing the κ_{\max} -fitting (i.e., recalculating the

κ_{\max} -fitted CS) at several smaller values of the endpoint of the range of values of κ_{\max} used for the fitting, and then comparing the values of c returned by the fitting procedure with the original (“optimal”) value, which corresponds to the absolute maximum of the mentioned endpoint (defined by Eq. (1.5.3)). The main purpose of the error test is determining the degree of correlation between two quantities related to the accuracy of extrapolation:

- 1) the relative difference between the fitted value of c and the original value of CS,
- 2) the relative difference between the fitted value of c and the exact value of CS.

Since the exact value of CS (corresponding to $\kappa_{\max} \rightarrow \infty$) is not always available, the fitted value corresponding to $\kappa_{\max} = K$ is used in its place if the relative correction of the CS due to the extrapolation is small enough (i.e., less than `tol_err_test`). If the correlation between the mentioned two quantities is strong enough, then it may become possible to formulate a simple rule (for example, multiplication by a constant factor) for determining an approximate upper bound of the relative uncertainty of the final estimate of the CS obtained by extrapolation, given the value of the first quantity, which is the one that is observed directly. The default value of parameter “`tol_err_test`” is 0 (i.e., the error test is not performed).

3.2.13. “**fitMode**” is an integer number equal to 0, ± 1 or 2. If `fitMode` \neq 0, then both the CS and the DCS data will be processed. If `fitMode` = 0, then only the CS will be fitted. If `fitMode` = -1 , then the nonlinear fitting of the DCS as a function of κ_{\max} will not be performed; only the smoothing (i.e., calculation of the moving average as described in Section 1.5.3) and the optional angular spline fitting and extrapolation (see Section 1.7.1) will be performed. If `fitMode` $>$ 0, then the mentioned κ_{\max} -fitting of the DCS will be performed (possibly followed by the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, as described in Section 1.7.2). The cases `fitMode` = 1 and `fitMode` = 2 differ only in treatment of irrecoverable errors during this fitting (see the description of parameter No. 3.14.3 “`nErrMax`”). The default value of parameter “`fitMode`” is 1.

3.2.14–15. “**shift_k_mode_CS**” and “**shift_k_mode_DCS**” (alias “`shift_k_mode`” for both) specify the method used for defining the κ_{\max} -fitting intervals (“shifts”) when fitting the dependence $CS(\kappa_{\max})$ or $DCS(\kappa_{\max})$, respectively. Each of these two parameters must be equal to 1, 2, or 3. The meanings of these values are explained below:

- 1 – shifting by 1 for `shift_k_max_(D)CS + 1` fits (see the description of parameters No. 3.2.7–8),
- 2 – `shift_k_max_(D)CS + 1` equidistant (and possibly overlapping) fitting intervals of fixed width (corresponding to `fitRange_(D)CS = 1` or 2) for `shift_k_max_(D)CS + 1` fits inside a wider interval defined by parameter “`fitRegionRatio_(D)CS`”,
- 3 – `shift_k_max_(D)CS + 1` fitting intervals with a fixed endpoint (equal to the maximum `kmax`), but with different and equidistant starting points for `shift_k_max+1` fits inside a wider interval defined by parameter “`fitRegionRatio_(D)CS`” (the value of parameter “`fitRange_(D)CS`” indicates in this case the width of the last, i.e., narrowest one of those intervals).

The default value of parameters “`shift_k_mode_CS`” and “`shift_k_mode_DCS`” is 1.

3.2.16–17. “**fitRegionRatio_CS**” and “**fitRegionRatio_DCS**” (alias “`fitRegionRatio`” for both) are used only when `shift_k_mode_(D)CS` $>$ 1. The value of each of these two parameters is interpreted as the ratio of the interval containing all the fitting intervals (“shifts”) to the maximum value of κ_{\max} when fitting the dependence $CS(\kappa_{\max})$ or $DCS(\kappa_{\max})$, respectively. The endpoint of the mentioned wider interval is equal to $\max(\kappa_{\max})$. The default value of these two parameters is equal to 0.8.

3.2.18–19. “**maxMovingAvgErrRatio_CS**” and “**maxMovingAvgErrRatio_DCS**” (alias “`maxMovingAvgErrRatio`” for both) are used only when `shift_k_mode_(D)CS` $>$ 1. The

value of each of these two parameters indicates the maximum allowed ratio of the moving average rms error to its minimum value among the shifts when fitting the dependence $CS(\kappa_{\max})$ or $DCS(\kappa_{\max})$, respectively. The shifts characterized by a greater value of the mentioned ratio are ignored. This is one of the three criteria used for shift selection when $\text{shift_k_mode_}(D)CS > 1$. The other two criteria are defined by parameters “range_ratio_max” and “maxShiftErrRatio_(D)CS”. The default value of parameters “maxMovingAvgErrRatio_CS” and “maxMovingAvgErrRatio_DCS” is very large (10^{30}), which is equivalent to absence of any constraints on the mentioned ratio.

3.2.20–21. “**maxShiftErrRatio_CS**” and “**maxShiftErrRatio_DCS**” (alias “maxShiftErrRatio” for both) are used only when $\text{shift_k_mode_}(D)CS > 1$. This is one of the three criteria used for shift selection when $\text{shift_k_mode_}(D)CS > 1$ (the other two criteria are defined by parameters “range_ratio_max” and “maxMovingAvgErrRatio_(D)CS”). This criterion is based on the value of a particular property of the fitted κ_{\max} -dependence of the (D)CS (such as the rms value of the residuals). The meaning of the mentioned property is defined by parameter “shiftSelection_CS” or “shiftSelection_DCS”, respectively (see the description of parameters No. 3.2.22–23). “maxShiftErrRatio_(D)CS” indicates the maximum allowed ratio of the variable defined by “shiftSelection_(D)CS” to its minimum value among the shifts. In the case “shiftSelection_(D)CS=2”, the valid values of the (D)CS are from $\text{optimalValue} / \text{maxShiftErrRatio_}(D)CS$ to $\text{optimalValue} * \text{maxShiftErrRatio_}(D)CS$, where “optimalValue” is either the maximum fitted (D)CS, or the minimum fitted (D)CS (see the description of parameters No. 3.2.22–23). Parameter “maxShiftErrRatio_(D)CS” can be greater than 1 only when parameter “Npasses_(D)CS” is equal to 1 (either by default, or as requested by the user). The default value of parameters “maxShiftErrRatio_CS” and “maxShiftErrRatio_DCS” is equal to 1 (this means that only one shift will be selected).

3.2.22–23. “**shiftSelection_CS**” and “**shiftSelection_DCS**” (alias “shiftSelection” for both) are used only when $\text{shift_k_mode_}(D)CS > 1$, in conjunction with parameter “maxShiftErrRatio_CS” or “maxShiftErrRatio_DCS”, respectively (see the description of parameters No. 3.2.20–21). Parameter “shiftSelection_(D)CS” defines the meaning of the variable that is minimized or maximized during the selection of the “optimal” fitting interval. The possible values of these two parameters are 1, 2, and 3. In addition, parameter “shiftSelection_DCS” is allowed to be equal to 4. The meanings of these values are explained below:

- 1 – minimum product of the rms residual and the uncertainty of the κ_{\max} -fitted (D)CS,
- 2 – maximum value of the κ_{\max} -fitted (D)CS if it is an increasing function of κ_{\max} , or minimum value otherwise,
- 3 – minimum autocorrelation of residuals of fitting the dependence $CS(\kappa_{\max})$ or $DCS(\kappa_{\max})$,
- 4 – minimum sum of the mean squared relative residual of the angular spline fitting (smoothing) and of the squared relative difference of the fitted CS and the angular integral of the κ_{\max} -fitted DCS (only “shiftSelection_DCS” is allowed to be equal to this value).

If parameter “shiftSelection_DCS” is equal to 1, 2 or 3, then the shift selection is performed for each value of the angle θ independently. Consequently, the κ_{\max} -fitting intervals for different angles may be different (their endpoints are written to the “DCS_parms_” file, which is described in Section 6.20). Conversely, the selection criterion defined by “shiftSelection_DCS=4” allows selection only of the *same* shift for all values of the angle, because this selection criterion is based on the overall shape of the angular dependence of the κ_{\max} -fitted DCS (after the angular spline fitting). The default values of parameters “shiftSelection_CS” and “shiftSelection_DCS” are equal to 1 and 4, respectively.

- 3.2.24–25. “**Npasses_CS**” and “**Npasses_DCS**” (alias “**Npasses**” for both) specify the number of overall “passes” when fitting the κ_{\max} -dependence of CS or DCS, respectively, in conjunction with the option `shift_k_mode_(D)CS > 1`. If `Npasses=2`, then the first pass will be used only to determine the optimal endpoints of the fitting interval for (D)CS (and for each angle). Those endpoints are stored in the arrays `kStart` and `kEnd`. The second pass will use those values of `kStart` and `kEnd` in a manner similar to the case “`shift_mode_(D)CS=1`”, i.e., by performing the κ_{\max} -fitting in several fitting intervals of equal width, which are shifted by 1 relative to each other (the mentioned values of `kStart` and `kEnd` correspond to “shift 0”, i.e., `kEnd` is used as the maximum value of κ_{\max}). Eight parameters are allowed to have different values for each of the two passes: “`fitRange_(D)CS`”, “`shift_k_max_(D)CS`”, “`thr_ratio_h_(D)CS`”, and “`fitFunc_(D)CS`”. The values of these parameters corresponding to pass 2 are specified by inserting “2” in the parameter name before “_CS” or “_DCS”: “`fitRange2_(D)CS`”, “`shift_k_max2_(D)CS`”, “`thr_ratio_h2_(D)CS`”, “`fitFunc2_(D)CS`”. The default value of parameter “`Npasses_(D)CS`” is equal to 1 when `shift_k_mode_(D)CS=1`, and to 2 when `shift_k_mode_(D)CS > 1`.
- 3.2.26–27. “**fitRange2_CS**” and “**fitRange2_DCS**” (alias “**fitRange2**” for both) specify the value of parameter “`fitRange_CS`” or “`fitRange_DCS`”, respectively, during pass No. 2 (see the descriptions of parameters No. 3.2.24–25 and No. 3.2.3–4). The default value of parameters “`fitRange2_CS`” and “`fitRange2_DCS`” is equal to 2.
- 3.2.28–29. “**shift_k_max2_CS**” and “**shift_k_max2_DCS**” (alias “**shift_k_max2**” for both) specify the value of parameter “`shift_k_max_CS`” or “`shift_k_max_DCS`”, respectively, during pass No. 2 (see the descriptions of parameters No. 3.2.24–25 and No. 3.2.7–8). The default value of these two parameters is equal to 19.

6.3. Parameters defining the set of angles

- 3.3.1–5. These parameters are the same as parameters No. 2.3.1–5 of Bremsstrahlung (see Section 5.3), i.e., they specify the limits of variation of the photon emission angle θ and the number of values of θ . If the calculation process starts from stage 3 (“`firstStage=3`”) and neither of these five parameters is specified by the user explicitly, then all angles will be read from the first column of the file with the DCS data created in stage 2 by subroutine “`Bremsstrahlung`” (or from the first line of this file, if it was created using a version of BREMS older than 1.5.0.0). If the calculation process starts from stage 3 and at least one of these parameters is specified explicitly, then the set of angles will be constructed as explained in the descriptions of parameters No. 2.3.1–5 of Bremsstrahlung (see Section 5.3), and the program will attempt to locate the corresponding lines (or columns, if the file was created using the version of BREMS older than 1.5.0.0) in the input file with the DCS data. If the data for at least one of the angles is not available, then the program will quit with an error message. *Note:* The option “`np1=0 np2=0`” is equivalent to the option “`fitMode=0`” (see also the description of parameter No. 3.2.13).

6.4. Parameters controlling the accuracy of intermediate calculations

- 3.4.1–3. “**tol1**”, “**tol2**”, and “**tol3**” (alias “**tol**” for all three) are, respectively, the tolerances of the three parameters c (or b'), d' , and h' of the nonlinear fitting function (1.5.1), respectively (see also Eqs. (1.5.7)). To be more precise, when c belongs to the set of independently varied parameters (whereas b is calculated by linear regression), `tol1` is the tolerance of the ratio $c / \Delta(D)CS$, where $\Delta(D)CS$ is the absolute range of variation of the original PW CS or PW DCS inside the κ_{\max} -fitting interval. The iterative fitting procedure is terminated when the change of the values of $c / \Delta(D)CS$ (or b'), d' , and h' between two iterations becomes less than the corresponding tolerances (if the absolute changes are greater than the specified tolerances, then fitting will be terminated when the relative changes become less than the relative tolerances defined by parameters No. 3.4.4–6). The recommended value of

parameters tol1 and tol2 is 10^{-6} or greater, and the recommended value of tol3 is 10^{-10} or greater. Smaller values may cause a very slow decrease of the sum of squared deviations, resulting in an apparent “lock-up” of the program. The default values of these three parameters are 10^{-6} , 10^{-6} and 10^{-9} , respectively.

- 3.4.4–6. “**rtol1**”, “**rtol2**”, and “**rtol3**” (alias “**rtol**” for all three) are, respectively, the relative tolerances of the three parameters c (or b'), d' , and h' of the nonlinear fitting function (1.5.1), respectively (see also Eqs. (1.5.7)). To be more precise, when c belongs to the set of independently varied parameters (whereas b is calculated by linear regression), rtol1 is the relative tolerance of $|c - (\text{D})\text{CS}_0|$, where $(\text{D})\text{CS}_0$ is the value of the original PW CS or PW DCS corresponding to the start of the fitting interval of κ_{max} . The relative change of a varied parameter is checked only if its absolute change is greater than the absolute tolerance defined by one of parameters No. 3.4.1–3. The default value of these three parameters is equal to 10^{-9} .
- 3.4.7. “**tol_range_max**” is the maximum relative range of CS or DCS allowed for skipping the nonlinear fitting (it should be noted that the CS and DCS, which are called “original” or “unfitted” in the following descriptions of the parameters, may have been smoothed with respect to κ_{max} (see Section 1.5.3) and fitted or extrapolated with respect to θ (see Section 1.7.1)). If the range of relative variation of $(\text{D})\text{CS}$ in the current range of values of κ_{max} is less than the variable “**tol_range**”, then the κ_{max} -fitting will not be performed, i.e., the final $(\text{D})\text{CS}$ will be set equal to the one obtained by truncating the series at the last (greatest) value of κ_{max} . Otherwise, the fitting will be performed and the final $(\text{D})\text{CS}$ will be set equal to the value of c returned by the fitting procedure. If the dependence of $(\text{D})\text{CS}$ on κ_{max} is not suitable for fitting (i.e., non-monotonous or with a wrong curvature or, in the case of the DCS, out-of-sequence with respect to the one corresponding to the previous value of θ), or if the fitted value is incorrect (i.e., it is on the wrong side of the range of variation of the $(\text{D})\text{CS}$, or negative, or exceeds the original value by a factor greater than 20, or differs from the original value by more than 200 widths of the range of variation in the case of the DCS or by more than 25 widths of the range of variation in the case of the CS), then **tol_range** will be increased by a factor of 2 or 2.5. This is done until the mentioned error condition does not occur or until **tol_range** becomes greater than or equal to **tol_range_max**. If **tol_range** is equal to **tol_range_max**, then the behavior of the program after detecting the mentioned error condition is different for CS and for DCS. In the case of fitting the CS, the program terminates the fitting for the current “shift” with an error message and flags this shift as a fitting failure (during the further processing, the CS fitting results corresponding to this shift will be excluded). In the case of fitting the DCS, each error point is replaced by the original “unfitted” value by default, as long as the number of consecutive error points in the angular dependence of DCS does not exceed a predefined value specified by parameter “**nErrMax**”. Otherwise, the further behavior of the program during the fitting of the DCS depends on the value of parameter No. 3.4.8 “**tol_range_max2**”. The starting value of **tol_range** is 10^{-3} , and the default value of parameter “**tol_range_max**” is 0.02.
- 3.4.8. “**tol_range_max2**” is used during κ_{max} -fitting of the DCS after the number of consecutive irrecoverable error points in the angular dependence of the DCS exceeds the value specified by parameter “**nErrMax**”. If **tol_range_max2** is equal to **tol_range_max**, then the program terminates the fitting for the current “shift” with an error message and flags this shift as a fitting failure (during the further processing, the DCS fitting results corresponding to this shift will be excluded). If **tol_range_max2** is greater than **tol_range_max**, then the variables **tol_range** and **tol_range_max** are increased simultaneously (in the same steps as before). This is done until the number of consecutive error points exceeds “**nErrMax**”, or until **tol_range_max** exceeds **tol_range_max2** (in the latter case, the current shift is flagged as a fitting failure). Parameter “**tol_range_max2**” makes it possible to increase **tol_range** not after the first fitting error, but only after the number of consecutive errors exceeds **nErrMax** (see

also the description of parameter No. 3.4.7 “tol_range_max”). Parameter “tol_range_max2” cannot be less than “tol_range_max”. The default value of “tol_range_max2” is 0.05.

One of the criteria used for determining if the DCS as a function of κ_{\max} at a given value of θ and in a given range of values of κ_{\max} may be fitted by the function (1.5.1) or (1.5.10) is whether the direction and rate of change of the DCS with increasing κ_{\max} are correct as compared to the DCS corresponding to the previous value of θ . Further on, the mentioned direction will be specified using the term “sign”: the sign is negative (“-1”) when the DCS decreases with decreasing rate, zero (“0”) when there is no significant change (i.e., when the relative range of the DCS in a given range of κ_{\max} is less than the mentioned variable tol_range), positive (“+1”) when the DCS increases with decreasing rate, and undefined (“+2”) when the DCS is a non-monotonous function of κ_{\max} or when its curvature is not consistent with a tendency to saturation (i.e., when the absolute value of the first derivative is not decreasing). The correct sequence of signs of the DCS corresponding to a set of increasing values of θ is the following:

- 1) a range of values of θ where all DCS have the sign +1,
- 2) a range of values of θ where all DCS have the sign 0,
- 3) a range of values of θ where all DCS have the sign -1.

One or two of these ranges may be absent, but their sequence may not be reversed. In short, the “sign” may not increase with increasing θ , and the sign “+2” is not allowed. However, the angular spline fitting of the angular dependence of the κ_{\max} -fitted DCS (see Section 1.7) may eliminate some types of deviations from this rule. In particular, a sequence of DCS with sign 0 interspersed with DCS with sign -1 is sometimes observed at large values of T_1 and k / T_1 , and the resulting “dips” in the angular dependence of the fitted DCS are eliminated by the mentioned angular spline fitting. Consequently, only two cases are treated as an error: (1) a non-monotonous dependence of CS or DCS on κ_{\max} (or a dependence that does not show a tendency to saturation), and (2) a DCS with sign -1 followed by a DCS with sign +1 (any number of DCS with sign 0 may be in between). In these cases, the variable “tol_range” is increased as explained above.

6.5. Parameters controlling usage of reference functions

Up to 2 user-specified reference functions may be used for the purpose of angular spline fitting of the ratio of the DCS and the reference function (see Section 1.7.1), or for the polynomial fitting of the ratio of the μ -corrected DCS and the reference function (see Section 1.5.4), or for the large-angle extrapolation in the case of small relative corrections (see Section 1.7.3), or for comparison of the final values of (D)CS with the corresponding reference values. The reference CS is calculated as the ratio of the reference DCS and the reference shape function (SF). Consequently, for each type of the reference function, there must be two data files: a file with the reference DCS data, and a file with the corresponding reference SF data. These files must contain at least two columns of numbers and a line with column headers. The first column must contain the values of the angle (in degrees), and the second column must contain the values of the reference DCS or SF. Parameters of this subgroup are used to specify the names of these files, the approximations to be used in order to create these files if they don’t exist, and the conditions for using the reference functions. Descriptions of these parameters are presented below.

3.5.1–2. “**prefix_ref_pn1**” (aliases “prefix_ref1”, “prefix_ref_pn”, “prefix_ref”) and “**prefix_ref_pn2**” (aliases “prefix_ref2”, “prefix_ref_pn”, “prefix_ref”) are the names of the folders containing the data files of point-nucleus reference functions No. 1 and No. 2, respectively (the folder names must end with the forward slash ‘/’ or backslash ‘\’). The suffix “_pn” indicates that those folders must be used only in the case of the point-nucleus approximation (see also the description of parameter No. 1.2.1 “nuclear_model”). If the corresponding files do not exist, then the analytical reference DDCS will be calculated using

the point-nucleus approximation (with the nuclear form factor equal to 1), and written to files, which will be created in those folders. By default, these two parameters are equal to the empty string, which means that the reference function data files must be in the current folder.

3.5.3–4. “**prefix_ref_fn1**” (aliases “**prefix_ref1**”, “**prefix_ref_fn**”, “**prefix_ref**”) and “**prefix_ref_fn2**” (aliases “**prefix_ref2**”, “**prefix_ref_fn**”, “**prefix_ref**”) are the names of the folders containing the data files of finite-nucleus reference functions No. 1 and No. 2, respectively (the folder names must end with the forward slash ‘/’ or backslash ‘\’). The suffix “_fn” indicates that those folders must be used only in the case of a finite-nucleus approximation (see also the description of parameter No. 1.2.1 “**nuclear_model**”). If the corresponding files do not exist, then the analytical reference DDCS will be calculated using the finite-nucleus approximation (with the nuclear form factor calculated according to Eq. (1.1.30b)), and written to files, which will be created in those folders. By default, these two parameters are equal to the empty string, which means that the reference function data files must be in the current folder.

3.5.5–6. “**suffix_ref1**” and “**suffix_ref2**” (alias “**suffix_ref**” for both) are the suffixes to be used when forming the names of the files with the data of reference functions No. 1 and No. 2, respectively. If **auto_naming_ref**=1 or **auto_naming_ref**=2 (see the description of parameters No. 3.5.7–8), then the suffix is inserted before the extension “.txt”. If **auto_naming_ref**=0 and the file name specified by parameter “**name_ref_DCS**” or “**name_ref_SF**” includes the extension “.txt” (see the descriptions of parameters No. 3.5.11–14), then the suffix is inserted before the extension. Otherwise, the suffix is appended to the file name (after the extension, if it exists), and the extension “.txt” is added (consequently, the suffix should not include the extension “.txt”). If the suffix is the empty string, then the file name specified by parameter “**name_ref_DCS**” or “**name_ref_SF**” is not modified (the extension “.txt” is not added in this case). The default value of parameters “**suffix_ref1**” and “**suffix_ref2**” is the empty string.

3.5.7–8. “**auto_naming_ref1**” and “**auto_naming_ref2**” (alias “**auto_naming_ref**” for both) are “switches” (0, 1 or 2) indicating if the names of the files (excluding the folder name specified by parameters No. 3.5.1–2) with the data of reference DCS No. 1 and No. 2, respectively, must be formed using the default naming rule. The default file name format is

$$\langle \text{prefix_ref}[\text{pn}, \text{fn}][1,2] \rangle \langle \text{prefix2} \rangle \text{Z_T.TE} \pm \text{XX_k.kkkE} \pm \text{YY} \langle \text{suffix_ref}[1,2] \rangle .\text{txt},$$

where “Z” is the atomic number, “T.TE±XX” is the kinetic energy of the incident electron (MeV) rounded to 2 significant digits in scientific notation, “k.kkkE±YY” is the energy of the bremsstrahlung photon (MeV) rounded to 4 significant digits in scientific notation (“E±XX” and “E±YY” are the respective decimal exponents), and “prefix2” is a prefix, which is either formed automatically (when **auto_naming_ref**=1) or obtained by concatenating the string “DCS” or “ShapeFn” with the prefix specified by parameter “**prefix2_ref1**” or “**prefix2_ref2**” (when **auto_naming_ref**=2). In the case “**auto_naming_ref**[1,2]=1”, prefix2 consists of three components, which are concatenated with each other:

- “DCS” or “ShapeFn” for the DCS and shape function data, respectively,
- “_Born_”, “_SM_LO_” or “_SM_NLO_” indicating the approximation used (Born, leading-order Sommerfeld-Maue, or next-to-leading order Sommerfeld-Maue, respectively),
- “_screened_”, which is included only when screening of the nuclear charge by the electron cloud is taken into account.

If this parameter is 2, then “prefix2” is formed by concatenating the string “DCS” or “ShapeFn” with the string specified by parameter “**prefix2_ref1**” or “**prefix2_ref2**” (No. 3.5.9–10). If this parameter is 0, then the name of the reference DCS data file must be

specified by parameters No. 3.5.11–12, and the name of the file with the reference shape function data must be specified by parameters No. 3.5.13–14. If this parameter is 1, then the default naming rule is used. In such a case, the second and third components of “prefix2” (see above) are determined from the values of parameters “appr_ref[1,2]” (No. 3.5.17–18) and “IV_ref[1,2]” (No. 3.5.19–20), respectively. The default value of parameters “auto_naming_ref[1,2]” is equal to 1, indicating the default naming rule.

3.5.9–10. “**prefix2_ref1**” and “**prefix2_ref2**” (alias “prefix2_ref” for both) are the prefixes to be inserted after the string “DCS” or “ShapeFn” at the beginning of the names of the files with the data of reference DCS No.1 and No.2, respectively, when parameter “auto_naming_ref1” or “auto_naming_ref2” is equal to 2 (see the description of parameters No. 3.5.7–8). The default value of those two parameters is “_fitted_”.

3.5.11–12. “**name_ref_DCS1**” and “**name_ref_DCS2**” (aliases “name_ref_DCS” for both) are the names of the files (including the extension, but excluding the folder name specified by parameters No. 3.5.1–2) with the data of reference DCS No. 1 and No. 2, respectively, which must be used when parameter “auto_naming_ref1” or “auto_naming_ref2” is 0. The default values of these two parameters are “ref1_DCS.txt” and “ref2_DCS.txt”, respectively.

3.5.13–14. “**name_ref_SF1**” and “**name_ref_SF2**” (aliases “name_ref_SF” for both) are the names of the files (including the extension, but excluding the folder name specified by parameters No. 3.5.1–2) with the data of reference shape function No. 1 and No. 2, respectively, which must be used when parameter “auto_naming_ref1” or “auto_naming_ref2” is equal to 0. The default values of these two parameters are “ref1_SF.txt” and “ref2_SF.txt”, respectively.

3.5.15–16. “**col_ref1**” and “**col_ref2**” (aliases “col_ref” for both) is the sequence number of the column with the values of reference function No.1 and No.2, respectively, in the corresponding data file. This number cannot be less than 2, because the first column is always assumed to contain the values of the photon emission angle θ . The default value of these two parameters is equal to 2.

3.5.17–18. “**appr_ref1**” and “**appr_ref2**” (alias “appr_ref” for both) indicate the approximation that must be used in order to create the DCS and SF data files corresponding to reference function No. 1 and No. 2, respectively, if these files do not exist. In addition, these parameters are used when forming the default names of the reference DCS and SF data files (see the description of parameters No. 3.5.7–8). The allowed values of these parameters are the same as the allowed values of parameter “appr” when BREMS is used for calculating the angular dependence of the DCS according to one of the approximations described in Section 1.1.2 and Section 1.1.3 (this mode of operation of BREMS is described in Section 7). I.e., three values are allowed:

- 0 – Born approximation (calculated by integrating Eq. (1.1.28) with respect to Ω_{p_2} numerically, or by evaluating the analytical expression (1.1.36) or (1.1.32)),
- 1 – leading-order Sommerfeld-Maue approximation (numerical integral of Eq. (1.1.40) with respect to Ω_{p_2} , plus the screening correction according to Eq. (1.1.46)),
- 2 – Sommerfeld-Maue approximation with the next-to-leading order (NLO) correction (the NLO correction term is calculated by numerical integration of Eq. (1.1.44) with respect to Ω_{p_2}).

The default values of parameters “appr_ref1” and “appr_ref2” are equal to 0 and –2, respectively.

3.5.19–20. “**IV_ref1**” and “**IV_ref2**” (alias “IV_ref” for both) indicate presence or absence of the screening correction when calculating the approximate DCS and SF using the approximation defined by parameter “appr_ref1” or “appr_ref2”, respectively. In addition, these parameters are used when forming the default names of the reference DCS and SF data files (see the description of parameters No. 3.5.7–8). Four values are allowed:

± 1 – no screening (pure Coulomb potential),

± 2 – screening function equal to a linear combination of exponentials (1.1.34a),

A negative value of “IV_ref1” or “IV_ref2” indicates that the program must quit with an error message instead of attempting to re-create the missing DCS or SF data file.

The default value of parameters “IV_ref1” and “IV_ref2” is equal to $\min(\text{IV}, 2)$, where “IV” is the type of the interaction potential, indicated by the value of parameter No. 1.1.5.

Note: The other parameters controlling the calculation of the mentioned approximate DCS are described in Section 7.

3.5.21. “**relErr_tol_ref**” (alias “rel_err_tol”) is the relative tolerance when checking the angular dependence of a reference DCS loaded from a file for existence of extra inflection points or extrema. The default value of this parameter is equal to 0.002.

The next twenty parameters define the minimum values T_1 , T_2 and k (in MeV), and the maximum values of $Z\alpha$ and $Z\alpha/\beta_2$ for using the reference DCS No. 1 or No. 2 (here, Z is the atomic number, the variables α and β are defined as in Eq. (1.1.27), and the subscript “2” in “ β_2 ” refers to the outgoing electron). “Using” a particular reference DCS means that it is used during the angular spline fitting of the PW DCS or of the κ_{\max} -fitted DCS as described in Section 1.7, or for the polynomial fitting of the ratio of the μ -corrected DCS and the reference function (see Section 1.5.4), or for comparison with the final fitted DCS at the end of the calculation. The mentioned five thresholds are defined separately for each of the two reference DCS, and for each of the two mentioned types of the angular spline fitting (the angular spline fitting of the PW DCS, and the angular spline fitting of the κ_{\max} -fitted DCS). If at least one of the mentioned five threshold values prevents reference DCS No. 1 or No. 2 from being used for the angular spline fitting of the PW DCS, then the value of “splineRef1” or “splineRef2” will be reset to zero automatically (see the description of parameters No. 3.7.22–24). Similarly, if at least one of the mentioned five threshold values prevents reference DCS No. 1 or No. 2 from being used for the angular spline fitting of the κ_{\max} -fitted DCS, then the value of “splineRef_fitted1” or “splineRef_fitted2” will be reset to zero automatically (see the description of parameters No. 3.8.20–23). If the threshold values do not prevent a particular reference DCS from being used either for the angular spline fitting of the PW DCS or for the angular spline fitting of the κ_{\max} -fitted DCS, then that reference DCS will be also used for the comparison with the final fitted DCS at the end of the calculation, and for the polynomial fitting of the μ -corrected DCS as described in Section 1.5.4, and for the large-angle extrapolation as described in Section 1.7.3 (if the latter uses of that reference DCS have been requested). The reference DCS is identified by the suffix “_1” or “_2” at the end of the parameter name used for specifying a particular threshold value.

3.5.22–23. “**T1_thr0_1**” (aliases “T1_thr1”, “T1_thr0”, and “T1_thr”) and “**T1_thr0_2**” (aliases “T1_thr2”, “T1_thr0”, and “T1_thr”) are the threshold values of T_1 such that the reference DCS No. 1 or No. 2 (respectively) will not be used for the angular spline fitting of the PW DCS if T_1 is less than the corresponding threshold value. If the type of the corresponding screening potential (indicated by the absolute value of “IV_ref1” or “IV_ref2”, respectively) is equal to 1 (no screening), or if the type of the corresponding approximation (indicated by “appr_ref1” or “appr_ref2”, respectively) is equal to 0 (Born approximation), then the default value of the corresponding threshold is equal to 0, and otherwise it is equal to $5 \cdot 10^{-5}$ (the value of zero means that there are no constraints on the magnitude of T_1).

3.5.24–25. “**T2_thr0_1**” (aliases “T2_thr1”, “T2_thr0”, and “T2_thr”) and “**T2_thr0_2**” (aliases “T2_thr2”, “T2_thr0”, and “T2_thr”) are the threshold values of T_2 such that the reference DCS No. 1 or No. 2 (respectively) will not be used for the angular spline fitting of the PW DCS if T_2 is less than the corresponding threshold value. If the type of the corresponding screening potential (indicated by the absolute value of “IV_ref1” or “IV_ref2”, respectively) is equal to 1 (no screening), or if the type of the corresponding approximation (indicated by “appr_ref1” or “appr_ref2”, respectively) is equal to 0 (Born approximation), then the

default value of the corresponding threshold is equal to 0, and otherwise it is equal to $2.5 \cdot 10^{-6}$ (the value of zero means that there are no constraints on the magnitude of T_2).

- 3.5.26–27. “**Ep_thr0_1**” (aliases “Ep_thr1”, “Ep_thr0”, and “Ep_thr”) and “**Ep_thr0_2**” (aliases “Ep_thr2”, “Ep_thr0”, and “Ep_thr”) are the threshold values of the photon energy k such that the reference DCS No. 1 or No. 2 (respectively) will not be used for the angular spline fitting of the PW DCS if k is less than the corresponding threshold value. If the type of the corresponding approximation (indicated by “appr_ref1” or “appr_ref2”, respectively) is equal to 0 (Born approximation), then the default value of the corresponding threshold is equal to 0, and otherwise it is equal to 10^{-10} (the value of zero means that there are no constraints on the magnitude of k).
- 3.5.28–29. “**Z_a_thr0_1**” (aliases “Z_a_thr1”, “Z_a_thr0”, and “Z_a_thr”) and “**Z_a_thr0_2**” (aliases “Z_a_thr2”, “Z_a_thr0”, and “Z_a_thr”) are the threshold values of $Z\alpha$ such that the reference DCS No. 1 or No. 2 (respectively) can be used for the angular spline fitting of the PW DCS only if $Z\alpha$ is less than the corresponding threshold value. The default value of these two parameters is 1 (this is practically equivalent to absence of any constraints on $Z\alpha$, because $Z\alpha < 1$ when $Z \leq 137$).
- 3.5.30–31. “**Z_a_b_thr0_1**” (aliases “Z_a_b_thr1”, “Z_a_b_thr0”, and “Z_a_b_thr”) and “**Z_a_b_thr0_2**” (aliases “Z_a_b_thr2”, “Z_a_b_thr0”, and “Z_a_b_thr”) are the threshold values of $Z\alpha / \beta_2$ such that the reference DCS No. 1 or No. 2 (respectively) can be used for the angular spline fitting of the PW DCS only if $Z\alpha / \beta_2$ is less than the corresponding threshold value. The default value of these two parameters is 10^{10} (this is equivalent to absence of any constraints on $Z\alpha / \beta_2$, because the threshold value is extremely large).
- 3.5.32–33. “**T1_thr_fitted_1**” (aliases “T1_thr1”, “T1_thr_fitted”, and “T1_thr”) and “**T1_thr_fitted_2**” (aliases “T1_thr2”, “T1_thr_fitted”, and “T1_thr”) are the threshold values of T_1 such that the reference DCS No. 1 or No. 2 (respectively) will not be used for the angular spline fitting of the κ_{\max} -fitted DCS if T_1 is less than the corresponding threshold value. If the type of the corresponding screening potential (indicated by the absolute value of “IV_ref1” or “IV_ref2”, respectively) is equal to 1 (no screening), or if the type of the corresponding approximation (indicated by “appr_ref1” or “appr_ref2”, respectively) is equal to 0 (Born approximation), then the default value of the corresponding threshold is equal to 0, and otherwise it is equal to $5 \cdot 10^{-5}$ (the value of zero means that there are no constraints on the magnitude of T_1).
- 3.5.34–35. “**T2_thr_fitted_1**” (aliases “T2_thr1”, “T2_thr_fitted”, and “T2_thr”) and “**T2_thr_fitted_2**” (aliases “T2_thr2”, “T2_thr_fitted”, and “T2_thr”) are the threshold values of T_2 such that the reference DCS No. 1 or No. 2 (respectively) will not be used for the angular spline fitting of the κ_{\max} -fitted DCS if T_2 is less than the corresponding threshold value. If the type of the corresponding screening potential (indicated by the absolute value of “IV_ref1” or “IV_ref2”, respectively) is equal to 1 (no screening), or if the type of the corresponding approximation (indicated by “appr_ref1” or “appr_ref2”, respectively) is equal to 0 (Born approximation), then the default value of the corresponding threshold is equal to 0, and otherwise it is equal to $2.5 \cdot 10^{-6}$ (the value of zero means that there are no constraints on the magnitude of T_2).
- 3.5.36–37. “**Ep_thr_fitted_1**” (aliases “Ep_thr1”, “Ep_thr_fitted”, and “Ep_thr”) and “**Ep_thr_fitted_2**” (aliases “Ep_thr2”, “Ep_thr_fitted”, and “Ep_thr”) are the threshold values of the photon energy k such that the reference DCS No. 1 or No. 2 (respectively) will not be used for the angular spline fitting of the κ_{\max} -fitted DCS if k is less than the corresponding threshold value. If the type of the corresponding approximation (indicated by “appr_ref1” or “appr_ref2”, respectively) is equal to 0 (Born approximation), then the default value of the corresponding threshold is equal to 0, and otherwise it is equal to 10^{-10} (the value of zero means that there are no constraints on the magnitude of k).

3.5.38–39. “**Z_a_thr_fitted_1**” (aliases “Z_a_thr1”, “Z_a_thr_fitted”, and “Z_a_thr”) and “**Z_a_thr_fitted_2**” (aliases “Z_a_thr2”, “Z_a_thr_fitted”, and “Z_a_thr”) are the threshold values of $Z\alpha$ such that the reference DCS No. 1 or No. 2 can be used for the angular spline fitting of the κ_{\max} -fitted DCS only if $Z\alpha$ is less than the corresponding threshold value. The default value of these two parameters is 1 (this is practically equivalent to absence of any constraints on $Z\alpha$, because $Z\alpha < 1$ when $Z \leq 137$).

3.5.40–41. “**Z_a_b_thr_fitted_1**” (aliases “Z_a_b_thr1”, “Z_a_b_thr_fitted”, and “Z_a_b_thr”) and “**Z_a_b_thr_fitted_2**” (aliases “Z_a_b_thr2”, “Z_a_b_thr_fitted”, and “Z_a_b_thr”) are the threshold values of $Z\alpha / \beta_2$ such that the reference DCS No. 1 or No. 2 (respectively) can be used for the angular spline fitting of the κ_{\max} -fitted DCS only if $Z\alpha / \beta_2$ is less than the corresponding threshold value. The default value of these two parameters is 10^{10} (this is equivalent to absence of constraints on $Z\alpha / \beta_2$, because the threshold value is very large).

6.6. Parameters controlling the μ -correction of the partial-wave DCS

Parameters of this subgroup are used to define the conditions of the “ μ -correction” of the DCS (see Section 1.5.4), i.e., optimization of the scale factor μ in Eq. (1.5.12b) and the replacement of the κ_{\max} -fitted DCS obtained by the nonlinear fitting described in Sections 1.5.1 and 1.5.2 with the “ μ -corrected” DCS calculated according to Eq. (1.5.12b).

3.6.1. “**mode_mu**” is used to specify the method of the μ -correction of the DCS (including the method of determining the optimal value of μ) in each “shift”, if the angular interval $\theta_{\text{start}} \leq \theta \leq \theta_{\text{end}}$ with an approximately constant scale factor μ has been found:

(a) if **mode_mu**=-1 and a fixed value of the final scale ratio μ is available (either specified by the user or calculated by the program), then the κ_{\max} -fitted DCS is replaced with the μ -corrected DCS defined by Eq. (1.5.12b) inside the angular range $\theta \geq \theta_{\text{start}}$ or $\theta \leq \theta_{\text{end}}$, depending on whether the PW DCS is a decreasing or increasing function of κ_{\max} , respectively, but the angular polynomial fitting and extrapolation of the μ -corrected DCS is not performed. If a fixed value of the final scale ratio μ is not available or cannot be determined, then the μ -correction is not performed in the current shift and in all subsequent shifts;

(b) if **mode_mu**=0, then the only effect of constant μ is the additional moving-average smoothing of the angular dependence of the normalized PW DCS inside the interval of constant μ prior to the κ_{\max} -fitting (see the end of Section 1.5.4), i.e., the further μ -correction is not performed (which also implies that the program does not attempt to determine the scale factor μ). Instead, the κ_{\max} -fitting by the stretched exponential or polynomial approximation is performed, using the values of the DCS obtained after the mentioned moving-average smoothing. Since this smoothing is always performed prior to the subsequent μ -correction if an angular range with approximately constant μ exists, the option “**mode_mu**=0” corresponds to the least effect of constant μ on processing of the DCS in comparison with non-zero values of parameter “**mode_mu**”;

(c) if **mode_mu**=1, then the values of μ for each shift are optimized by minimizing the deviation of the μ -corrected DCS from the fitting polynomial in the extrapolation range, whereas the degree of the fitting polynomial (**fitDegree_mu**) and the type of the “reference function” used for the mentioned fitting (**fitRef_mu_opt**) are the same for all shifts and determined at the start of stage 3 by minimizing the standard deviation of the μ -corrected DCS over different values of the endpoint of the fitting interval, defined in terms of its offset from the first irregularity of the μ -corrected DCS (**fitEndOffset_mu**), or by minimizing the distortion of the μ -corrected DCS in the extrapolation interval (if only one value of **fitEndOffset_mu** is used);

(d) if mode_mu=2, then fitDegree_mu and fitRef_mu_opt are determined at the start of stage 3 (as in the case mode_mu=1), but the values of μ for each shift are determined as described at the end of Section 1.5.4, i.e., by stretched-exponential extrapolation of the scale ratio $\mu(\kappa_{\max}) = (\text{DCS}(\kappa_{\max}, \theta) - \text{DCS}(K', \theta)) / (\text{DCS}(K, \theta) - \text{DCS}(K', \theta))$, averaged over the angular interval where the absolute value of the relative correction of the PW DCS due to the κ_{\max} -fitting is between the values defined by parameters No. 3.6.2 (“maxCorr_mu”) and No. 3.6.3 (“thrCorr_mu”), if the maximum absolute deviation of the empirical values of μ from 1 (calculated using $\text{DCS}(\kappa_{\max} \rightarrow \infty, \theta)$ instead of $\text{DCS}(\kappa_{\max}, \theta)$ in the above expression of μ) inside the mentioned angular interval is less than the value defined by parameter No. 3.6.4 (“maxDev_mu”). In this case, the polynomial fitting is performed only once for each degree of the fitting polynomial and each value of fitEndOffset_mu, in order to calculate the extrapolated μ -corrected DCS corresponding to the mentioned extrapolated value of μ . If no such angular interval exists, or if its width is less than the parameter No. 3.6.5 (“minWidth_mu”), or if the number of data points inside this interval is less than the value of parameter No. 3.6.6 (“minPoints_mu”), then μ is optimized as in the case mode_mu=1 (i.e., the case mode_mu=2 then becomes equivalent to the case mode_mu=1);

(e) if mode_mu=3, then the values of μ for each shift are determined as in the case mode_mu=2, whereas fitDegree_mu and fitRef_mu_opt are determined for each shift separately by minimizing the standard deviation over different values of fitEndOffset_mu, or the distortion of the μ -corrected DCS in the extrapolation interval (using the previously-determined fixed value of μ).

Note: The μ -correction is not applied in the current shift and in all subsequent shifts if the relative correction of the DCS due to the κ_{\max} -fitting is less than 0.001 inside the entire angular range where the μ -correction would be applied (i.e., at $\theta \geq \theta_{\text{start}}$ if the partial-wave DCS is a decreasing function of κ_{\max} , or at $\theta \leq \theta_{\text{end}}$ if the partial-wave DCS is an increasing function of κ_{\max}).

The default value of parameter “mode_mu” is equal to 3.

In order to minimize the standard deviation of the μ -corrected DCS over different values of the endpoint of the fitting interval (defined in terms of the variable fitEndOffset_mu, which is the offset of the mentioned endpoint from the first irregularity of the μ -corrected DCS), several equidistant values of fitEndOffset_mu are tested. The standard deviation that is being minimized includes an additional term, which reflects the quality of the fit inside the polynomial fitting interval (see Section 1.5.4, in the paragraph following Eq. (1.5.23)). The endpoints of the range of fitEndOffset_mu to be tested are defined by parameters No. 3.6.17–18 (“fitEndOffset_mu_min” and “fitEndOffset_mu_max”), or No. 3.6.20–21 (“fitEndOffset_mu0_min” and “fitEndOffset_mu0_max”), and the number of values of fitEndOffset_mu is specified using parameter No. 3.6.19 (“n_fitEndOffset_mu”). The mentioned optimization of the degree of the fitting polynomial (fitDegree_mu) is performed by testing several values – from the minimum degree defined by parameter No. 3.6.31 (“fitDegree_mu_min2”) to the maximum degree defined by parameter No. 3.6.32 (“fitDegree_mu_max2”) – and selecting the one that corresponds to the least sensitivity of the values of the fitting polynomial in the fitting and extrapolation intervals to the choice of the value of fitEndOffset_mu. The number “2” at the end of the names of the latter two parameters indicates that they must be used only when the PW DCS is a decreasing function of κ_{\max} . Otherwise, parameters No. 3.6.29–30 (“fitDegree_mu_min1” and “fitDegree_mu_max1”) are used. However, they are not allowed to be different from each other (unlike parameters “fitDegree_mu_min2” and “fitDegree_mu_max2”). I.e., when the PW DCS is an increasing function of κ_{\max} , only one value of fitDegree_mu is allowed (it may be specified using the alias “fitDegree_mu1”).

- 3.6.2. “**maxCorr_mu**” (alias “max_corr_mu”) is the maximum relative correction of the PW DCS due to the κ_{\max} -fitting, to be used for determining the optimal value of the scale factor μ for individual “shifts” in the case mode_mu=2 or mode_mu=3 (see the description of parameter No. 3.6.1 “mode_mu”). The default value of this parameter is equal to 0.3.
- 3.6.3. “**thrCorr_mu**” is the minimum (“threshold”) relative correction of the PW DCS due to the κ_{\max} -fitting, to be used for determining the optimal value of the scale factor μ for individual “shifts” in the case mode_mu=2 or mode_mu=3 (see the description of parameter No. 3.6.1 “mode_mu”). In order to include a given value of θ into the set of values used for averaging the scale ratio $\mu(\kappa_{\max}) = (\text{DCS}(\kappa_{\max}, \theta) - \text{DCS}(K', \theta)) / (\text{DCS}(K, \theta) - \text{DCS}(K', \theta))$, the absolute value of the relative correction at that value of θ must be strictly greater than thrCorr_mu. The default value of this parameter is equal to 0. This means that the angles where the κ_{\max} -fitting was not performed (and the relative correction is consequently zero) will never be used for the angular averaging of the scale ratio $\mu(\kappa_{\max})$.
- 3.6.4. “**maxDev_mu**” is the maximum absolute deviation of the scale ratios calculated using the κ_{\max} -fitted DCS (i.e., $\mu = (\text{DCS}(\kappa_{\max} \rightarrow \infty, \theta) - \text{DCS}(K', \theta)) / (\text{DCS}(K, \theta) - \text{DCS}(K', \theta))$) from 1 (calculated inside the angular interval where the absolute value of the relative correction of the DCS due to the κ_{\max} -fitting is between the values specified using parameters No. 3.6.2 “maxCorr_mu” and No. 3.6.3 “thrCorr_mu”), to be used for determining the optimal value of the scale factor μ for individual “shifts” in the case mode_mu=2 or mode_mu=3 (see the description of parameter No. 3.6.1 “mode_mu”). The default value of this parameter is equal to 0.02.
- 3.6.5–6. “**minWidth_mu**” (alias “min_width_mu”) and “**minPoints_mu**” are the minimum width (in degrees) of the angular interval where the absolute value of the relative correction of the DCS due to the κ_{\max} -fitting is between the values specified using parameters No. 3.6.2 “maxCorr_mu” and No. 3.6.3 “thrCorr_mu”, and the minimum number of data points in this interval, respectively. The default values of these two parameters are 20 and 30, respectively.
- 3.6.7. “**kmax_ratio_mu**” is the ratio of the starting and ending values of the interval of κ_{\max} (i.e., K'/K) where the scale factor $\mu = (\text{DCS}(\kappa_{\max}, \theta) - \text{DCS}(K', \theta)) / (\text{DCS}(K, \theta) - \text{DCS}(K', \theta))$ (see Eq. (1.5.12a)) must be initially calculated for the purpose of locating the angular range where μ is approximately constant. The default value of this parameter is equal to 0.5.
- 3.6.8–9. “**start_angle_mu**” and “**end_angle_mu**” are the starting and ending angles of the angular interval where the value of the scaling factor μ in Eq. (1.5.12b) must be calculated (in degrees). If start_angle_mu < 0 or start_angle_mu \geq 180, then the starting angle will be determined using parameters thr_range_mu[1,2] (No. 3.6.12–13) and tol_mu[1,2] (No. 3.6.14–15). Similarly, if end_angle_mu \leq 0 or end_angle_mu > 180, then the ending angle will be determined using parameters thr_range_mu[1,2] and tol_mu[1,2]. The default value of parameters “start_angle_mu” and “end_angle_mu” is equal to -1 (i.e., both endpoints of the mentioned angular interval are defined using parameters thr_range_mu[1,2] and tol_mu[1,2] by default).
- 3.6.10–11. “**tol_range_ratio_mu1**” and “**tol_range_ratio_mu2**” (alias “tol_range_ratio_mu” for both) are used to specify the maximum allowed “gap” between the angle 0° (if the PW DCS is an increasing function of κ_{\max}) or 180° (if the PW DCS is a decreasing function of κ_{\max}) and the nearest endpoint of the mentioned angular range where the scale factor μ in Eq. (1.5.12b) must be calculated (in the current description, those endpoints will be denoted “start_angle_mu” or “end_angle_mu”, respectively, including the case when their values are determined using parameters thr_range_mu[1,2] and tol_mu[1,2]). The mentioned “gap” should not be too large, because this would reduce the accuracy of the angular extrapolation. Parameter “tol_range_ratio_mu1” is used to specify the maximum allowed value of the ratio

start_angle_mu / (end_angle_mu – start_angle_mu) if the PW DCS is an increasing function of κ_{\max} . Parameter “tol_range_ratio_mu2” is used to specify the maximum allowed value of the ratio $(180 - \text{end_angle_mu}) / (\text{end_angle_mu} - \text{start_angle_mu})$ if the PW DCS is a decreasing function of κ_{\max} . If this maximum is not exceeded, then the “ μ correction”, i.e., replacement of the κ_{\max} -fitted DCS by the μ -corrected DCS defined by Eq. (1.5.12b), inside the angular interval $[0^\circ, \text{end_angle_mu}]$ or $[\text{start_angle_mu}, 180^\circ]$, respectively, can be applied. In addition, parameter “tol_range_ratio_mu1” “doubles up” as the maximum allowed value of the ratio $\text{fitStartOffset_mu} / (\text{end_angle_mu} - \text{start_angle_mu})$ if the PW DCS is an increasing function of κ_{\max} , and tol_range_ratio_mu2 “doubles up” as the maximum allowed value of $\text{fitEndOffset_mu_max} / (\text{end_angle_mu} - \text{start_angle_mu})$ if the PW DCS is a decreasing function of κ_{\max} . If the original value of the ratio of fitStartOffset_mu (parameter No. 3.6.23) or fitEndOffset_mu_max (parameter No. 3.6.18) to end_angle_mu – start_angle_mu is greater than tol_range_ratio_mu1 or tol_range_ratio_mu2, respectively, then fitStartOffset_mu or fitEndOffset_mu_min and fitEndOffset_mu_max will be reduced, so that the value of the mentioned ratio becomes equal to tol_range_ratio_mu1 or tol_range_ratio2, respectively. The default value of parameters “tol_range_ratio_mu1” and “tol_range_ratio_mu2” is equal to 0.3.

- 3.6.12–13. “**thr_range_mu1**” and “**thr_range_mu2**” (alias “thr_range_mu” for both) are used to specify the minimum width of the angular range where the scale factor μ in Eq. (1.5.12a) is approximately independent of the angle θ when the DCS is an increasing or decreasing function of κ_{\max} , respectively (in degrees). The test for a constant value of μ is performed only when $\text{fit_SF_DCS} = 2$ or ± 3 (see the description of parameter No. 3.2.11 “fit_SF_DCS”). If $|\text{fit_SF_DCS}| = 3$ and the width of the mentioned interval is not less than thr_range_mu1 and the DCS increases with κ_{\max} , then the first angle greater than the right endpoint of the mentioned interval is treated as the point where the switch from fitting the DCS to fitting the SF must occur (see also the description of parameters No. 3.2.11 “fit_SF_DCS” and No. 3.6.14–15 “tol_mu[1,2]”). If thr_range_mu[1,2] > 180, then fit_SF_DCS is reset to 2, and the mentioned test is not performed. The default values of parameters “thr_range_mu1” and “thr_range_mu2” are equal to 181 and 120, respectively.
- 3.6.14–15. “**tol_mu1**” and “**tol_mu2**” (alias “tol_mu” for both) are used to specify the maximum allowed range of variation of the normalized differential of DCS over all angles belonging to the angular interval where the test for stability of the scale factor μ in Eq. (1.5.12a) is performed (the normalized differential of $\text{DCS}(\kappa_{\max})$ is defined at the end of Section 1.5.4). Parameter “tol_mu1” is used when the DCS is an increasing function of κ_{\max} , and parameter “tol_mu2” is used when the DCS is a decreasing function of κ_{\max} . If at least one of the endpoints of the mentioned angular interval is not specified explicitly (using parameters No. 3.6.8–9 “start_angle_mu” and “end_angle_mu”), then this interval is defined as the widest interval among all angular intervals where the mentioned range of variation is less than tol_mu, excluding the intervals whose width is less than the value of parameter “thr_range_mu1” (No. 3.6.12) or “thr_range_mu2” (No. 3.6.13), respectively. The default value of parameters “tol_mu1” and “tol_mu2” is equal to 0.1.
- 3.6.16. “**fitStart_mu**” is the starting angle of the angular range for fitting of the μ -corrected DCS by a polynomial of $\cos \theta$ when the partial-wave DCS is a decreasing function of κ_{\max} . The default value of this parameter is equal to 90.
- 3.6.17–19. “**fitEndOffset_mu_min**”, “**fitEndOffset_mu_max**” (alias “fitEndOffset_mu” or “fit_end_offset_mu” for both), and “**n_fitEndOffset_mu**” are the minimum and maximum values of the offset that must be subtracted from the angle corresponding to the first irregularity in the angular dependence of the μ -corrected DCS in order to obtain the endpoint of the angular range (θ') for polynomial fitting of the μ -corrected DCS as a function of $\cos \theta$ when the partial-wave DCS is a decreasing function of κ_{\max} , and the

number of equidistant values of this offset to be tested (see also the description of parameter No. 3.6.1 “mode_mu”). If no irregularity is found, or if the resulting maximum θ' (corresponding to the minimum offset) is greater than the endpoint θ_{end} of the range of constant μ (or greater than “end_angle_mu”), then the maximum θ' is set equal to θ_{end} (and all smaller values of θ' are increased by the same amount, so that the intervals between the adjacent values of θ' do not change). Otherwise, the maximum θ' can still be increased (although by a smaller amount), depending on parameter No. 3.6.22 (“tol_corr_mu”). The default values of these three parameters are equal to 20, 30, and 11, respectively.

Note: Parameters “fitEndOffset_mu_min” and “fitEndOffset_mu_max” (No. 3.6.17–18) are used only when the scale factor μ is determined by minimizing the angular integral of the difference of the μ -corrected DCS and its polynomial approximation in the extrapolation interval (see Eq. (1.5.24a)). Otherwise, parameters “fitEndOffset_mu0_min” and “fitEndOffset_mu0_max” (No. 3.6.20–21) are used.

- 3.6.20–21. “**fitEndOffset_mu0_min**” and “**fitEndOffset_mu0_max**” (alias “fitEndOffset_mu0” or “fit_end_offset_mu” for both) are the alternative values of parameters “fitEndOffset_mu_min” and “fitEndOffset_mu_max” (No. 3.6.17–18), to be used when the scale factor μ is not determined by minimizing the angular integral of the difference of the μ -corrected DCS and its polynomial approximation in the extrapolation interval (see Eq. (1.5.24a)), but is determined by an alternative method (for example, by averaging expression (1.5.26), or by least squares optimization of parameters λ and C in Eq. (1.5.28)). The default values of these two parameters are equal to 2 and 12, respectively.
- 3.6.22. “**tol_corr_mu**” is the tolerance of the relative change of the DCS due to the replacement of the PW DCS by the μ -corrected DCS (1.5.12b). This parameter is used to increase the maximum endpoint of the angular range (θ') for fitting of the μ -corrected DCS by a polynomial of $\cos \theta$ when the partial-wave DCS is a decreasing function of κ_{max} and an irregularity is found in the angular dependence of the μ -corrected DCS (see also the description of parameter No. 3.6.17 “fitEndOffset_mu_min”). The mentioned increase occurs after locating the angular range where the values of the mentioned relative change are less than tol_corr_mu. If the endpoint of the latter angular range (θ_{tol}) is greater than the angle corresponding to the mentioned irregularity (θ_{irreg}), then the maximum θ' is set equal to $\min(\theta_{\text{tol}}, \theta_{\text{end}})$, where θ_{end} is the endpoint of the range of constant μ (or the value of parameter “end_angle_mu”). If θ_{tol} is less than θ_{irreg} , but greater than $\theta_{\text{irreg}} - (\text{fitEndOffset_mu_min} / 2)$, then the maximum θ' is set equal to the value that is symmetric to the angle of the irregularity relative to θ_{tol} , unless the value obtained in this way is greater than θ_{end} . I.e., in this case the maximum θ' is equal to $\min(2\theta_{\text{tol}} - \theta_{\text{irreg}}, \theta_{\text{end}})$. In any case, all smaller values of θ' are increased by the same amount, so that the intervals between the adjacent values of θ' do not change. The default value of this parameter is equal to 0.5.
- 3.6.23. “**fitStartOffset_mu**” is the offset that must be added to the angle corresponding to the start of the range where the scale factor μ is approximately constant (or to “start_angle_mu”) in order to obtain the starting point of the angular range for polynomial fitting of the μ -corrected DCS as a function of $\cos \theta$ when the partial-wave DCS is an increasing function of κ_{max} . The default value of this parameter is equal to 0.
- 3.6.24. “**fitEnd_mu**” is the endpoint of the angular range for fitting of the μ -corrected DCS by a polynomial of $\cos \theta$ when the partial-wave DCS is an increasing function of κ_{max} . The default value of this parameter is equal to 80.
- 3.6.25–26. “**fitRef_mu1**” and “**fitRef_mu2**” (alias “fitRef_mu” for both) is the integer number from -2 to 4 indicating the set of reference functions that must be used as the divisor of the μ -corrected DCS in order to obtain the dependent variable of the polynomial fitting (see

Eq. (1.5.22) in Section 1.5.4) when the partial-wave DCS is an increasing function of κ_{\max} or a decreasing function of κ_{\max} , respectively. If this parameter is equal to 0, 1, or 2, then only one reference function, whose sequence number is equal to the indicated value, will be tried (the value of 0 corresponds to absence of the mentioned divisor, i.e., the reference function equal to 1). In other cases, the optimal reference function is chosen on the basis of the balance between the quality of the polynomial fit inside the angular fitting interval and the stability of the polynomial extrapolation (outside the fitting interval) with respect to the different values of the endpoint of the fitting interval (see also Section 1.5.4, the paragraph after Eq. (1.5.23)). The values -2, -1, 3, 4 correspond to the following combinations of reference functions:

- 2 – No. 0 and No. 2,
- 1 – No. 0 and No. 1,
- 3 – No. 1 and No. 2,
- 4 – No. 0, No. 1, and No. 2.

The default value of parameters “fitRef_mu1” and “fitRef_mu2” is equal to -1.

Note: If the set of reference functions includes reference function No. 0 and if it is not the only reference function, then it will most likely be removed automatically from the set of reference functions before the μ -fitting. This happens when the overall relative correction of the PW DCS due to the κ_{\max} -fitting is categorized as “large”, i.e., when an angular interval satisfying the constraints defined by parameters No. 3.6.45–46 (“maxCorr_mu2” and “minWidth_mu2”) does not exist.

- 3.6.27–28. “fitLog_mu1” and “fitLog_mu2” (alias “fitLog_mu” for both) is the integer number 0, 1, or 2, indicating if the polynomial fitting must be applied to the logarithm of the ratio of the μ -corrected DCS and the reference function (instead of the actual ratio $DCS_{\mu} / DCS_{\text{ref}}$ as in the case of Eq. (1.5.22)) when the partial-wave DCS is an increasing function of κ_{\max} or a decreasing function of κ_{\max} , respectively. If this parameter is equal to 0, then the logarithm will not be used. If this parameter is equal to 1, then only the logarithm will be used. If this parameter is equal to 2, then both approaches will be tried, and the optimal method will be selected using the same criteria that are used for choosing the optimal degree of the fitting polynomial and the optimal reference function (see Section 1.5.4). The default value of parameters “fitLog_mu1” and “fitLog_mu2” is equal to 0 (i.e., the logarithm is not used by default).
- 3.6.29–30. “fitDegree_mu_min1” and “fitDegree_mu_max1” (aliases “fitDegree_mu1” and “fitDegree_mu” for both) are the minimum and maximum values of the degree of the polynomial used for fitting the μ -corrected DCS (see Section 1.5.4) when the partial-wave DCS is an increasing function of κ_{\max} . If either fitDegree_mu_min1 or fitDegree_mu_max1 is specified with the minus sign, then cubic spline fitting will be applied instead of the polynomial fitting, and the absolute values of these two parameters will be interpreted as the minimum and maximum number of inter-knot intervals (this number is one less than the number of “knots”, i.e., breakpoints of the piecewise cubic spline function). The knots are equidistant. The absolute value of these two parameters must be equal to each other (see also the description of parameter No. 3.6.1 “mode_mu”). The arguments of the fitting polynomial and the cubic spline are equal to $\sin^2(\theta/2)$ and $-\cos\theta$, respectively. The default value of parameters “fitDegree_mu_min1” and “fitDegree_mu_max1” is equal to 3.
- 3.6.31–32. “fitDegree_mu_min2” and “fitDegree_mu_max2” (aliases “fitDegree_mu2” and “fitDegree_mu” for both) are the minimum and maximum values of the degree of the polynomial used for fitting the μ -corrected DCS (see Section 1.5.4) when the partial-wave DCS is a decreasing function of κ_{\max} (see also the description of parameter No. 3.6.1 “mode_mu”). If either fitDegree_mu_min2 or fitDegree_mu_max2 is specified with the minus sign, then cubic spline fitting will be applied instead of the polynomial fitting, and the

absolute values of these two parameters will be interpreted as the minimum and maximum number of inter-knot intervals (this number is one less than the number of “knots”, i.e., breakpoints of the piecewise cubic spline function). The knots are equidistant. The arguments of the fitting polynomial and the cubic spline are equal to $\sin^2(\theta/2)$ and $-\cos\theta$, respectively. The default values of parameters “fitDegree_mu_min2” and “fitDegree_mu_max2” are equal to 1 and 20, respectively.

Note: In the files “mu_range.txt” and “mu.txt”, the spline fitting is indicated by a negative number in column “fitDegree_mu” (in such a case, the mentioned number is opposite to the number of inter-knot intervals).

3.6.33–34. “**polyn_mode_mu1**” and “**polyn_mode_mu2**” (alias “polyn_mode_mu” for both) indicates the point of joining the unfitted μ -corrected DCS with its polynomial approximation when constructing the final DCS when the partial-wave DCS is an increasing function of κ_{\max} or a decreasing function of κ_{\max} , respectively. Four values are allowed:

- 1 – it is the ending (starting) point of the polynomial fitting interval if the PW DCS decreases (increases) with κ_{\max} ,
- 2 – it is the starting (ending) point of the polynomial fitting interval if the PW DCS decreases (increases) with κ_{\max} ,
- 0 or 3 – the polynomial fit is not used for constructing the final DCS (it is used only for optimization of the scale factor μ in Eq. (1.5.12b)).

In the case 1 or 2, the polynomial fit will be used for constructing the final DCS (i.e., it will replace the original κ_{\max} -fitted DCS obtained from the nonlinear fit by the function (1.5.1) or (1.5.10)) at all angles greater than the indicated point if the PW DCS decreases with κ_{\max} , and at all smaller angles otherwise. The default value of parameters “polyn_mode_mu1” and “polyn_mode_mu2” is equal to 2.

3.6.35. “**compRef_mu**” is the sequence number (1 or 2) of the reference function that must be used for comparison with the μ -corrected PW DCS at the start of stage 3. The results of this comparison are written to the two or three files belonging to the fifth group of files defined in Section 6.20, if `output_mu = ±1` or `output_mu = 2` (see the description of parameter No. 3.10.5). The default value of parameter “compRef_mu” is equal to 1 (reference function No. 1 is by default calculated using the Born approximation).

3.6.36. “**mu**” is a fixed non-zero value of the scale factor μ in Eq. (1.5.12b) to be used in conjunction with the option “output_mu=-1” (see the description of parameter No. 3.10.5). This parameter can be non-zero only when `output_mu=-1`. If `mu = 0`, then the value of the scale factor μ will be optimized iteratively (this is always the case when `output_mu ≥ 0`). The default value of parameter “mu” is equal to 0.

3.6.37. “**MA_period_theta_mu**” is the moving average (MA) period used for the additional angular MA smoothing of the PW DCS inside the angular interval of constant scale factor μ (see end of Section 1.5.4). If this parameter is zero (the default value), then its value will be determined from the absolute value of “theta_mu” (No. 3.6.38). In such a case, `MA_period_theta_mu` will be set equal to the number of points from $180^\circ - |\text{theta_mu}|$ to $|\text{theta_mu}|$. Depending on whether the PW DCS is a decreasing or increasing function of κ_{\max} inside the angular range of constant μ , the mentioned moving average is either “trailing” (i.e., calculated using the current point and previous `MA_period_theta_mu - 1` points), or “leading” (i.e., calculated using the current point and next `MA_period_theta_mu - 1` points).

3.6.38. “**theta_mu**” is the value of the angle θ where the fixed value of the scale factor μ must be calculated using the corresponding value of the κ_{\max} -fitted DCS when the other methods of determining a fixed value of μ fail. This approach relies on the fact that the values of the PW DCS used for the κ_{\max} -fitting are preprocessed by normalizing and averaging over a large

number of consecutive values of θ (this number is specified by parameter No. 3.6.37 “MA_period_theta_mu”). Consequently, it is reasonable to expect that the random errors in those values of PW DCS are sufficiently small to ensure a high accuracy of the κ_{\max} -fitted DCS, especially if all the values of θ used for the mentioned averaging can be grouped in pairs of values symmetric with respect to 90° . $|\theta_{\mu}|$ cannot be less than 90 . If $\theta_{\mu} > 0$, then this approach will be applied if the other methods of determining a fixed value of μ fail. If the PW DCS increases with κ_{\max} , then the fixed value of μ will be determined at the angle that is symmetrical to the specified value of θ_{μ} with respect to 90° , i.e., at $180^\circ - \theta_{\mu}$. For example, if θ_{μ} is 110 and the PW DCS increases with κ_{\max} , then the fixed value of μ will be determined for the angle of 70° . If $\theta_{\mu} < 0$, then this method of determining a fixed value of μ will not be applied (however, $|\theta_{\mu}|$ may still be used for determining MA_period_theta_mu, as explained in the description of parameter No. 3.6.37). Parameter θ_{μ} cannot be less than 90 . Its default value is -110 .

3.6.39–44. “polyn_thr_mu1”, “polyn_thr_mu2”, “maxDeg_mu1”, “maxDeg_mu2”, “minDeg_mu1”, and “minDeg_mu2” are counterparts of the six parameters “polyn_thr_DCS1” (No. 3.11.2), “polyn_thr_DCS2” (No. 3.11.3), “maxDeg_DCS1” (No. 3.11.5), “maxDeg_DCS2” (No. 3.11.6), “minDeg_DCS1” (No. 3.11.8), and “minDeg_DCS2” (No. 3.11.9), respectively, to be used inside the interval of constant μ . The aliases of the six parameters whose names end with “_mu<1,2>” can be obtained from the aliases of their counterparts whose names end with “_DCS<1,2>” by removing the aliases whose names do not include the string “_DCS” and by replacing “DCS” with “mu”. The default values of these six parameters are the same as of the corresponding parameters whose names end with “_DCS<1,2>”.

3.6.45–46. “maxCorr_mu2” (alias “max_corr_mu”) and “minWidth_mu2” (alias “min_width_mu”) are the maximum relative correction of the PW DCS due to the κ_{\max} -fitting and the minimum width of the corresponding angular interval, respectively, to be used for applying an alternative definition of the objective function (OF), which is minimized during the μ -fitting. The mentioned alternative OF is defined using parameters OF_type_mu (No. 3.6.47) and DCS_fit_mu (No. 3.6.48), and it is applied after finding a sufficiently wide angular range where the absolute value of the mentioned relative correction is less than maxCorr_mu2. The minimum allowed width of the mentioned interval is defined using parameter minPoints_mu. The default values of these two parameters are 0.02 and 140 , respectively.

3.6.47. “OF_type_mu” is an integer number equal to 1 , 2 , or 3 , indicating one of the three alternative definitions of the objective function (OF), which is minimized during the μ -fitting. The method of μ -fitting described in Section 1.5.4 is based on minimization of the absolute value of the left-hand side of Eq. (1.5.24a) or Eq. (1.5.24b), using the simplex method. The corresponding OF is defined as the left-hand side of Eq. (1.5.24a,b) squared. This OF is the main one, and it corresponds to OF_type_mu = 1 . This definition of the OF is always applied for individual “shifts” when an angular range satisfying the constraints defined by parameters No. 3.6.45–46 (“maxCorr_mu2” and “minWidth_mu”) does not exist. I.e., parameter “OF_type_mu” is then ignored (as well as parameter “DCS_fit_mu”). The OF indicated by this parameter will be used only when the mentioned angular range is found, or for the initial μ -fitting at the start of stage 3 (before the κ_{\max} -fitting). “OF_type_mu=2” indicates the sum of squared relative deviations of $DCS_{\text{ext}} - DCS(K'')$ from $DCS_{\mu} - DCS(K'')$, i.e., the OF is in this case equal to $\sum ((DCS_{\text{ext}} - DCS(K'')) / (DCS_{\mu} - DCS(K'')) - 1)^2$. The summation is performed inside the same interval that would be used for the calculation of the angular integral if the main OF was used, i.e., at $\theta' \leq \theta \leq 180^\circ$ if the PW DCS is a decreasing function of κ_{\max} (see Eq. (1.5.24a)) or at $0^\circ \leq \theta \leq \theta'$ if the PW DCS is an increasing function of κ_{\max} (see

Eq. (1.5.24b)). In the case “OF_type_mu=3”, each term of this sum is additionally multiplied by $\sin^2 \theta$. The default value of parameter “OF_type_mu” is equal to 2.

Note: Parameter “OF_type_mu” has been added after noticing that the main OF is not the optimal one in the case of relatively small overall corrections of the PW DCS due to the κ_{\max} -fitting. The mentioned two parameters No. 3.6.45–46 (“maxCorr_mu2” and “minWidth_mu2”) are used to categorize the overall correction as “small” or “large”: if an angular interval satisfying the constraints defined by parameters No. 3.6.45–46 is found, then the overall correction is categorized as sufficiently small to use an alternative OF. However, in the case of the default values of parameters “maxCorr_mu2” and “minWidth_mu2”, the overall correction is then usually sufficiently small for applicability of the simpler method of large-angle polynomial extrapolation (see Section 1.7.3), eliminating the need for the μ -fitting. As a result, the modifications of the μ -fitting procedure defined by parameters “OF_type_mu” and “DCS_fit_mu” are unlikely to be applied in practice if the default values of parameters “maxCorr_mu2” and “minWidth_mu2” are used.

3.6.48. “DCS_fit_mu” is an integer number equal to 0, 1, or 2, which indicates if the relative deviations of the μ -corrected DCS from the κ_{\max} -fitted DCS must be taken into account during optimization of the parameters of the μ -corrected DCS (i.e., the scale factor μ , the choice of the reference function, and the degree of the fitting polynomial) for individual “shifts” when mode_mu ≥ 2 and the alternative definition of the OF defined by parameter “OF_type_mu” is applied (see also the description of parameter No. 3.6.47). If the alternative definition of the OF is not applied (i.e., when an angular interval satisfying the constraints defined by parameters No. 3.6.45–46 does not exist), then the mentioned relative deviations and the value of “DCS_fit_mu” are always ignored. Thus, parameter DCS_fit_mu acts only as a modifier of the *alternative* OF. In the case “DCS_fit_mu=0”, the mentioned relative deviations are ignored. In the case “DCS_fit_mu=1”, the mentioned relative deviations are included in the final standard deviation after the simplex optimization of the scale factor μ , but they are not used in the actual definition of the OF that is minimized during this simplex fitting. In the case “DCS_fit_mu=2”, the mentioned relative deviations are used both when calculating the final standard deviation after the simplex fitting and in the definition of the OF for the simplex fitting. “DCS_fit_mu=2” is allowed only with “OF_type_mu=2” or “OF_type_mu=3”. In the case “DCS_fit_mu=2”, a sum of squared relative deviations of the μ -corrected DCS from the κ_{\max} -fitted DCS is added to the OF. Inside the angular interval of the polynomial fitting (see Eq. (1.5.22)), this sum is defined as $\sum ((DCS_{\text{ext}} - DCS(K'')) / (DCS_{\text{fitted}} - DCS(K'')) - 1)^2$ (or the same sum with each term multiplied by $\sin^2 \theta$ in the case “OF_type_mu=3”). Outside the interval of the polynomial fitting, the additional sum is defined as $\sum ((DCS_{\mu} - DCS(K'')) / (DCS_{\text{fitted}} - DCS(K'')) - 1)^2$ (or the same sum with each term multiplied by $\sin^2 \theta$ in the case “OF_type_mu=3”). Thus, the two values that are compared with each other when calculating each term of this sum are additionally reduced by the value of the PW DCS corresponding to the endpoint of the current κ_{\max} -fitting interval ($DCS(K'')$). The summation in this sum is performed using only the data points that belong to the angular interval satisfying the constraints defined by the four parameters No. 3.6.2 (“maxCorr_mu”), No. 3.6.3 (“thrCorr_mu”), No. 3.6.5 (“minWidth_mu”), and No. 3.6.6 (“minPoints_mu”). In no such angular interval exists, then the mentioned additional sum of squared relative deviations will not be added to the OF for the simplex optimization of μ , and those standard deviations will be also ignored when calculating the final standard deviation (after the simplex fitting), regardless of the value of DCS_fit_mu. The default value of parameter “DCS_fit_mu” is equal to 2.

- 3.6.49. “**mu_ref_max**” controls the conditions when an alternative method of choosing the optimal reference function $DCS_{ref}(\theta)$ in the definition of the fitting polynomial (Eq. (1.5.22)) must be applied. This method is based on comparison of the μ -fitting results obtained using each of the requested reference functions with the results corresponding to the reference function optimized for a fixed “reference” value of the scale factor μ . The latter reference value of μ is calculated before the μ -correction using the values of the κ_{max} -fitted DCS inside the angular interval satisfying the constraints defined by the four parameters No. 3.6.2 (“maxCorr_mu”), No. 3.6.3 (“thrCorr_mu”), No. 3.6.5 (“minWidth_mu”), and No. 3.6.6 (“minPoints_mu”). If no such angular interval is found, then the mentioned alternative method will not be applied regardless of the value of “mu_ref_max”. Since this alternative method has not been found to be superior to the default one, it is recommended to leave parameter “mu_ref_max” equal to its default value (–1), which ensures that only the original method (without usage of the reference value of μ) will be applied. For the same reason, the exact meaning of this parameter and the method of the mentioned comparison will not be described here.
- 3.6.50. “**verbosity_mu**” is a “switch” (0 or 1) controlling output of messages about μ -fitting errors at the start of stage 3, when the initial analysis of the scaling properties of the angular dependence of the partial-wave DCS is performed. If verbosity_mu=0, then only the messages corresponding to the first (smallest) degree of the μ -fitting polynomial will be output. If verbosity_mu=1, then the error messages corresponding to all fitting degrees will be output (see also description of parameter No. 3.6.1 “mode_mu”). The default value of this parameter is equal to 0.

6.7. Parameters controlling the angular spline fitting and extrapolation of the partial-wave DCS

- 3.7.1. “**kmax_spline**” indicates the value of κ_{max} to be used for the spline fitting of the angular dependence of the partial-wave DCS. The default value of this parameter is equal to -1, which indicates that the mentioned value of κ_{max} must be set equal to the maximum κ_{max} used in stage 3 (see also the description of parameter No. 3.2.1 “kmax_fit” in Section 6.2).
- 3.7.2–4. “**spline_theta_min1**”, “**spline_theta_min2**” (aliases “spline_theta_min”, “spl_theta_min” for both) and “**n_spline_theta_min**” define the set of equidistant angles to be used as the starting point (θ_{min}) of the angular spline-fitting interval when fitting the partial-wave (PW) DCS (see also Section 1.7.1). “spline_theta_min1” and “spline_theta_min2” are the first and last angles of the set, respectively, and “n_spline_theta_min” is the number of equidistant angles in the set. The angles must be specified in degrees. If spline_theta_min1 = spline_theta_min2, then n_spline_theta_min is reset to 1. If n_spline_theta_min=1, then spline_theta_min2 is reset to spline_theta_min1. The default values of these three parameters are the following: spline_theta_min1=10, spline_theta_min2=10, n_spline_theta_min=1.
- 3.7.5–7. “**spline_theta_max1**”, “**spline_theta_max2**” (alias “spline_theta_max”, “spl_theta_max” for both) and “**n_spline_theta_max**” define the set of equidistant angles to be used as the ending point (θ_{max}) of the angular spline-fitting interval (see also Section 1.7.1). “spline_theta_max1” and “spline_theta_max2” are the first and last angles of the set, respectively, and “n_spline_theta_max” is the number of equidistant angles in the set. The angles must be specified in degrees. If spline_theta_max1 = spline_theta_max2, then n_spline_theta_max is reset to 1. If n_spline_theta_max=1, then spline_theta_max2 is reset to spline_theta_max1. The default values of these three parameters are the following: spline_theta_max1=170, spline_theta_max2=180, n_spline_theta_max=6.
- 3.7.8. “**spline_theta_max_thr**” defines the start of the angular range where the PW DCS is checked for existence of an extra maximum (i.e., a large-angle distortion, such as illustrated in Fig. 8b in Section 1.7.1). If “spline_theta_max_thr” is specified with the minus sign and a

large-angle distortion is found, then the values of “spline_theta_max1” and “spline_theta_max2” will be adjusted automatically. The adjusted value of spline_theta_max2 is determined as described in Section 1.7.1 (condition “(a)”), i.e., it corresponds to the last point in the “undistorted” part of the DCS, defined as the last point satisfying the condition $DCS(\theta) > DCS(180^\circ)$, where the DCS corresponds to the maximum value of κ_{\max} (assuming that the distortion occurs after the angle |spline_theta_max_thr|). In such a case, the value of spline_theta_max1 is modified, too, so that the difference spline_theta_max2 – spline_theta_max1 stays the same (the value of n_spline_theta_max is unchanged). The default value of “spline_theta_max_thr” is equal to 80.

3.7.9. “**relRange_thr**” controls an additional increase of θ_{\max} in the case spline_theta_max_thr<0 after finding a large-angle distortion in the angular dependence of the DCS, as described in Section 1.7.1 (condition “(b)”). If the relative variation of the DCS over the last N_{fit} values of κ_{\max} (i.e., $K - N_{\text{fit}} + 1 \leq \kappa_{\max} \leq K$, where N_{fit} is calculated according to Eq. (1.5.11a) or is specified using parameter “Nfit_DCS”) at the value of θ_{\max} determined as described previously (according to condition “(a)” in Section 1.7.1) is less than relRange_thr, then the program will attempt to increase θ_{\max} . The cycle of incrementing θ_{\max} will end after finding the point where the mentioned relative variation is greater than relRange_thr, or after reaching the point where the DCS corresponding to $\kappa_{\max} = K$ starts to increase as a function of θ (whichever happens first). The default value of parameter “relRange_thr” is 0.1.

3.7.10. “**splineExt**” defines the additional conditions for performing the angular extrapolation (both large-angle and small-angle), which may override the values of θ_{\min} and θ_{\max} defined by parameters No. 3.7.2–9. The allowed values of this parameter are 0, ± 1 , ± 2 :

splineExt=0: the angular extrapolation will not be performed ($\theta_{\min} = 0^\circ$, $\theta_{\max} = 180^\circ$),

splineExt<0: the angular extrapolation will always be performed,

splineExt>0: the angular extrapolation (both large-angle and small-angle) will be performed only after finding a large-angle distortion of the DCS,

splineExt= ± 2 : the data corresponding to $\theta < \theta_{\min}$ will not be modified (i.e., they will not be replaced by the angular dependence extrapolated to small angles).

The default value of parameter “splineExt” is 0 (i.e., the angular extrapolation of the PW DCS is not performed by default).

3.7.11–13. “**splineIntRatio_min1**” (aliases “splineIntRatio_min”, “splineIntRatio1”, “spl_int_ratio_min1”, “splineIntRatio1_thr_min”, and “spl_int_ratio1_thr_min”), “**splineIntRatio_max1**” (aliases “splineIntRatio_max”, “splineIntRatio1”, and “spl_int_ratio_max1”) and “**n_splineIntRatio1**” (aliases “n_splineIntRatio” and “n_spl_int_ratio1”) define the set of values of the first parameter controlling the variation of knot density (this parameter is denoted ε_1 in Section 1.7). This set of values is used during the search for the optimal value of ε_1 , which minimizes the objective function (OF) defined by Eq. (1.7.7). “splineIntRatio_min1” and “splineIntRatio_max1” are the first and last values of the set, respectively, and “n_splineIntRatio1” is the number of values in the set. All values are equidistant on the logarithmic scale. If n_splineIntRatio1<0, then the “best” value in the set will be subsequently used as the starting value for simplex minimization of the OF (see Section 1.7.1). If splineIntRatio_min1<0, then the knot positions are determined on the basis of the curvature (second derivative) of the PW DCS as a function of θ : a larger absolute value of the second derivative corresponds to a larger knot density (smaller inter-knot intervals). This provides a unique value of each knot, so that no iterative optimization is needed and parameters No. 3.7.12–17 are not used. The knots are found in this case by projecting uniformly spaced points onto a density function, which is proportional to the cumulative integral of the square root of the absolute value of the second derivative of the spline-smoothed PW DCS. The absolute value of splineIntRatio_min1 is interpreted in this

case as the minimum number of points inside one inter-knot interval to be used for the mentioned spline smoothing of the PW DCS (which is needed for construction of the mentioned density function). The default values of these three parameters are the following: $\text{splineIntRatio_min1}=10^{-10}$, $\text{splineIntRatio_max1}=10^{10}$, $\text{n_splineIntRatio1}=-21$.

- 3.7.14–16. “**splineIntRatio_min2**” (aliases “splineIntRatio_min”, “splineIntRatio2”, and “spl_int_ratio_min2”), “**splineIntRatio_max2**” (aliases “splineIntRatio_max”, “splineIntRatio2”, and “spl_int_ratio_max2”) and “**n_splineIntRatio2**” (aliases “n_splineIntRatio” and “n_spl_int_ratio2”) define the set of values of the second parameter controlling the variation of knot density (this parameter is denoted ε_2 in Section 1.7). Usage and default values of these parameters are identical to usage and default values of parameters No. 3.7.11–13. The only difference is that n_splineIntRatio2 is allowed to be equal to 0. In such a case, only the first knot-density parameter (ε_1) is used, and the inter-knot intervals form a geometric progression (see Eq. (1.7.4)).
- 3.7.17. “**splineIntRatio1_thr**” (aliases “spline_int_ratio1_thr”, “splineIntRatio1_thr_min”, and “spl_int_ratio1_thr_min”) is the minimum allowed value of the first parameter controlling the variation of knot density (this parameter is denoted ε_1 in Section 1.7). If this parameter is equal to 0 (the default value), then the only constraint on ε_1 is the requirement that ε_1 must be positive.
- 3.7.18. “**splineLastIntRatio_thr**” (alias “spl_lastIntRatio_thr”) is the minimum allowed ratio of the width of the last inter-knot interval (ending at θ_{\max}) and the width of the large-angle extrapolation interval (i.e., $180^\circ - \theta_{\max}$). The default value of this parameter is equal to 1 (i.e., the interval between the last two knots of the optimal spline function cannot be narrower than the large-angle extrapolation interval). Larger values of this parameter would improve stability of the large-angle extrapolation, but may cause deterioration of accuracy of the spline fitting at $\theta < \theta_{\max}$. This parameter is not used when the large-angle extrapolation is not performed (i.e., when $\theta_{\max} = 180^\circ$).
- 3.7.19–20. “**splineInt_min**” (aliases “splineInt”, “spl_int_min”, “spl_int”) and “**splineInt_max**” (aliases “splineInt”, “spl_int_max”, “spl_int”) are positive integer numbers indicating, respectively, the minimum and maximum values of the approximate average inter-knot interval (\bar{w}) inside the spline-fitting interval (in degrees). \bar{w} is used to calculate the number of inter-knot intervals. The latter number is equal to the width of the spline-fitting interval divided by \bar{w} (this ratio is rounded to the nearest integer, or is set equal to 1 if the nearest integer is zero). The number of knots (N) is greater by 1. The program will test several integer values of \bar{w} starting with splineInt_max and ending with splineInt_min . Each new value of \bar{w} is chosen so that the new value of N (calculated as described above) is greater than the previous value. The optimal value of N is the one that yields the smallest value of the objective function (1.7.7). The default values of parameters “splineInt_min” and “splineInt_max” are 3 and 60, respectively.
- 3.7.21. “**nSplineKnots_max**” (alias “n_spl_knots_max”) is the maximum allowed number of spline knots when fitting the angular dependence of the original PW DCS. This parameter is used to impose an additional limitation on the number of knots (the other two parameters controlling the number of spline knots are No. 3.7.19 “splineInt_min” and No. 3.7.20 “splineInt_max”). The default value of this parameter is 62, which is equivalent to absence of additional limitation, because the minimum allowed value of parameter “splineInt_min” is 3 (this value of the average inter-knot interval \bar{w} corresponds to 61 knots).
- 3.7.22–24. “**splineRef0**”, “**splineRef1**” and “**splineRef2**” (alias “splineRef” for all three) are “switches” (± 1 or 0) controlling the choice of the reference function for the angular spline fitting and extrapolation of the original PW DCS (see also Section 1.7.1). The number after “splineRef” indicates the reference function: reference function No. 0 is equal to 1 (i.e., no modification of the original PW DCS), whereas reference functions No. 1 and No. 2 are

defined by parameters No. 3.5.1–20. If $\text{splineRef}[0,1,2]=\pm 1$, then the angular spline fitting (and extrapolation) of the ratio of the original PW DCS and the corresponding reference DCS may be performed, and if $\text{splineRef}[0,1,2]=0$, then the mentioned fitting will not be performed. If $\text{splineRef0}=+1$, then the angular spline fitting of the PW DCS using reference function No. 0 will be performed only when at least one of the two alternative reference DCS No. 1 and No. 2 is used (the five criteria for using each of the two reference DCS No. 1 and No. 2 are defined by parameters No. 3.5.22–31). If $\text{splineRef0}=-1$, then the angular spline fitting of the PW DCS using reference function No. 0 will be performed regardless of whether the reference DCS No. 1 or No. 2 is used or not. If $\text{splineRef1}=-1$ and $\text{splineRef2}=-1$, then only one of the two reference DCS No. 1 and No. 2 will be used for the angular spline fitting: it is the DCS that is most similar to the original PW DCS inside the angular spline-fitting interval. If two or more reference functions are used for the angular spline fitting of the PW DCS, then the optimal reference function is the one that yields the smallest value of the objective function (1.7.7). The default value of parameter “splineRef2” is equal to 0. The default values of parameters “splineRef0” and “splineRef1” is equal to +1, except in the case $T_1 > 3 \text{ MeV}$, $T_2 / T_1 \leq 10^{-4}$, when these parameters are equal to 0 (i.e., the cubic spline fitting of the PW DCS is not performed near the tip of the photon spectrum at electron energies higher than 3 MeV).

3.7.25–26. “**splineArg1**” and “**splineArg2**” (aliases “splineArg” and “spl_arg” for both) are integer numbers 1, 2 or 3 indicating the first and last definition of the spline argument to be tested:

- 1 – the spline argument is equal to θ ,
- 2 – the spline argument is equal to $-\cos \theta$,
- 3 – the spline argument is equal to $\ln[(1 - \cos \theta) / 2]$.

All definitions starting with No. splineArg1 and ending with No. splineArg2 will be tested (see also Section 1.7.1). The optimal definition of the spline argument is the one that yields the smallest value of the objective function (1.7.7). The default values of parameters “splineArg1” and “splineArg2” are equal to 1 and 2, respectively.

3.7.27. “**splineLog**” (alias “spl_log”) controls the optional replacement of the original function by its logarithm during the angular spline fitting. Three values are allowed:

- 0 – do not replace the original function by its logarithm,
- 1 – perform the angular spline fitting only with the logarithm of the original function,
- 2 – perform the angular spline fitting both with the original function and with its logarithm.

In the latter case, the optimal option is the one that yields the smallest value of the objective function (1.7.7). The default value of parameter “splineLog” is equal to 2.

3.7.28. “**minDeg_cos**” (aliases “min_deg_cos”, “deg_cos0”, “deg_cos”) is used to specify the minimum degree of the approximating polynomial in the case of two knots when the spline argument is equal to $-\cos \theta$ (see the note at the end of Section 1.7.1). The default value of this parameter is equal to 1.

3.7.29. “**maxDeg_cos**” (aliases “max_deg_cos”, “deg_cos0”, “deg_cos”) is used to specify the maximum degree of the approximating polynomial when the spline argument is equal to $-\cos \theta$ (see the note at the end of Section 1.7.1). If this parameter is less than 3, then the number of knots will not be allowed to be greater than 2 when the spline argument is equal to $-\cos \theta$. If this parameters is equal to 0, then $-\cos \theta$ will not be used as the argument of a polynomial or of a spline function approximating the angular dependence of the original PW DCS (regardless of the values of parameters “splineArg1” and “splineArg2”). The default value of this parameter is equal to 3.

3.7.30. “**tol_spline**” (alias “tol_spl”) is used to specify the absolute tolerance of the change of the natural logarithm of the two spline knot-density parameters (denoted ε_1 and ε_2 in Section 1.7)

during their optimization by the simplex method, as a part of the angular spline fitting of the partial-wave DCS. The default value of this parameter is equal to 10^{-4} .

- 3.7.31. **“maxRelDev_spl_ratio”** is the maximum allowed ratio of two maximum relative deviations of the spline-fitted PW DCS from the original PW DCS: one of them is calculated using the angular dependence of the spline-fitted DCS corresponding to the current value of κ_{\max} (i.e., the maximum value of $|\kappa_2|$ used in the current “shift”), and another one is calculated using the spline-fitted DCS corresponding to $\kappa_{\max} = \text{kmax_spline}$, i.e., the value of κ_{\max} , for which the knot positions are optimized (see the description of parameter No. 3.7.1). If this ratio is exceeded and if the larger one of the two mentioned relative deviations is greater than the value of parameter No. 3.7.32 (“maxRelDev_spl”), then stage 3 is restarted without the spline fitting of the PW DCS, and the intermediate file with the spline-fitted DCS data are deleted. The default value of this parameter is equal to 10.
- 3.7.32. **“maxRelDev_spl”** is the larger one of the two maximum relative deviations of the spline-fitted DCS from the original PW DCS that must be exceeded in order to calculate their ratio and to perform the check mentioned in the description of parameter No. 3.7.31 (“maxRelDev_spl_ratio”). The default value of this parameter is equal to 0.1.

The next six parameters define the objective function (OF) that is minimized during the angular spline fitting of the original PW DCS. Although the default definition of the OF consists of only one term equal to the squared rms value of the relative residuals δ_{res} of the linear regression optimizing the spline values at the optimal set of knots (see Eq. (1.7.7)), there is an option to add two more terms reflecting other properties of the spline function, which are related to the accuracy of the spline approximation – rms value of the uncertainty δ_{unc} (see Eq. (1.7.6)) and relative difference between the CS and the angular integral of the spline-fitted DCS with respect to the solid angle of photon emission. In addition, there is an option to use either the arithmetic average or the geometric average of the mentioned terms when calculating the OF. Thus, the most general expression of the OF used for the angular spline fitting of the original PW DCS is the following:

$$f = f_n [(a_{\text{unc}} \delta_{\text{unc}})^2 + (a_{\text{res}} \delta_{\text{res}})^2 + (a_{\text{CS}} \delta_{\text{CS}})^2], \quad (6.7.1a)$$

or

$$f = (\delta_{\text{unc}}^{2a_{\text{unc}}} \delta_{\text{res}}^{2a_{\text{res}}} \delta_{\text{CS}}^{2a_{\text{CS}}}) f_n, \quad (6.7.1b)$$

where δ_{res} is the root-mean-square (rms) value of relative residuals of the spline fitting inside the interval $\theta_{\min} \leq \theta \leq \theta_{\max}$, and δ_{CS} is the relative difference between the original PW CS and the mentioned angular integral of the spline function, which approximates the corresponding PW DCS. Each of the three coefficients a_{unc} , a_{res} and a_{CS} can be either 1 or 0. f_n is the “normalization factor” equal to the inverse number of terms included in the definition of the OF (i.e., the inverse number of non-zero a -coefficients in Eqs. (6.7.1a,b)). The next six parameters are used to specify the three coefficients a_{unc} , a_{res} and a_{CS} in Eqs. (6.7.1a,b), and the method of combining the terms of the OF:

- 3.7.33. **“splineUnc_wt”** (alias “spl_unc_wt”) is a “switch” (1 or 0) indicating the value of the first coefficient (a_{unc}) in Eqs. (6.7.1a,b). The default value of this parameter is equal to 0.
- 3.7.34. **“splineRes_wt”** (alias “spl_res_wt”) is a “switch” (1 or 0) indicating the value of the second coefficient (a_{res}) in Eqs. (6.7.1a,b). The default value of this parameter is equal to 1.
- 3.7.35. **“splineCS_wt”** (alias “spl_CS_wt”) is a “switch” (1 or 0) indicating the value of the third coefficient (a_{CS}) in Eqs. (6.7.1a,b). The default value of this parameter is equal to 0.
- 3.7.36. **“geomAvg”** (alias “geom_avg”) is a “switch” (1 or 0) indicating whether the objective function must be defined as the arithmetic average (6.7.1a) (“geomAvg=0”) or as the geometric average (6.7.1b) (“geomAvg=1”). This parameter has no effect if only one type of relative deviation is used in the definition of the OF (for example, in the case of the default definition (1.7.7)). The default value of this parameter is 1 (indicating geometric average).
- 3.7.37. **“mainDevType”** (alias “main_dev_type”) indicates the type of relative deviation that must determine the value of the OF when two or more types of relative deviation are included in

the definition of the OF. Since the value of the arithmetic average (6.7.1a) is determined by the largest of the terms used to calculate it, the values of all other terms (corresponding to the other types of relative deviation) are set equal to the value of the “main” relative deviation if they are greater than it and the option “geomAvg=0” is used (it is also possible to replace the original term with the geometric average of the original term and the “main” relative deviation, depending on the value of parameter No. 3.7.38 “devCapType”). Since the value of the geometric average (6.7.1b) is determined by the smallest of the factors used to calculate it, the values of all other factors (corresponding to the other types of relative deviation) are set equal to the value of the “main” relative deviation if they are less than it and the option “geomAvg=1” is used (it is also possible to replace the original factor with the geometric average of the original factor and the “main” relative deviation, depending on the value of parameter No. 3.7.38 “devCapType”). When mainDevType=0, all included types of relative deviation are treated equally when calculating the OF. This parameter is ignored when only one type of relative deviation is used in the definition of the OF (for example, in the case of the default definition (1.7.7)). The allowed non-zero values of parameter “mainDevType” are:

- 2 – δ_{unc} (first term of Eqs. (6.7.1a,b)),
- 3 – δ_{res} (second term of Eqs. (6.7.1a,b)),
- 4 – δ_{CS} (third term of Eqs. (6.7.1a,b)).

Such numbering of the deviation types is used in order to be consistent with the numbering used in the case of spline fitting of the κ_{max} -fitted DCS (in the latter case, two other deviation types with numbers 1 and 5 are available). The default value of this parameter is 2.

3.7.38. “**devCapType**” (alias “**dev_cap_type**”) is the number 1 or 2 indicating the type of the replacement applied to a term or factor in the definition of the OF when that term or factor is greater than the “main” relative deviation (in the case “geomAvg=0”) or less than the “main” relative deviation (in the case “geomAvg=1”), which is specified by parameter No. 3.7.37 (“mainDevType”). If devCapType = 1, then the mentioned term or factor is set equal to the absolute value of the “main” relative deviation. If devCapType = 2, then the mentioned term or factor is set equal to the geometric average of the original term or factor and the “main” relative deviation (i.e., to the square root of the product of the latter two terms). The default value of parameter “devCapType” is equal to 2.

6.8. Parameters controlling the angular spline fitting and extrapolation of the κ_{max} -fitted DCS

3.8.1–3. “**spline_theta_min_fitted1**”, “**spline_theta_min_fitted2**” (aliases “**spline_theta_min_fitted**”, “**spl_theta_min**” for both) and “**n_spline_theta_min_fitted**” define the set of equidistant angles to be used as the starting point (θ_{min}) of the angular spline-fitting interval when spline-fitting the κ_{max} -fitted DCS (see also Section 1.7.2). “**spline_theta_min_fitted1**” and “**spline_theta_min_fitted2**” are the first and last angles of the set, respectively, and “**n_spline_theta_min_fitted**” is the number of equidistant angles in the set. The angles must be specified in degrees. If **spline_theta_min_fitted1** is equal to **spline_theta_min_fitted2**, then **n_spline_theta_min_fitted** is reset to 1. If **n_spline_theta_min_fitted**=1, then **spline_theta_min_fitted2** is reset to **spline_theta_min_fitted1**. If the “ μ -correction” is not applied (see Sections 1.5.4 and 6.6), or the “alternative CS-fitting mode” is not applied (see Section 6.12), or **mode_mu** = 0, or the partial-wave DCS is an increasing function of κ_{max} , then $\theta_{\text{min}} = 0$ by default, i.e., **spline_theta_min_fitted1** = **spline_theta_min_fitted2** = 0. In other cases, $\theta_{\text{min}} = \theta_{\text{start}}$ (the starting point of the interval of constant scale factor μ , or the angle specified by parameter “**start_angle_mu**”), i.e., **spline_theta_min_fitted1** = **spline_theta_min_fitted2** = θ_{start} .

3.8.4–6. “**spline_theta_max_fitted1**”, “**spline_theta_max_fitted2**” (aliases “**spline_theta_max_fitted**” and “**spl_theta_max**”) and “**n_spline_theta_max_fitted**” define

the set of angles to be used as the ending point (θ_{\max}) of the angular spline-fitting interval when spline-fitting the κ_{\max} -fitted DCS (see also Section 1.7.2). “spline_theta_max_fitted1” and “spline_theta_max_fitted2” are the first and last angles of the set, respectively, and “n_spline_theta_max_fitted” is the number of equidistant angles in the set. The angles must be specified in degrees. If spline_theta_max_fitted1 = spline_theta_max_fitted2, then n_spline_theta_max_fitted is reset to 1. If n_spline_theta_max_fitted=1, then spline_theta_max_fitted2 is reset to spline_theta_max_fitted1. If the μ -correction is applied and mode_mu ≥ 1 (see the description of parameter No. 3.6.1), and the PW DCS decreases with κ_{\max} and the overall relative correction of the PW DCS due to the κ_{\max} -fitting is categorized as “large” (i.e., if there is no angular interval satisfying the constraints defined by parameters No. 3.6.45–46 “maxCorr_mu2” and “minWidth_mu2”), then θ_{\max} is by default equal to θ' (the endpoint of the polynomial fitting interval used for the μ -correction), i.e., spline_theta_max_fitted1 = spline_theta_max_fitted2 = θ' . If the μ -correction is applied and parameter “mode_mu” is equal to -1 or 0 or the PW DCS is a decreasing function of κ_{\max} , but the overall relative correction of the PW DCS due to the κ_{\max} -fitting is categorized as “small” (i.e., if an angular interval satisfying the constraints defined by parameters No. 3.6.45–46 exists), or if the simple polynomial extrapolation described in Section 1.7.3 is applied at large angles, or if $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$, then $\theta_{\max} = 180^\circ$, i.e., spline_theta_max_fitted1=spline_theta_max_fitted2=180. In other cases, the default values of those parameters are: spline_theta_max_fitted1=100, spline_theta_max_fitted2=180, n_spline_theta_max_fitted=17.

3.8.7. “**splineExt_fitted**” defines the additional conditions for performing the angular extrapolation (both large-angle and small-angle) of the κ_{\max} -fitted DCS, which may override the values of θ_{\min} and θ_{\max} defined by parameters No. 3.8.1–6. The allowed values of this parameter are 0, ± 1 , and ± 2 :

splineExt_fitted = 0: the angular extrapolation will not be performed ($\theta_{\min} = 0^\circ$, $\theta_{\max} = 180^\circ$),

splineExt_fitted < 0: the angular extrapolation will always be performed,

splineExt_fitted > 0: the angular extrapolation will be performed only after finding an extra maximum or minimum of the κ_{\max} -fitted DCS in the large-angle extrapolation range, or in the case of an irrecoverable fitting error inside the angular range $\theta < (180^\circ + |\text{spline_theta_max_thr}|) / 2$, or in the case of a large relative correction of the DCS due to the κ_{\max} -fitting (averaged over different “shifts”) at any angle (see the description of parameter No. 3.8.8 “relCorr_thr”). Since the default value of parameter “spline_theta_max_thr” is 80 (see the description of parameter No. 3.7.8), the endpoint of the angular range where a check for an irrecoverable fitting error is performed is 130° .

splineExt_fitted = ± 2 : the data corresponding to $\theta < \theta_{\min}$ will not be modified (i.e., they will not be replaced by the angular dependence extrapolated to small angles).

The default value of parameter “splineExt_fitted” is -2, except when the “alternative” CS-fitting mode described in Section 6.12 is applied (then splineExt_fitted is equal to -1 by default). See also the descriptions of parameters No. 3.8.41 and No. 3.8.45.

3.8.8. “**relCorr_thr**” defines an alternative condition for performing the angular extrapolation of the κ_{\max} -fitted DCS in the case “splineExt_fitted=1” (see the description of parameter No. 3.8.7): the angular extrapolation will be performed if the relative correction of the DCS due to the κ_{\max} -fitting (averaged over different “shifts”) at any angle is greater than |relCorr_thr| when positive, or greater than |relCorr_thr|/(1+|relCorr_thr|) in absolute value when negative. If relCorr_thr > 0 or if the spline fitting of the original PW DCS has not been

performed, then the correction is calculated relative to the moving average of the original PW DCS, otherwise it is relative to the spline approximation of the original PW DCS (possibly with the large-angle extrapolation applied). The default value of parameter “relCorr_thr” is -0.3.

3.8.9–11. **“splineIntRatio_min_fitted1”** (aliases “splineIntRatio_min_fitted”, “splineIntRatio_fitted1”, “spl_int_ratio_min1”, “splineIntRatio1_thr_min_fitted”, “spl_int_ratio1_thr_min”), **“splineIntRatio_max_fitted1”** (aliases “spl_int_ratio_max1”, “splineIntRatio_max_fitted”, “splineIntRatio_fitted1”) and **“n_splineIntRatio_fitted1”** (aliases “n_splineIntRatio_fitted” and “n_spl_int_ratio1”) define the set of values of the first parameter controlling the variation of knot density (this parameter is denoted ε_1 in Section 1.7). This set of values is used during the search for the optimal value of ε_1 , which minimizes the objective function defined by Eq. (1.7.8a) or Eq. (1.7.8b). “splineIntRatio_min_fitted1” and “splineIntRatio_max_fitted1” are the first and last values of the set, respectively, and “n_splineIntRatio_fitted1” is the number of values in the set. All values are equidistant on the logarithmic scale. If n_splineIntRatio_fitted1 < 0, then the “best” value in the set will be subsequently used as the starting value for simplex minimization of the objective function (see Section 1.7). If splineIntRatio_min_fitted1 < 0, then the knot positions are determined on the basis of the curvature (second derivative) of the κ_{\max} -fitted DCS as a function of θ : a larger absolute value of the second derivative corresponds to a larger knot density (smaller inter-knot intervals). This provides a unique value of each knot, so that no iterative optimization is needed and parameters No. 3.8.10–15 are not used. The knots are found in this case by projecting uniformly spaced points onto a density function, which is proportional to the cumulative integral of the square root of the absolute value of the second derivative of the spline-smoothed κ_{\max} -fitted DCS. The absolute value of splineIntRatio_min_fitted1 is interpreted in this case as the minimum number of points inside one inter-knot interval to be used for the mentioned spline smoothing of the κ_{\max} -fitted DCS (which is needed for construction of the mentioned density function). The default values of these three parameters are: splineIntRatio_min_fitted1 = 10^{-10} , splineIntRatio_max_fitted1 = 10^{10} , n_splineIntRatio_fitted1 = -21.

3.8.12–14. **“splineIntRatio_min_fitted2”** (aliases “splineIntRatio_min_fitted”, “splineIntRatio_fitted2”, and “spl_int_ratio_min2”), **“splineIntRatio_max_fitted2”** (aliases “splineIntRatio_max_fitted”, “splineIntRatio_fitted2”, and “spl_int_ratio_max2”) and **“n_splineIntRatio_fitted2”** (aliases “n_splineIntRatio_fitted” and “n_spl_int_ratio2”) define the set of values of the second parameter controlling the knot density (this parameter is denoted ε_2 in Section 1.7). Usage of these parameters is identical to usage of parameters No. 3.8.9–11. The only difference is that n_splineIntRatio_fitted2 = 0 is allowed. Then only the first knot-density parameter (ε_1) is used, and the inter-knot intervals form a geometric progression (see Eq. (1.7.4)). The default values of these three parameters are the same as the default values of parameters No. 3.8.9–11, i.e., splineIntRatio_min_fitted2 = 10^{-10} , splineIntRatio_max_fitted2 = 10^{10} , n_splineIntRatio_fitted2 = -21.

3.8.15. **“splineIntRatio1_thr_fitted”** (aliases “spline_int_ratio1_thr”, “spl_int_ratio1_thr_min”, and “splineIntRatio1_thr_min_fitted”) is the minimum allowed value of the first parameter controlling the variation of knot density (this parameter is denoted ε_1 in Section 1.7). If this parameter is equal to 0 (the default value), then the only constraint on ε_1 is the requirement that ε_1 must be positive.

Note: If only one knot-density parameter is used (i.e., if n_splineIntRatio_fitted2 = 0), then it may be necessary to use the option “splineIntRatio1_thr_fitted = 1” in order to ensure that the inter-knot intervals do not form a decreasing sequence. Otherwise, the optimized spline function may be affected too much by the large-angle errors of the

angular dependence of the κ_{\max} -fitted DCS (relative errors of κ_{\max} -fitting are typically greatest at large angles).

- 3.8.16. **“splineLastIntRatio_thr_fitted”** (alias **“spl_lastIntRatio_thr”**) is the minimum allowed ratio of the width of the last inter-knot interval (ending at θ_{\max}) and the width of the large-angle extrapolation interval (i.e., $180^\circ - \theta_{\max}$). The default value of this parameter is equal to 1 (i.e., the interval between the last two knots of the optimal spline function cannot be narrower than the large-angle extrapolation interval). Larger values of this parameter would improve stability of the large-angle extrapolation, but may cause deterioration of accuracy of the spline fitting at $\theta < \theta_{\max}$. This parameter is not used when the large-angle extrapolation is not performed (i.e., when $\theta_{\max} = 180^\circ$).
- 3.8.17–18. **“splineInt_min_fitted”** (aliases **“splineInt_fitted”** and **“spl_int_min”**) and **“splineInt_max_fitted”** (aliases **“splineInt_fitted”** and **“spl_int_max”**) are integer numbers indicating, respectively, the minimum and maximum values of the approximate average inter-knot interval (\bar{w}) inside the spline-fitting interval (in degrees). \bar{w} is used to calculate the number of inter-knot intervals. The latter number is equal to the width of the spline-fitting interval divided by \bar{w} (this ratio is rounded to the nearest integer, or is set equal to 1 if the nearest integer is zero). The number of knots (N) is greater by 1. The program will test several integer values of \bar{w} starting with $|\text{splineInt_max_fitted}|$ and ending with $\text{splineInt_min_fitted}$. Each new value of \bar{w} is chosen so that the new value of N (calculated as described above) is greater than the previous value. If $\text{splineInt_max_fitted} > 0$, then the optimal value of N is the one that yields the smallest value of the objective function (1.7.8a) or (1.7.8b). If $\text{splineInt_max_fitted} < 0$, then the program will select the first (smallest) value of N such that the other adjustable parameters can be determined successfully (i.e., there is no angular spline fitting error). The default values of parameters **“splineInt_min_fitted”** and **“splineInt_max_fitted”** are 10 and 180, respectively. This means that the number of knots cannot be greater than 19. If $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$, then a different default value of $\text{splineInt_min_fitted}$ is used: in this case, $\text{splineInt_min_fitted}$ is equal to $\min(5, \text{splineInt_max_fitted})$ by default. If the **“alternative”** CS-fitting mode described in Section 6.12 is applied, then $\text{splineInt_min_fitted}$ is equal to 20 by default.
- 3.8.19. **“nSplineKnots_max_fitted”** (alias **“n_spl_knots_max”**) is the maximum allowed number of spline knots when fitting the angular dependence of the κ_{\max} -fitted DCS. This parameter is used to impose an additional limitation on the number of knots (the other two parameters controlling the number of spline knots are No. 3.8.17 **“splineInt_min_fitted”** and No. 3.8.18 **“splineInt_max_fitted”**). The default value of this parameter is 62, which is equivalent to absence of additional limitation, because the minimum allowed value of parameter **“splineInt_min_fitted”** is 3 (this value of the average inter-knot interval corresponds to 61 knots).
- 3.8.20–23. **“splineRef_fitted0”**, **“splineRef_fitted1”**, **“splineRef_fitted2”**, and **“splineRef_fitted3”** (alias **“splineRef_fitted”** for all four) are **“switches”** (± 1 or 0) controlling the choice of the reference function for the angular spline fitting and extrapolation of the κ_{\max} -fitted DCS (see also Section 1.7). The number after **“splineRef_fitted”** indicates the reference function: reference function No. 0 is equal to 1 (i.e., no modification of the original κ_{\max} -fitted DCS), reference functions No. 1 and No. 2 are defined by parameters No. 3.5.1–20, and reference function No. 3 is the PW DCS corresponding to $\kappa_{\max} = K$ (this PW DCS may have been spline-fitted and extrapolated as described in Section 1.7.1, depending on the values of parameters No. 3.7.1–38). If $\text{splineRef_fitted}[0,1,2,3] = \pm 1$, then the angular spline fitting (and extrapolation) of the ratio of the original PW DCS and the corresponding reference DCS may be performed, and if $\text{splineRef_fitted}[0,1,2,3] = 0$, then the mentioned fitting will not be performed. If $\text{splineRef_fitted0} = +1$ or $\text{splineRef_fitted3} = +1$, then the angular spline fitting of the PW

DCS using reference function No. 0 or No. 3, respectively, will be performed only when at least one of the two alternative reference DCS No. 1 and No. 2 is used (the five criteria for using each of the two reference DCS No. 1 and No. 2 are defined by parameters No. 3.5.32–41). If `splineRef_fitted0=-1` or `splineRef_fitted3=-1`, then the angular spline fitting of the PW DCS using reference function No. 0 or No. 3, respectively, will be performed regardless of whether the reference DCS No. 1 or No. 2 is used or not. If `splineRef_fitted1=-1` and `splineRef_fitted2=-1`, then only one of the two reference DCS No. 1 and No. 2 will be used for the angular spline fitting: it is the DCS that is most similar to the original κ_{\max} -fitted DCS inside the angular spline-fitting interval. If `splineRef_fitted1=-1` or `splineRef_fitted1*splineRef_fitted2=-1`, and $|\text{splineRef_fitted3}|=1$, then the same criterion will be used for choosing between reference DCS No. 1 and reference DCS No. 3. Similarly, if `splineRef_fitted2=-1` or `splineRef_fitted1*splineRef_fitted2=-1`, and $|\text{splineRef_fitted3}|=1$, then the same criterion will be used for choosing between reference DCS No. 2 and reference DCS No. 3. In those cases, reference DCS No. 3 will not be used if its angular dependence is irregular. If two or more reference functions are used for the angular spline fitting of the κ_{\max} -fitted DCS, then the optimal reference function is the one that yields the smallest value of the objective function (1.7.7). The default values of these four parameters are the following: `splineRef_fitted0=-1`, `splineRef_fitted1=1`, `splineRef_fitted2=0`, `splineRef_fitted3=-1`. If the “alternative” CS-fitting mode described in Section 6.12 is applied, then the default value of parameter `splineRef_fitted0` is changed to 0.

Note: If `splineRef_fitted0` is initially nonzero and the μ -fitting is performed (see Sections 1.5.4 and 3.6), then `splineRef_fitted0` will most likely be automatically reset to zero before the spline fitting for individual “shifts”. This happens when the overall relative correction of the PW DCS due to the κ_{\max} -fitting is categorized as “large”, i.e., when an angular interval satisfying the constraints defined by parameters No. 3.6.45–46 (“`maxCorr_mu2`” and “`minWidth_mu2`”) does not exist.

3.8.24–25. “**splineArg_fitted1**” and “**splineArg_fitted2**” (aliases “`splineArg_fitted`” and “`spl_arg`” for both) are integer numbers 1, 2 or 3 indicating the first and last definition of the spline argument to be tested:

- 1 – the spline argument is equal to θ ,
- 2 – the spline argument is equal to $-\cos \theta$,
- 3 – the spline argument is equal to $\ln[(1 - \cos \theta) / 2]$.

All definitions starting with No. `splineArg_fitted1` and ending with No. `splineArg_fitted2` will be tested (see also Section 1.7). The optimal definition of the spline argument is the one that yields the smallest value of the objective function (1.7.7). The default value of parameters “`splineArg_fitted1`” and “`splineArg_fitted2`” is 2 (i.e., the spline argument is equal to $-\cos \theta$ by default).

3.8.26. “**splineLog_fitted**” (alias “`spl_log`”) controls the optional replacement of the original function by its logarithm during the angular spline fitting. Three values are allowed:

- 0 – do not replace the original function by its logarithm,
- 1 – perform the angular spline fitting only with the logarithm of the original function,
- 2 – perform the angular spline fitting both with the original function and with its logarithm.

In the latter case, the optimal option is the one that yields the smallest value of the objective function (1.7.7). The default value of parameter “`splineLog_fitted`” is equal to 2.

3.8.27. “**minDeg_cos_fitted**” (aliases “`min_deg_cos`”, “`deg_cos_fitted`”, “`deg_cos`”) is used to specify the minimum degree of the approximating polynomial in the case of two knots when the spline argument is equal to $-\cos \theta$ (see the note at the end of Section 1.7.1). The default value of this parameter is equal to 1.

- 3.8.28. “**maxDeg_cos_fitted**” (aliases “max_deg_cos”, “deg_cos_fitted”, “deg_cos”) is used to specify the maximum degree of the approximating polynomial when the spline argument is equal to $-\cos \theta$ (see the note at the end of Section 1.7.1). If this parameter is less than 3, then the number of knots will not be allowed to be greater than 2 when the spline argument is equal to $-\cos \theta$. If this parameter is equal to 0, then $-\cos \theta$ will not be used as the argument of a polynomial or of a spline function approximating the angular dependence of the κ_{\max} -fitted DCS (regardless of the values of parameters “splineArg_fitted1” and “splineArg_fitted2”). The default value of this parameter is equal to 3.
- 3.8.29. “**tol_spline_fitted**” (alias “tol_spl”) is used to specify the absolute tolerance of the change of the natural logarithm of the two spline knot-density parameters (denoted ε_1 and ε_2 in Section 1.7) during their optimization by the simplex method, as a part of the angular spline fitting of the κ_{\max} -fitted DCS. The default value of this parameter is equal to 10^{-4} .
- 3.8.30. “**spline_combine**” indicates if the κ_{\max} -fitted DCS data for different “shifts” must be combined into a single dataset for the subsequent spline fitting and extrapolation. This is possible only in the case `shift_k_mode_DCS=1`. If `spline_combine=0`, or if `shift_k_mode_DCS>1`, then the κ_{\max} -fitted DCS data for different shifts are spline-fitted and extrapolated separately, whereupon the spline fitting results are averaged over the valid shifts (with optional weighting) and spline-fitted again. In this case, the first coefficient (a_{diff}) in the full definition of the objective function (6.8.1a,b) is equal to zero and the term δ_{diff} is excluded, because it is defined only when the number of shifts used for optimization of the spline-fitting parameters is greater than 1. If `spline_combine=1`, then the linear part of the spline fitting (i.e., optimization of the spline values at a fixed set of knots) will also be performed separately for each shift, but the search for the optimal values of the other adjustable parameters (such as the endpoints of the angular spline-fitting interval and the knot density parameters) will be performed taking into account all shifts simultaneously, using the full definition of the objective function (6.8.1a,b). After that, the spline fitting results will be averaged over the valid shifts (with optional weighting) and spline-fitted again (as in the case “`spline_combine=0`”). When `spline_combine=1`, all adjustable parameters of the spline fitting, excluding the values of the spline function at the knots, are the same for all shifts (unlike in the case “`spline_combine=0`”, when those parameters are determined for each shift separately). If `spline_combine=2`, then the initial angular spline fitting of the κ_{\max} -fitted DCS will be skipped, and only the average of the κ_{\max} -fitted DCS (averaged over all shifts) will be spline-fitted. The default value of this parameter is equal to 0. If $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$, then a different default value of `spline_combine` is used: in this case, `spline_combine` is equal to 2 by default.
- 3.8.31. “**spline_maxRelErr**” is the maximum allowed relative uncertainty (returned by the κ_{\max} -fitting procedure) for using a given data point of the angular dependence of the κ_{\max} -fitted DCS for the angular spline fitting. If the mentioned relative uncertainty is greater than the value of this parameter, then the corresponding data point will not be used for the angular spline fitting (i.e., it will be assigned a zero weight). If parameter “`spline_maxRelErr`” is zero or negative, then it will be ignored (i.e., the relative uncertainty will not be taken into account when determining whether a given data point must be used for the angular spline fitting). The default value of this parameter is 0.1.
- 3.8.32. “**tol_0wt**” is the maximum allowed fraction of points with zero weights in the angular dependence of the κ_{\max} -fitted DCS. A point can be assigned a zero weight due to an error of κ_{\max} fitting, or due to a large value of its relative uncertainty (see the description of parameter No. 3.8.31). If the final fraction of the points that have been assigned a zero weight is greater than the value of this parameter, then the program will terminate with an error message. The default value of this parameter is equal to 0.5.

- 3.8.33. “**spline_tolRelSD**” is the initial value of the maximum allowed relative standard deviation (calculated over multiple “shifts”) for using a given data point of the κ_{\max} -fitted DCS for the angular spline fitting. If the total number of points rejected due to this criterion is greater than half the initial number of points with non-zero weights, then `spline_tolRelSD` will be increased by a factor of 1.25. This will be repeated until the total number of the rejected points becomes less than half of the initial number of points with non-zero weights. If parameter “`spline_tolRelSD`” is zero or negative, then it will be ignored (i.e., the standard deviation will not be taken into account when determining whether a given data point must be used for the angular spline fitting). The default value of this parameter is equal to 0.01.
- 3.8.34. “**relErr_tol_spl**” is the relative tolerance when checking the angular dependence of a spline-fitted DCS for existence of extra inflection points or extrema. The default value of this parameter is equal to 10^{-4} .

Although parameters No. 3.8.1–6 are normally sufficient for defining the set of angular spline-fitting intervals to be tested when processing the κ_{\max} -fitted DCS data, there is also an option to define the mentioned set of angular intervals using additional criteria:

- (a) the minimum and maximum width of the spline-fitting interval (i.e., the difference $\theta_{\max} - \theta_{\min}$),
- (b) the maximum allowed range of the relative correction of the original PW DCS due to the initial angular spline fitting and the subsequent κ_{\max} -fitting,
- (c) the maximum allowed fraction of the angular integral of the κ_{\max} -fitted DCS (with respect to the solid angle of photon emission) corresponding to the small-angle extrapolation range ($0 \leq \theta \leq \theta_{\min}$).

The six parameters (No. 3.8.35–40) defining those criteria are described below:

- 3.8.35–36. “**spline_theta_rangeMin**” and “**spline_theta_rangeMax**” (alias “`spline_theta_range`” for both) are the minimum and maximum allowed values of the interval width ($\theta_{\max} - \theta_{\min}$), respectively. If the current value of this width is greater than the maximum allowed value, then this interval will be rejected. Otherwise, the width of the angular spline-fitting interval may be increased by increasing θ_{\max} or decreasing θ_{\min} . This increase of the interval width depends on the magnitude of the range of the relative correction of the original PW DCS due to the initial angular spline fitting and the subsequent κ_{\max} -fitting (see the description of parameters No. 3.8.37–39). The default values of parameters “`spline_theta_rangeMin`” and “`spline_theta_rangeMax`” are equal to `spline_theta_max_fitted1 - spline_theta_min_fitted2` and `spline_theta_max_fitted2 - spline_theta_min_fitted1`, respectively (this means that all angular intervals constructed using parameters No. 3.8.1–6 are acceptable by default).
- 3.8.37–39. “**relCorrRangeMax1**”, “**relCorrRangeMax2**” (alias “`relCorrRangeMax`” for both) and “**n_relCorrRangeMax**” define the set of equidistant values of the maximum allowed range (“`corrRange_max`”) of the relative correction of the original PW DCS due to the initial angular spline fitting and the subsequent κ_{\max} -fitting, to be used when choosing among the angular intervals whose width are between the limiting values defined by parameters No. 3.8.35–36. This correction may be either relative to the moving average of the original PW DCS, or relative to the spline approximation of it, depending on the sign of parameter No. 3.8.8 (“`relCorr_thr`”): the moving average of the original PW DCS will be used as the “base” value if `relCorr_thr` ≥ 0 , and the spline approximation of the PW DCS will be used if `relCorr_thr` < 0 . The range of the relative correction “`relCorr_range`” is defined as the difference of the maximum and minimum values of the relative correction “`relCorr`” in the current angular interval. If the value of `relCorr_range` corresponding to the initial angular interval (which is one of the intervals defined by parameters No. 3.8.1–6) is less than the current value of `corrRange_max`, then the program will attempt to increase the width of the angular spline-fitting interval by decreasing θ_{\min} or increasing θ_{\max} . In general, there are several such intervals with equal width, containing the initial interval. In such a case, the

optimal interval is the one where the value of `relCorr_range` is smallest. If this value is also less than `corrRange_max`, then the width will be increased again. This process will be continued until the interval width reaches `spline_theta_rangeMax`, or `relCorr_range` becomes greater than `corrRange_max` (whichever happens first). If `corrRange_max` is equal to 0, then the value of the relative correction will be ignored. The default values of these parameters are the following: `relCorrRangeMax1=0`, `relCorrRangeMax2=0`, `n_relCorrRangeMax=1` (i.e., the value of the relative correction is ignored by default).

Note: In order to eliminate the asymmetry in the magnitudes of positive and negative relative corrections (the former ranging from 0 to $+\infty$, the latter ranging from 0 to -1), the negative values of the relative correction “`relCorr`” are redefined in the code of BREMS as `relCorr/(1+relCorr)`. This note applies only to the values of the relative correction used during the angular spline fitting as described above. Everywhere else (for example, in the “`DCS_fitted_`” file), negative relative corrections are defined conventionally (i.e., their absolute value is always less than 1).

3.8.40. “**smallAngleFraction**” is the maximum allowed fraction of the angular integral of the κ_{\max} -fitted DCS (with respect to the solid angle of photon emission) corresponding to the small-angle extrapolation range ($0 \leq \theta \leq \theta_{\min}$). If the ratio of the integral of `DCS(θ) \cdot sin(θ)` from 0° to θ_{\min} with respect to θ and the total integral (from 0° to 180°) is greater than `smallAngleFraction`, then θ_{\min} will be reduced to comply with the mentioned requirement. The default value of this parameter is equal to 1 (i.e., all values of θ_{\min} are allowed).

The next nine parameters define the objective function (OF) that is minimized during the angular spline fitting of the κ_{\max} -fitted DCS. Although the default definition of the OF consists of three or two terms (see Eq. (1.7.8a) and Eq. (1.7.8b)), there is an option to add two more terms reflecting other properties of the spline function, which are related to the accuracy of the spline approximation –relative differences between values of the κ_{\max} -fitted DCS corresponding to different fitting intervals (when `spline_combine=1`), and relative deviations of the spline-fitted shape function (SF) from the reference SF No. 1 or No. 2 (which by default correspond to the Born approximation and Sommerfeld-Maue approximation, respectively). Thus, the most general expression of the OF used for the angular spline fitting of the κ_{\max} -fitted DCS is the following:

$$f = f_n [(a_{\text{diff}} \delta_{\text{diff}})^2 + (a_{\text{unc}} \delta_{\text{unc}})^2 + (a_{\text{res}} \delta_{\text{res}})^2 + (a_{\text{CS}} \delta_{\text{CS}})^2 + (a_{\text{SF}} \delta_{\text{SF}})^2], \quad (6.8.1a)$$

or

$$f = (\delta_{\text{diff}}^{2a_{\text{diff}}} \delta_{\text{unc}}^{2a_{\text{unc}}} \delta_{\text{res}}^{2a_{\text{res}}} \delta_{\text{CS}}^{2a_{\text{CS}}} \delta_{\text{SF}}^{2a_{\text{SF}}})^{f_n}, \quad (6.8.1b)$$

where δ_{diff} is the rms value of the relative deviation of a value of the κ_{\max} -fitted DCS from the average κ_{\max} -fitted DCS, calculated over all fitting intervals (i.e., the standard relative deviation), and δ_{SF} is the rms value of the relative deviation of the κ_{\max} -fitted SF from the reference SF, calculated over the entire angular range $0^\circ \leq \theta \leq 180^\circ$. Each of the five coefficients a_{diff} , a_{unc} , a_{res} , a_{CS} and a_{SF} can be either 1 or 0. f_n is the “normalization factor” equal to the inverse number of terms included in the definition of the OF (i.e., the inverse number of non-zero a -coefficients in Eqs. (6.8.1a,b)). The next nine parameters are used to specify the five coefficients a_{diff} , a_{unc} , a_{res} , a_{CS} and a_{SF} in Eqs. (6.8.1a,b), the method of combining the terms of the OF, and the definition of the mentioned reference CS:

3.8.41. “**CS_ref_spline**” is the “reference CS” for calculation of the term δ_{CS} in the definition of the objective function (6.8.1a) or (6.8.1b) (see also Section 1.7.2). This term is included only when `splineCS_wt_fitted=1` (see the description of parameter No. 3.8.45). If `CS_ref_spline=0` and `splineCS_wt_fitted=1`, then `CS_ref_spline` will be assigned the default value, which is equal to the saturation value of the partial-wave CS as a function of κ_{\max} obtained by nonlinear least squares fitting.

Notes: 1) If $CS_ref_spline > 0$ and $splineCS_wt_fitted = 1$ and the “alternative” CS-fitting mode is applied (see Section 6.12), then the default value of parameter “splineExt_fitted” (No. 3.8.7) is changed from -2 to -1.

2) It is possible to replace CS_ref_spline with the interpolated value returned by subroutine $Brems_CS_interp$. This is achieved by setting parameter “CS_int” to a value greater than 1 (see the description of parameter No. 6.1.5 in Section 9.1).

- 3.8.42. “**splineDiff_wt**” is a “switch” (1 or 0) indicating the value of the first coefficient (a_{diff}) in Eqs. (6.8.1a,b). The default value of this parameter is equal to 1.
- 3.8.43. “**splineUnc_wt_fitted**” (alias “spl_unc_wt”) is a “switch” (1 or 0) indicating the value of the second coefficient (a_{unc}) in (6.8.1a,b). The default value of this parameter is equal to 1.
- 3.8.44. “**splineRes_wt_fitted**” (alias “spl_res_wt”) is a “switch” (1 or 0) indicating the value of the third coefficient (a_{res}) in Eqs. (6.8.1a,b). The default value of this parameter is equal to 1.
- 3.8.45. “**splineCS_wt_fitted**” (alias “spl_CS_wt”) is a “switch” (1 or 0) indicating the value of the fourth coefficient (a_{CS}) in Eqs. (6.8.1a,b). The default value of this parameter is equal to 1.
- 3.8.46. “**splineSF_wt**” can be either 0 or the sequence number (1 or 2) of the reference SF to be used when calculating the rms relative deviation δ_{SF} in the fifth term of Eqs. (6.8.1a,b). When $splineSF_wt$ is equal to 0, this term is excluded ($a_{SF} = 0$). When $splineSF_wt$ is equal to 1 or 2, this term is included ($a_{SF} = 1$). The default value of this parameter is equal to 0.
- 3.8.47. “**geomAvg_fitted**” (alias “geom_avg”) is a “switch” (1 or 0) indicating whether the OF must be defined as the arithmetic average (6.8.1a) (“geomAvg_fitted=0”) or as the geometric average (6.8.1b) (“geomAvg_fitted=1”). This parameter has no effect if only one term is used in the definition of the OF (for example, if OF is defined according to Eq. (1.7.7)). The default value of this parameter is equal to 0 (indicating arithmetic average).
- 3.8.48. “**mainDevType_fitted**” (alias “main_dev_type”) indicates the type of relative deviation that must determine the value of the OF when two or more types of relative deviation are included in the definition of the OF. Since the value of the arithmetic average (6.8.1a) is determined by the largest of the terms used to calculate it, the values of all other terms (corresponding to the other types of relative deviation) are set equal to the value of the “main” relative deviation if they are greater than it and the option “geomAvg_fitted=0” is used (it is also possible to replace the original term with the geometric average of the original term and the “main” relative deviation, depending on the value of parameter No. 3.8.49 “devCapType_fitted”). Since the value of the geometric average (6.8.1b) is determined by the smallest of the factors used to calculate it, the values of all other factors (corresponding to the other types of relative deviation) are set equal to the value of the “main” relative deviation if they are less than it and the option “geomAvg_fitted=1” is used (it is also possible to replace the original factor with the geometric average of the original factor and the “main” relative deviation, depending on the value of parameter No. 3.8.49 “devCapType_fitted”). When $mainDevType_fitted=0$, all included types of relative deviation are treated equally when calculating the OF. This parameter is ignored when only one type of relative deviation is used in the definition of the OF. The allowed non-zero values of parameter “mainDevType_fitted” are the following:

- 1 – δ_{diff} (first term of Eqs. (6.8.1a,b)),
- 2 – δ_{unc} (second term of Eqs. (6.8.1a,b)),
- 3 – δ_{res} (third term of Eqs. (6.8.1a,b)),
- 4 – δ_{CS} (fourth term of Eqs. (6.8.1a,b)),
- 5 – δ_{SF} (fifth term of Eqs. (6.8.1a,b)).

The default value of this parameter is equal to 3, except when the “alternative” CS-fitting mode is applied, in which case it is equal to 4 (see also Section 6.12).

3.8.49. “**devCapType_fitted**” (alias “**dev_cap_type**”) is the number 1 or 2 indicating the type of the replacement applied to a term or factor in the definition of the OF when that term or factor is greater than the “main” relative deviation (in the case “**geomAvg_fitted=0**”) or less than the “main” relative deviation (in the case “**geomAvg_fitted=1**”), which is specified by parameter No. 3.8.48 (“**mainDevType_fitted**”). If **devCapType_fitted** = 1, then the mentioned term or factor is set equal to the absolute value of the “main” relative deviation. If **devCapType_fitted** = 2, then the mentioned term or factor is set equal to the geometric average of the original term or factor and the “main” relative deviation (i.e., to the square root of the product of the latter two terms). The default value of parameter “**devCapType_fitted**” is equal to 2.

6.9. Parameters controlling the large-angle polynomial extrapolation at small relative corrections

The large-angle polynomial extrapolation, which is controlled by parameters of this subgroup, is not applied for fitting the “original” DCS if both the μ -correction and the alternative method of improving accuracy of the final κ_{\max} -fitted DCS are used simultaneously (the latter method is described in Section 1.8, and the corresponding parameters are described in Section 6.18). In such a case, the large-angle polynomial extrapolation (and the parameters described below) will be applied only for fitting the “alternative” DCS.

3.9.1–2. “**degree_extrap_min**” and “**degree_extrap_max**” (alias “**degree_extrap**” for both) are the minimum and maximum degree of the polynomial used for the angular fitting and large-angle extrapolation (this degree is denoted L in Eq. (1.7.9) in Section 1.7.3). The default values of these two parameters are equal to 1 and 10, respectively.

3.9.3. “**fitRef_extrap**” is the integer number from 0, 1 or 2 equal to the sequence number of the reference function that must be used as the divisor of the extrapolated DCS in order to obtain the dependent variable of the polynomial fitting (see Eq. (1.7.9) in Section 1.7.3). The value of 0 corresponds to absence of the mentioned divisor, i.e., the reference function equal to 1. The default value of this parameter is 1 (this value by default corresponds to the screened Born-approximation DCS).

3.9.4–5. “**thrCorr_extrap1**” and “**thrCorr_extrap2**” (alias “**thrCorr_extrap**” for both) are the two threshold absolute values of the relative correction, which were denoted t_1 and t_2 in Section 1.7.3. The second one cannot be less than the first one. If both these parameters are equal to 0, then the large-angle polynomial extrapolation will not be performed. If $T_1 \leq 3$ MeV or $T_2 / T_1 > 0.02$, then the default values of these two parameters are equal to 0.05 and 0.3, respectively (otherwise, they are both equal to zero).

3.9.6. “**maxPosCorr_extrap**” is the maximum allowed positive relative correction. If the relative correction of the PW DCS due to the κ_{\max} -fitting is positive and greater than this value at any angle, then the large-angle polynomial extrapolation will not be performed, and other large-angle extrapolation methods will be applied. The default value of this parameter is equal to 1 (i.e., if the κ_{\max} -fitting causes an increase of the DCS by a factor greater than 2 at any angle, then the large-angle polynomial extrapolation will not be performed).

3.9.7. “**start_extrap**” is the starting angle (in degrees) of the polynomial fitting interval. The default value of this parameter is equal to 110.

3.9.8–9. “**thrAngle_extrap1**” and “**thrAngle_extrap2**” (alias “**thrAngle_extrap**” for both) are the two threshold values of the endpoint of the polynomial fitting interval (in degrees), which were denoted θ_{e1} and θ_{e2} in Section 1.7.3. The second one cannot be less than the first one. The default values of these two parameters are equal to 160 and 170, respectively.

3.9.10. “**nFit_extrap**” is the number of polynomial fitting cycles. Each polynomial fitting differs from the previous one by a smaller value of the endpoint of the fitting interval. The current fitting interval is obtained from the previous one by excluding the last data point (see also Section 1.7.3). The default value of this parameter is equal to 21.

3.9.11. “**minPoints_extrap**” is the smallest allowed number of data points used for the polynomial fitting. The default value of this parameter is equal to 31.

Note: Taking into account that the number of points used for the polynomial fitting may be reduced by up to $nFit_extrap - 1$ points (see the description of parameter No. 3.9.10), the number of points from the starting angle (parameter No. 3.9.7 “start_extrap”) to the maximum ending angle (denoted θ_p in Section 1.7.3) cannot be less than $minPoints + nFit_extrap - 1$. The default value of the latter sum is equal to 51.

3.9.12. “**minRatio_extrap**” is the smallest allowed ratio of the polynomial in the expression (1.7.9) of the extrapolated DCS (after the weighted averaging over all fitting cycles, as explained in Section 1.7.3) at any point inside the large-angle extrapolation interval to the value of the same polynomial at the starting angle of this interval, as well as the smallest allowed value of the inverse ratio. If the value of the mentioned ratio at a particular point inside the extrapolation range is less than $minRatio_extrap$ or greater than $1/minRatio_extrap$, then the extrapolation results will be rejected (i.e., other large-angle extrapolation methods will be applied instead of the polynomial extrapolation). The default value of this parameter is equal to 0.03.

3.9.13. “**maxChange_extrap**” is the maximum allowed relative deviation of the extrapolated DCS corresponding to the degree $L + 1$ (i.e., one greater than the value of parameter No. 3.9.1 “degree_extrap”) from the extrapolated DCS corresponding to the degree L (specified by parameter “degree_extrap”) at any point inside the large-angle extrapolation interval. If the maximum relative deviation of the larger one of the mentioned two values from the smaller one is greater than $maxChange_extrap$, then the extrapolation results will be rejected (i.e., other large-angle extrapolation methods will be applied instead of the polynomial extrapolation). The default value of this parameter is equal to 0.4.

3.9.14. “**maxDiff_mu_extrap**” controls the extension of the polynomial fitting interval on the basis of the relative deviation of the μ -corrected DCS (calculated using the value of the scale factor μ corresponding to smaller angles) from the κ_{max} -fitted DCS. This interval will be extended by adding all points where the mentioned relative deviation is less than $maxDiff_mu_extrap$ in absolute value. The default value of this parameter is equal to 0 (no extension).

6.10. Parameters controlling the type and number of additional datasets to be created

3.10.1. “**additionalFiles_fit**” is a “switch” (1 or 0) indicating if the files of the second and third group of output files defined in Section 6.20 must be updated. The default value of this parameter is equal to 0 (i.e., the mentioned files are not updated).

3.10.2. “**extrap_files**” is a “switch” (1 or 0) indicating if the file with the values of the spline-fitted and extrapolated PW DCS for all angles and all values of κ_{max} must be created (this file belongs to the fourth group of output files described in Section 6.20). The name of this file is controlled by parameters “suffix_spline”, “suffix_extrap”, and “suffix3a” (see the descriptions of parameters No. 3.15.5–6 and No. 3.15.8). The default value of parameter “extrap_files” is equal to 0 (indicating that the mentioned file must not be created).

3.10.3. “**output_interm0**” (alias “output_interm”) is a “switch” (1 or 0) indicating if the file with the values of the κ_{max} -fitted DCS for all angles and all “shifts” that were not flagged as κ_{max} -fitting failures must be created (this file belongs to the fourth group of output files described in Section 6.20). The default value of parameter “output_interm0” is 0 (indicating that the mentioned file must not be created).

3.10.4. “**output_interm1**” (alias “output_interm”) is a “switch” (1 or 0) indicating if the file with the values of the spline-fitted and extrapolated κ_{max} -fitted DCS for all angles and all “shifts” that were not flagged as κ_{max} -fitting failures must be created, and if the file “Data_interm1.txt” with the optimal values of all adjustable parameters defining the optimal

spline fit of the κ_{\max} -fitted DCS corresponding to each “shift” that has not been flagged as a fitting failure must be updated (these two files belong to the fourth group of output files described in Section 6.20). The default value of parameter “output_interm1” is 0 (indicating that the mentioned two files must not be created or updated).

- 3.10.5. “**output_mu**” is a “switch” (0, ± 1 , or 2) indicating if the files “mu_range.txt” and “mu.txt” with the values of endpoints of the “optimum” angular interval for calculation of the scale factor μ in Eq. (1.5.12b) and the values of the rms and maximum relative deviations of the μ -corrected DCS from the reference DCS indicated by parameter “compRef_mu” (No. 3.6.35) must be updated, and if the file “DCS_mu_....txt” with the values of the μ -corrected DCS for all angles must be created (those files belong to the fifth group of files defined in Section 6.20). If parameter “output_mu” is equal to 0, then those files will not be updated. If “output_mu” is equal to ± 1 , then only the files “mu_range.txt” and “DCS_mu_....txt” will be updated. If output_mu=-1, then the program will quit immediately after updating those two files (i.e., the κ_{\max} -fitting will not be performed). If output_mu=2, then all three mentioned files will be updated. The default value of parameter “output_mu” is equal to 0 (indicating that the mentioned three files must not be updated or created).
- 3.10.6. “**MA_file**” is a “switch” (0 or 1) indicating if the file with the values of the moving average (MA) of the original partial-wave DCS must be created. The default value of this parameter is equal to 0 (indicating that the mentioned file must not be created). The name of this file is controlled by parameters “suffix_MA” and “suffix3a” (see the descriptions of parameters No. 3.15.7–8). *Note:* The file with the MA values will not be created if the MA is not used (i.e., if the MA period is equal to 1), regardless of the value of parameter “MA_file”.

6.11. Parameters controlling the choice of the fitting function during the κ_{\max} -fitting

- 3.11.1–3. “**polyn_thr_CS**” (aliases “polyn_thr” and “polyn_thr_incr”), “**polyn_thr_DCS1**” (aliases “polyn_thr”, “polyn_thr_incr”, and “polyn_thr_DCS”), and “**polyn_thr_DCS2**” (aliases “polyn_thr” and “polyn_thr_DCS”) are the threshold values of the relative correction of the CS or DCS due to the stretched exponential fitting of the dependence (D)CS(κ_{\max}), which must be exceeded in order to use the polynomial (1.5.10) as the fitting function, where x is defined by Eq. (1.5.8) with b , d and h optimized for the case of a first-degree polynomial ($M = 1$). It is also possible to use $h = 0$ and an arbitrary positive value of d (see the description of parameters No. 3.11.19–21). The polynomial fitting will be also applied in the case of a fitting error during the stretched exponential fitting. Parameter “polyn_thr_DCS1” is used when the dependence DCS(κ_{\max}) is an increasing function, and “polyn_thr_DCS2” is used when the dependence DCS(κ_{\max}) is a decreasing function. If polyn_thr_(D)CS[1,2]<0, then the polynomial fitting will be performed only in the case of an error during the preceding stretched-exponential fitting. If polyn_thr_(D)CS[1,2]=0, then the polynomial fitting will always be preferred to the stretched exponential fitting, regardless of the magnitude of the relative correction. The initial stretched exponential fitting is performed using the fitting function defined by Eq. (1.5.1). The default values of those three parameters are equal to 0.2, 0.2, and -1 , respectively (since the latter value is negative, the polynomial fitting is never performed by default when DCS(κ_{\max}) is a decreasing function).
- 3.11.4–6. “**maxDeg_CS**” (aliases “maxDeg”, “deg_CS”, “deg_incr”), “**maxDeg_DCS1**” (aliases “maxDeg”, “deg_DCS”, “deg_DCS1”, “maxDeg_DCS”, “deg_incr”), and “**maxDeg_DCS2**” (aliases “maxDeg”, “deg_DCS”, “deg_DCS2”, “maxDeg_DCS”) indicate the maximum degree of the polynomial (M) defined by Eq. (1.5.10) and Eq. (1.5.8) to be used during the κ_{\max} fitting of the CS or DCS (the choice of the optimal degree is explained in Section 1.5.2). The suffixes “1” and “2” indicate an increase or a decrease of the PW DCS as a function of κ_{\max} , respectively. The default value of these three parameters is equal to 6.
- 3.11.7–9. “**minDeg_CS**” (aliases “minDeg”, “deg_CS”, “deg_incr”), “**minDeg_DCS1**” (aliases “minDeg”, “deg_DCS”, “deg_DCS1”, “minDeg_DCS”, “deg_incr”), and “**minDeg_DCS2**”

(aliases “minDeg”, “deg_DCS”, “deg_DCS2”, “minDeg_DCS”) indicate the minimum degree of the polynomial (M) defined by Eq. (1.5.10) and Eq. (1.5.8) to be used during the κ_{\max} fitting of the CS or DCS (the choice of the optimal degree is explained in Section 1.5.2). The suffixes “1” and “2” indicate an increase or a decrease of the PW DCS as a function of κ_{\max} , respectively. The default value of these three parameters is equal to 0.

- 3.11.10. “**polyn_relErr_tol**” is the maximum allowed relative uncertainty of the zero-degree term obtained by the polynomial κ_{\max} -fitting (i.e., the term c in Eq. (1.5.10)). The default value of this parameter is equal to 0.05.
- 3.11.11–12. “**simple_exp_CS**” and “**simple_exp_DCS**” (alias “simple_exp” for both) indicate if the “simple exponential” approximation of the dependence of (D)CS on κ_{\max} may be used. In this case, the value of parameter h in Eq. (1.5.1) is equal to zero, whereas the value of the stretching exponent d is fixed. Any positive value of d is allowed (thus, a more accurate term for this approximation is “fixed- d approximation” rather than “simple exponential”, because the latter term usually implies $d = 1$). This option is applied either in the region of increase of (D)CS with κ_{\max} (simple_exp_(D)CS=1), or in the region of decrease with κ_{\max} (simple_exp_(D)CS=2), or both (simple_exp_(D)CS=3), if the reduced sum of squared residuals corresponding to the three-parameter “simple exponential” approximation does not exceed the reduced sum of squared residuals corresponding to the four-parameter stretched exponential approximation (defined by Eq. (1.5.1) with $h = 0$ and with d optimized) by a factor greater than $1 + \text{simple_exp_thr_}(D)CS$ (see also the description of parameters No. 3.11.13–15). The fixed value of the stretching exponent d used for the “simple exponential” approximation is defined by one of the three parameters No. 3.11.16–18 (“d_exp_CS”, “d_exp_DCS1”, or “d_exp_DCS2”). The default values of parameters “simple_exp_CS” and “simple_exp_DCS” are equal to 0 and 2, respectively.
- 3.11.13–15. “**simple_exp_thr_CS**” (aliases “simple_exp_thr” and “simple_exp_thr_incr”), “**simple_exp_thr_DCS1**” (aliases “simple_exp_thr”, “simple_exp_thr_incr”, and “simple_exp_thr_DCS”), and “**simple_exp_thr_DCS2**” (aliases “simple_exp_thr” and “simple_exp_thr_DCS”) are the threshold values of the relative deviation of the reduced sum of squared residuals (i.e., the sum of squared residuals divided by the number of degrees of freedom) obtained using a three-parameter “simple exponential” approximation of the function (D)CS(κ_{\max}) (with a predefined fixed value of the stretching exponent d) from the corresponding reduced sum of squared residuals obtained using the four-parameter stretched exponential approximation (1.5.1) with $h = 0$ and with d optimized by least squares. If the mentioned relative deviation is greater than the threshold value, then the latter approximation will be preferred to the simple exponential approximation. Otherwise, the simple exponential approximation will be preferred. The suffixes “1” and “2” indicate an increase or a decrease of the PW DCS as a function of κ_{\max} , respectively. The default value of these three parameters is equal to 0.01.
- 3.11.16–18. “**d_exp_CS**” (aliases “d_exp”, “d_exp_incr”), “**d_exp_DCS1**” (aliases “d_exp”, “d_exp_DCS”, “d_exp_incr”), and “**d_exp_DCS2**” (aliases “d_exp”, “d_exp_DCS”) are used to specify the mentioned fixed value of the stretching exponent d for the “simple exponential” fit (see the description of parameters No. 3.11.11–15). The suffix “1” or “2” corresponds to increase or decrease of the PW DCS with κ_{\max} , respectively. If a value of an exponent is specified with the minus sign, then the simple exponential fitting will be performed using the absolute value of the specified exponent, and if this fitting fails, then a more general four- or five-parameter fitting (with adjustable d) will be performed instead. If the specified value of the exponent is positive, then there will be no second fitting attempt using the four- or five-parameter stretched-exponential fitting function after a failure of simple three-parameter exponential fitting. The default value of these three parameters is 1.

- 3.11.19–21. “**d_polyn_CS**” (aliases “d_polyn”, “d_polyn_incr”), “**d_polyn_DCS1**” (aliases “d_polyn”, “d_polyn_DCS”, “d_polyn_incr”), and “**d_polyn_DCS2**” (aliases “d_polyn”, “d_polyn_DCS”) are used to specify the value of the stretching exponent d in the expression of the argument of the fitting polynomial (Eq. (1.5.8) with $h = 0$), when d has to be fixed (rather than optimized by least squares at $M = 1$). The suffix “1” or “2” corresponds to increase or decrease of the PW DCS with κ_{\max} , respectively. If $d_{\text{polyn}} > 0$, then the polynomial fitting will always use $d = d_{\text{polyn}}$, $h = 0$, and a non-adjustable initial value of the optimized parameter b (see Eq. (1.5.8)). If $d_{\text{polyn}} < 0$, then the values $d = |d_{\text{polyn}}|$, $h = 0$ and a non-adjustable initial value of b would be used only in the case of a failure of the previous three-, four- or five-parameter stretched-exponential fitting. In other cases, the argument of the polynomial would be set equal to the exponential obtained by the previous stretched-exponential fitting (possibly with $h > 0$). The default value of these three parameters is equal to 0.5 (since this value is positive, the values of b and d used in Eq. (1.5.8) are independent of the values obtained in the preceding stretched-exponential fitting, whereas $h = 0$).
- 3.11.22–24. “**d_init_CS**” (aliases “d_init”, “d_init_incr”), “**d_init_DCS1**” (aliases “d_init”, “d_init_DCS”, “d_init_incr”), and “**d_init_DCS2**” (aliases “d_init”, “d_init_DCS”) are used to specify the initial value of the stretching exponent d for the stretched-exponential fit when $\text{vary_h_}(D)\text{CS}=0$ or $\text{vary_h_}(D)\text{CS}=1$. If $\text{vary_h_}(D)\text{CS} \geq 2$, then the value of parameter “d_init_(D)CS<1,2>” means the geometric average of the maximum and minimum initial values of d to be tested (the range of variation of $\ln(d)$ is in such a case equal to 10). The suffix “1” or “2” corresponds to increase or decrease of the PW DCS with κ_{\max} , respectively. The default value of these three parameters is equal to $e^{-5} = 0.00673794699908547$.
- 3.11.25–26. “**vary_h_CS**” and “**vary_h_DCS**” (alias “vary_h” for both) indicate the method of calculating parameter h in Eq. (1.5.1) when fitting the CS or the DCS, respectively: (1) if $\text{vary_h}=0$, h will be equal to zero; (2) if $|\text{vary_h}| > 0$, h will be calculated as the value corresponding to the smallest sum of squared absolute deviations after performing the fitting $|\text{vary_h}|$ times. If $|\text{vary_h}| > 1$, then the initial values of the natural logarithm of parameter d used for each fitting attempt are equidistant and range from $\ln(d_{\text{init}})-5$ to $\ln(d_{\text{init}})+5$, where “d_init” is one of three parameters “d_init_CS”, “d_init_DCS1”, “d_init_DCS2” (No. 3.11.22–24). If $\text{vary_h} > 0$, then parameter h will be allowed to be non-zero only when the (D)CS increases with κ_{\max} . If $\text{vary_h} < 0$, then h will be allowed to be non-zero regardless of the direction of change of the DCS as a function of κ_{\max} . By default, $\text{vary_h_CS}=10$ in the case “accuracy_level=1”, and $\text{vary_h_CS}=20$ in the case “accuracy_level=2”. The default value of vary_h_DCS is 0.
- 3.11.27–28. “**tol_corr_CS**” and “**tol_corr_DCS**” (alias “tol_corr” for both) are used to specify the threshold value of the relative correction of the CS or DCS due to nonlinear fitting, respectively, which must be exceeded in order to perform the five-parameter stretched exponential fitting by the expression (1.5.1) (with parameter h varied) or the polynomial fitting by the expression (1.5.10). Before performing the five-parameter stretched exponential fitting or the polynomial fitting of $\text{CS}(\kappa_{\max})$ or $\text{DCS}(\kappa_{\max})$ (i.e., optimizing parameters a, b, c, d and h in Eq. (1.5.1), or parameters c, c_1, c_2, \dots, c_M in Eq. (1.5.10)), the three- or four-parameter stretched exponential fitting with $h = 0$ is performed, and if the relative correction of the CS or DCS due to this fitting is less than parameter “tol_corr_CS” or “tol_corr_DCS” respectively, then the result of the three- or four-parameter stretched exponential fitting is accepted without attempting the other two mentioned types of fitting. The default value of these two parameters is 0.005.

Notes: 1) The five-parameter stretched exponential fitting or the polynomial fitting is never attempted if the number of points in the fitting interval (N_{fit}) is less than the value of parameter No. 3.11.29 (“tol_Nfit”).

- 2) The choice between the five-parameter stretched exponential fitting and the polynomial fitting is controlled by parameters No. 3.11.1–3 (“polyn_thr_CS”, “polyn_thr_DCS1”, and “polyn_thr_DCS2”).

- 3.11.29. “**tol_Nfit**” specifies the minimum number of values of κ_{\max} in the fitting interval (N_{fit}) needed for the five-parameter stretched exponential fitting (i.e., least squares optimization of all five parameters of the fitting function defined by Eq. (1.5.1)) or the fitting by the polynomial (1.5.10) to be possible (if N_{fit} is less than **tol_Nfit**, then only the three- or four-parameter stretched-exponential fitting with $h = 0$ will be performed). The default value of this parameter is 10. **Notes:** 1) The five-parameter stretched exponential fitting or the polynomial fitting is never attempted if the relative correction of the CS or DCS due to the four-parameter stretched exponential fitting is less than the value of parameter No. 3.11.27 (“**tol_corr_CS**”) or No. 3.11.28 (“**tol_corr_DCS**”), respectively. 2) Another factor determining the choice between the four- and five-parameter stretched exponential fitting is the value of the uncertainty of the optimal value of the varied parameter c returned by the fitting procedure. This uncertainty is calculated using Eq. (1.6.2a). If the difference of the two least-squares estimates of the (D)CS (obtained using the four- and five-parameter stretched exponential fitting) is less than the larger of the two corresponding uncertainties multiplied by parameter No. 3.11.30 or No. 3.11.31 (“**thr_ratio_h_CS**” or “**thr_ratio_h_DCS**”), then the result with the smaller uncertainty is preferred, otherwise the estimate obtained by the five-parameter stretched exponential fitting is preferred.
- 3.11.30–31. “**thr_ratio_h_CS**” and “**thr_ratio_h_DCS**” (alias “**thr_ratio_h**” for both) control the condition to perform the comparison of the absolute uncertainties of the fitted (D)CS needed to determine which of the two variants of the stretched exponential fitting (with $h = 0$ or $h > 0$) must be preferred. This parameter defines the threshold value of the ratio of the absolute difference between the two estimates of the fitted (D)CS and the larger of the two corresponding absolute uncertainties, which must be exceeded in order to use the result corresponding to $h > 0$ unconditionally (i.e., without the additional requirement for the uncertainty corresponding to $h > 0$ to be less than the uncertainty corresponding to $h = 0$). If **thr_ratio_h**(D)CS=0, then the result corresponding to $h > 0$ will always be used (i.e., the uncertainties corresponding to $h = 0$ and $h > 0$ will not be compared). If **thr_ratio_h**(D)CS=1, then the additional requirement will be applied only when the larger of the two confidence intervals contains the value of the fitted (D)CS corresponding to the other fitting mode. If **thr_ratio_h**(D)CS is equal to a very large value, then the two uncertainties will always be compared, and the result corresponding to the smaller uncertainty will be used. Parameter “**thr_ratio_h**(D)CS” has an effect only when parameter “**vary_h**(D)CS” is non-zero (see the description of parameters No. 3.11.25–26). The default values of parameters “**thr_ratio_h_CS**” and “**thr_ratio_h_DCS**” are 1 and 10^{10} , respectively.
- 3.11.32–33. “**fitFunc_CS**” and “**fitFunc_DCS**” (alias “**fitFunc**” for both) control the choice between the two definitions of the fitting function – the stretched exponential (1.5.1) and the power function (1.5.6) – when fitting the dependence CS(κ_{\max}) or DCS(κ_{\max}), respectively. If **fitFunc**(D)CS=1, then the power function (1.5.6) will be used. If **fitFunc**(D)CS=2, then the stretched exponential (1.5.1) will be used. In any case, h may be one of the optimized parameters, or it may be fixed at zero, depending on the values of parameters No. 3.11.25–26. If **fitFunc**(D)CS=3, then the program will calculate the value of the left-hand side of inequality (1.5.4) after performing the fitting with the stretched exponential (1.5.1), and if this value is less than parameter No. 3.11.34 “**d_h_thr**”, the fitting will be redone using the power-function approximation (1.5.6) (which has one less varied parameter than the fitting function used for the previous fitting attempt). The default value of parameters “**fitFunc_CS**” and “**fitFunc_DCS**” is 2.
- 3.11.34. “**d_h_thr**” is the threshold value of the expression on the left-hand side of inequality (1.5.4), which must be exceeded in order to use the stretched exponential definition of the

- fitting function (1.5.1) (with up to five varied parameters) when `fitFunc_(D)CS=3` (see the description of parameters No. 3.11.32–33). Parameter “`d_h_thr`” is equal to 0.002 by default.
- 3.11.35–36. “**simple_fit_CS**” and “**simple_fit_DCS**” (alias “`simple_fit`” for both) are “switches” (0 or 1) indicating if the stretched-exponential fitting (Eq. (1.5.1)) of the dependence $CS(\kappa_{\max})$ or $DCS(\kappa_{\max})$, respectively, must be simplified by requiring that the fitted values corresponding to the initial and ending points of the κ_{\max} -fitting interval are exactly equal to the corresponding empirical values. This requirement causes a reduction of the number of varied parameters by 2. The default value of these two parameters is 0 (i.e., the mentioned simplification is not applied by default).
- 3.11.37–38. “**thr_ratio_h2_CS**” and “**thr_ratio_h2_DCS**” (alias “`thr_ratio_h2`” for both) specify the value of parameter “`thr_ratio_h_CS`” or “`thr_ratio_h_DCS`”, respectively, during pass No. 2 when `Npasses=2` (see the descriptions of parameters No. 3.2.24–25 and No. 3.11.30–31). The default values of parameters “`thr_ratio_h2_CS`” and “`thr_ratio_h2_DCS`” are 1 and 10^{10} , respectively.
- 3.11.39–40. “**fitFunc2_CS**” and “**fitFunc2_DCS**” (alias “`fitFunc2`” for both) specify the value of parameter “`fitFunc_CS`” or “`fitFunc_DCS`”, respectively, during pass No. 2 when `Npasses=2` (see the descriptions of parameters No. 3.2.24–25 and No. 3.11.32–33). The default value of parameters “`fitFunc_CS`” and “`fitFunc_DCS`” is 2.

6.12. Parameters controlling the alternative CS-fitting mode

Parameters described in this section define the conditions of applying the “alternative CS-fitting mode”, which is characterized by skipping the step of fitting the dependence of the partial-wave SDCS (referred to as “CS”) on κ_{\max} . The value of SDCS is calculated in this mode entirely from the dependence of the DDCS (referred to as “DCS”) on κ_{\max} and θ (unlike in the “normal” CS-fitting mode, when the final SDCS is set equal to the arithmetic average of the saturation value of the mentioned dependence $CS(\kappa_{\max})$ obtained by nonlinear fitting and the angular integral of the κ_{\max} -fitted DCS, and with their difference contributing to the estimate of the overall uncertainty of the κ_{\max} -fitted CS, as explained in Section 1.6). More precisely, the final κ_{\max} -fitted CS is equal in the alternative mode to the angular integral of the final κ_{\max} -fitted DCS (i.e., $\int DCS d\Omega$), whereas the uncertainty of the final κ_{\max} -fitted CS is equal to the angular integral of the absolute value of the uncertainty of the final κ_{\max} -fitted DCS (i.e., $\int |\Delta DCS| d\Omega$). In the alternative CS-fitting mode, a greater importance is assigned to the value of parameter “`CS_ref_spline`” (No. 3.8.41), because its value is the main factor determining the final DCS at small angles when the angular dependence of the DCS is strongly peaked in the forward direction. This greater importance of `CS_ref_spline` (which may be either specified by the user or determined by spline fitting and interpolation of the dependence $\ln CS(\ln T_1)$, as explained in Section 1.7.2 and Section 9) is caused by resetting the default value of the starting point of the angular spline-fitting interval from 0 to θ_{start} , which is defined as the starting point of the angular interval where the scale factor μ (defined by Eq. (1.5.25)) is approximately angle-independent. Since the value of θ_{start} is always much greater than the most probably angle of photon emission (which corresponds to the maximum of $\sin \theta \cdot DCS(\theta)$), the value of CS is determined by values of $DCS(\theta)$ in the excluded angular interval $[0, \theta_{\text{start}}]$. The mentioned values of $DCS(\theta)$ are calculated by angular cubic-spline fitting and small-angle extrapolation, using `CS_ref_spline` as one of criteria for minimization of the “objective function”, which is defined according to Eq. (1.7.8a). Thus, in the alternative CS-fitting mode, the small-angle part of the angular dependence of the final κ_{\max} -fitted DCS is mainly determined by the value of `CS_ref_spline`, whereas the nonlinear fitting model defined by Eq. (1.5.1) is mainly used for estimation of the large-angle part of $DCS(\theta)$ and for optimization of the boundary conditions at $\theta = \theta_{\text{start}}$ for the mentioned small-angle cubic-spline extrapolation. The mentioned preference of small-angle cubic-spline extrapolation to direct estimation of parameters of Eq. (1.5.1) by nonlinear least squares stems from insufficient accuracy of the latter estimation at large electron energies (of

the order of 10 MeV or greater) and at small angles, in comparison with minimization of the objective function (1.7.8a) during spline fitting, if a sufficiently accurate “reference” value of the CS is available.

The default values of several parameters controlling the mentioned angular cubic-spline fitting are changed for the alternative CS-fitting mode: parameter “splineInt_min_fitted” (No. 3.8.17) is by default equal to 20, parameter “splineExt_fitted” (No. 3.8.7) is by default equal to -1, parameter “mainDevType_fitted” (No. 3.8.48) is by default equal to 4, and parameter “splineRef_fitted0” (No. 3.8.20) is by default equal to 0.

The main criterion for the choice of the alternative CS-fitting mode is a sufficiently large energy of the electron (both incident and outgoing). By default, this mode can be enabled only when $T_1 > 10$ MeV (parameter “T1_CS_mode_thr”), $T_2 > 3$ MeV (parameter “T2_CS_mode_thr”), $T_2 / T_1 > \text{tip_thr}$ (see also the description of parameter No. 9 at the end of Section 2), and the photon energy is non-zero. However, even when all those conditions are satisfied, the “normal” mode may be selected instead. This happens when the following additional conditions are satisfied simultaneously: (a) the relative change of CS due to the κ_{max} -fitting is less than 30 % (parameter “relCorr_CS_mode_thr”), (b) the final relative uncertainty of the CS (after κ_{max} -fitting both the CS and the DCS) is less than 5 % (if $\text{CS_ref_spline} = 0$) or 0.5 % (if $\text{CS_ref_spline} \neq 0$) (parameters “relSD_CS_mode_thr1” and “relSD_CS_mode_thr2”, respectively), (c) $\text{CS_ref_spline} \neq 0$ and the absolute value of the relative deviation of the κ_{max} -fitted value of CS from CS_ref_spline is less than 2 % (parameter “relDiff_CS_mode_thr”). If the “normal” CS-fitting mode is selected, then parameter CS_ref_spline is set equal to zero, and the mentioned change of the default values of several parameters controlling the angular cubic-spline fitting is not applied, with the exception of parameter “splineInt_min_fitted” (No. 3.8.17), which is changed to 20 by default. In order to check if the mentioned additional conditions are satisfied, the “normal” κ_{max} -fitting of $\text{CS}(\kappa_{\text{max}})$ must be performed. Consequently, the alternative CS-fitting mode (with CS_ref_spline obtained by interpolation of $\ln \text{CS}(\ln T_1)$, or specified by the user, or equal to the default value of 0) is by default applied only after the mentioned “normal” κ_{max} -fitting if at least one of the mentioned three additional conditions is not satisfied, or in the case of a failure of the nonlinear fitting of the dependence of the partial-wave CS on κ_{max} , or a failure to join the “original” κ_{max} -fitted DCS with the alternative κ_{max} -fitted DCS (see also Section 1.8 and Section 6.18). It is also possible to apply the alternative mode immediately (without a preceding “normal” run), by setting to zero at least one of the mentioned four additional parameters “relCorr_CS_mode_thr”, “relSD_CS_mode_thr1” (if $\text{CS_ref_spline} = 0$), “relSD_CS_mode_thr2” (if $\text{CS_ref_spline} \neq 0$), or “relDiff_CS_mode_thr” (if $\text{CS_ref_spline} \neq 0$). Conversely, it is possible to apply only the normal CS-fitting mode (with $\text{CS_ref_spline}=0$ and with the mentioned change of the default value of parameter No. 3.8.17 “splineInt_min_fitted”) and quit with an error message if the normal mode fails or is rejected, instead of applying the alternative mode. In order to achieve this, the switch “retry_CS_mode” must be set to 0 (it is equal to 1 by default). This may be desirable in the case of the default options “CS_ref_spline=0” and “CS_int=0”, because the final κ_{max} -fitted CS and DCS obtained in the alternative mode may then deviate from the correct values by more than 50 %.

Below is the list of all parameters that are specific to the alternative CS-fitting mode. Explanations of the role of some parameters, which were provided above, are not repeated in the descriptions of parameters presented below.

3.12.1–2. “T1_CS_mode_thr” (alias “T1_mode_thr”) and “T2_CS_mode_thr” are the threshold values of the initial and final kinetic energies of the electron T_1 and T_2 (in MeV), respectively, which must be exceeded in order to enable the alternative CS-fitting mode described above. The default values of parameters T1_CS_mode_thr and T2_CS_mode_thr are equal to 10 and 3, respectively.

3.12.3. “relCorr_CS_mode_thr” is the threshold value of the relative correction of the partial-wave SDCS due to the κ_{max} -fitting. If the mentioned relative correction is greater than or equal to relCorr_CS_mode_thr, then the alternative CS-fitting mode described above will be

applied. Otherwise, the normal CS-fitting mode may be applied instead (depending on parameters No. 3.12.4–6). The default value of parameter “relCorr_CS_mode_thr” is equal to 0.3.

- 3.12.4–5. “**relSD_CS_mode_thr1**” and “**relSD_CS_mode_thr2**” (alias “relSD_CS_mode_thr” for both) are the threshold values of the final relative uncertainty (standard deviation) of the CS (after κ_{\max} -fitting both the CS and the DCS), to be used when the interpolated or user-specified value of parameter “CS_ref_spline” (No. 3.8.41) is zero or nonzero, respectively. If the mentioned relative uncertainty is greater than or equal to relSD_CS_mode_thr[1,2], then the alternative CS-fitting mode described above will be applied. Otherwise, the normal CS-fitting mode may be applied instead (depending on parameters No. 3.12.3 and No. 3.12.6). The default values of parameters “relSD_CS_mode_thr1” and “relSD_CS_mode_thr2” are equal to 0.05 and 0.005, respectively.
- 3.12.6. “**relDiff_CS_mode_thr**” is the threshold absolute value of the relative deviation of the κ_{\max} -fitted value of CS from the interpolated or user-specified value of parameter “CS_ref_spline” (No. 3.8.41). If CS_ref_spline $\neq 0$ and the absolute value of the mentioned relative deviation is greater than or equal to relCorr_CS_mode_thr, then the alternative CS-fitting mode described above will be applied. Otherwise, the normal CS-fitting mode may be applied instead (depending on parameters No. 3.12.3–5). The default value of parameter “relDiff_CS_mode_thr” is equal to 0.02.
- 3.12.7. “**retry_CS_mode**” is a “switch” (0 or 1), which indicates that the alternative CS-fitting mode must be applied after a failure of the preceding “normal” κ_{\max} -fitting. If this parameter is equal to 0, then the mentioned failure will cause the program to quit with an error message instead of redoing the fitting in the alternative mode. The default value of parameter “retry_CS_mode” is equal to 1.

6.13. Parameters defining the moving average interval of κ_{\max}

- 3.13.1–2. “**avg_period_min_CS**” and “**avg_period_min_DCS**” (aliases “avg_period_min” and “avg_period” for both) are equal to the minimum moving average interval for the nonlinear fitting of the functions CS(κ_{\max}) and DCS(κ_{\max}), respectively (see Section 1.5.3). If the partial-wave interpolation is applied, then the default value of avg_period_min is equal to parameter k2_step_last (i.e., the interval between the last two breakpoints of κ_{\max} if k2_step_last > k2_step_first, or the interval between the first two breakpoints of κ_{\max} if k2_step_last = k2_step_first). If the partial-wave interpolation is not applied, then the default value of avg_period_min_(D)CS is equal to 5 when $\max(\max|\kappa_1|, \max|\kappa_2|) \geq 80$, or to 1 otherwise.
- 3.13.3–4. “**avg_period_max_CS**” and “**avg_period_max_DCS**” (aliases “avg_period_max” and “avg_period” for both) are equal to the maximum moving average interval for the nonlinear fitting of the functions CS(κ_{\max}) and DCS(κ_{\max}), respectively (see Section 1.5.3). Parameter “avg_period_max_(D)CS” is one of two alternative parameters used to specify the maximum moving average interval. Another one is parameter No. 3.13.5 “avg_period_max_ratio”. The final value of the maximum moving average interval is equal to the smaller of the two values corresponding to each of the two parameters. The default value of parameter “avg_period_max_(D)CS” is very large (1000). Consequently, the maximum moving average interval is determined using only the value of parameter “avg_period_max_ratio” by default. **Note:** If the angular spline fitting of the PW DCS is performed (see Section 1.7.1), then only one value of the moving average interval is used (this value is defined by the corresponding parameter “avg_period_min_(D)CS”). Otherwise, if a fitting error occurs, the moving average interval is increased by 1 and the fitting is redone. This process is repeated until the fitting error does not occur or the maximum value of the moving average interval is reached.

3.13.5. “**avg_period_max_ratio**” is used for an alternative estimation of the maximum moving average interval. It is equal to the ratio of the required maximum moving average interval and N_{fit} (the meaning of N_{fit} is explained in Section 1.5.1). The actual value of the maximum moving average interval is equal to the smaller of two values: `avg_period_max_(D)CS` (described above) and `avg_period_max_ratio*Nfit`. In the case “`avg_period_max_ratio=0`”, no averaging will be applied. The default (and maximum allowed) value of this parameter is 0.25.

6.14. Parameters defining the error thresholds

3.14.1. “**maxRelErr**” is the maximum acceptable relative error of the single- and double differential cross sections calculated by Bremsstrahlung due to uncertainties of the S integrals. If this parameter is positive, then the “original” and “test” cross sections (in the files whose names end with “_test”) calculated by Bremsstrahlung will be compared, and the maximum value of κ_{max} will be reduced if their relative differences are greater than `maxRelErr`. The default value of this parameter is 0.05.

3.14.2. “**maxRelErr2**” is the maximum acceptable relative error of the single- and double differential cross sections calculated by Bremsstrahlung due to truncation of the sum (1.1.10) with respect to l . If this parameter is positive, then the “original” and “test” cross sections (in the files whose names end with “_test2”) calculated by Bremsstrahlung will be compared, and the maximum value of κ_{max} will be reduced if their relative differences are greater than `maxRelErr2`. The default value of this parameter is 0.001.

3.14.3. “**nErrMax**” is the maximum allowed number of consecutive irrecoverable error points in the angular dependence of the κ_{max} -fitted DCS. If the κ_{max} -fitting fails at a given value of θ and the number of consecutive irrecoverable errors (`nErr`) is less than `nErrMax`, then the κ_{max} -fitted DCS at the current value of θ will be replaced by a value calculated without the κ_{max} -fitting. The replacement value depends on the value of parameter No. 3.2.13 (“`fitMode`”). If `fitMode = 1`, then the replacement value is equal to the original (unfitted) DCS. If `fitMode = 2`, then the replacement value is calculated by log-linear interpolation between the two values of the fitted DCS corresponding to the two closest “bracketing” values of θ where the fitting has been successful. If `nErrMax = 0`, then the fitting procedure will be terminated after the first irrecoverable error. The default value of this parameter is 6 when $T_1 \leq 3$ MeV, and 12 otherwise. *Note*: The limitation on the number of consecutive errors is not applied inside the angular interval $\theta \geq (180^\circ + |\text{spline_theta_max_thr}|) / 2$ (see also the description of parameter No. 3.7.8).

3.14.4. “**max_min_ratio_thr**” is the maximum allowed ratio of the maximum and minimum values of the DCS in the entire angular interval $0^\circ \leq \theta \leq 180^\circ$ when the angular dependence of the DCS is allowed to have a minimum. I.e., if the value of the mentioned ratio is less than or equal to `max_min_ratio_thr`, then the DCS is allowed to have a minimum, and if the mentioned ratio is greater than `max_min_ratio_thr`, then the DCS is not allowed to have a minimum. This parameter is used in order to determine if the approximate angular dependence of the DCS obtained by cubic spline fitting and extrapolation is acceptable, or if it must be rejected (because of existence of additional extrema or inflection points). The default value of this parameter is equal to 10.

6.15. Parameters defining the names of input and output files, and the conditions for overwriting

3.15.1–2. “**prefix_fit_CS**” and “**prefix_fit_DCS**” (alias “`prefix_fit`” for both) are the names of the folders with the CS and DCS data files created by Bremsstrahlung. `Brems_fit` reads the (D)CS data from six files created by Bremsstrahlung: three files whose names start with “_CS_” and three files whose names start with “DCS_” (see the description of the files of the first group in Section 5.8). The program searches for the three “_CS_” files and three “DCS_” files in the folders specified by parameters “`prefix_fit_CS`” and “`prefix_fit_DCS`”,

respectively. The folder name must end with the slash '/'. If parameter “prefix_fit_(D)CS” is the empty string (specified by writing a space after “prefix_fit_(D)CS=”), then the mentioned three files must be in the current folder. This parameter is used only when firstStage = 3 and parameter No. 1.9.1 “prefix” (see Section 4.9) is not ‘.’. In other cases, or if this parameter is not specified, Brems_fit will search for the cross section data files in the current folder. The default value of parameters “prefix_fit_CS” and “prefix_fit_DCS” is the empty string.

- 3.15.3. “**suffix3**” (alias “suffix_3”) is the suffix that is appended to the names of files “DCS_fitted_...”, “ShapeFn_fitted_...”, “DCS_parms_...”, “DCS_interm0_...”, “DCS_interm1_...”, and “DCS_mu_...” (the contents of these files are described in Section 6.20). The default value of this parameter is the empty string.
- 3.15.4. “**iFit**” is a “switch” (1 or 0) indicating whether the existing data files with the fitted DCS and shape function data must be overwritten. This parameter is ignored if fitMode = 0 (see the description of parameter No. 3.2.13). If iFit = 0 and processing of the DCS is requested (fitMode ≠ 0), then Brems_fit will process the DCS data only if there is no file with the fitted DCS data (otherwise no files will be updated, and the program will quit with a corresponding message). If iFit = 1, the DCS data will be always processed, and the existing files with the fitted DCS and shape function data will be overwritten. The default value of this parameter is 1.
- 3.15.5–6. “**suffix_spline**” and “**suffix_extrap**” define the suffix to be used in the case “extrap_files=1” (see the description of parameter No. 3.10.2) when forming the name of the file with the values of the spline-fitted and extrapolated PW DCS for all angles and all values of κ_{\max} (this file belongs to the fourth group of output files described in Section 6.20). The suffix specified by parameter “suffix_spline” is used when the angular extrapolation is not performed, and the PW DCS is only spline-fitted in the entire angular range ($\theta_{\min} = 0^\circ$ and $\theta_{\max} = 180^\circ$, using the notations of Section 1.7.1). The suffix specified by parameter “suffix_extrap” is used when the angular extrapolation of the PW DCS outside of the spline-fitting range is performed ($\theta_{\min} > 0^\circ$, or $\theta_{\max} < 180^\circ$). In any case, the suffix is inserted before the extension “.txt”. The default values of parameters “suffix_spline” and “suffix_extrap” are “_spline” and “_spline_extrap”, respectively.
- 3.15.7. “**suffix_MA**” defines the suffix to be used in the case “MA_file=1” (see the description of parameter No. 3.10.6) when forming the name of the file with the values of the moving average of the original PW DCS. The default value of this parameter is “_MA”.
- 3.15.8. “**suffix3a**” (alias “suffix_3”) defines the additional suffix to be appended to the names of the “_spline” and “spline_extrap” files, and the moving-average file (after the suffix defined by parameters No. 3.15.5–7). The default value of this parameter is the empty string.

6.16. Parameters controlling calculation of the uncertainty of DCS

As mentioned in Section 1.3.2, the sum in Eq. (1.1.10) may be truncated, which means that the maximum value of l (denoted l_{\max}) in this sum may be less than the theoretical maximum of l (which is equal to $\max|\kappa_1| + \max|\kappa_2|$). In BREMS, the effect of this truncation is evaluated by calculating two sets of PW cross sections: the set corresponding to the original value of parameter No. 1.3.12 “lmax” (which may be either the default one or specified by the user), and the set corresponding to the reduced value of lmax, with the size of this reduction specified using parameter No. 2.2.19 “lmax_decr”. In stage 2, the latter set of cross sections is written to the files whose name includes the additional suffix “_test2” (see also Section 5.8). In stage 3, the relative change of the PW DCS caused by this reduction at the maximum value of κ_{\max} in the analyzed data may be used as a component of the overall relative uncertainty of the final κ_{\max} -fitted DCS (this component is added in quadrature to the other components, yielding the overall relative uncertainty). However, such estimate of the mentioned uncertainty would be very unreliable,

because it reflects only the difference between the cross sections corresponding to two arbitrary values of l_{\max} , both of which are less than the theoretical maximum of l . It is desirable to have at least a rough estimate of the relative change of the DCS caused by the reduction of l_{\max} from $\max|\kappa_1| + \max|\kappa_2|$ to the value of l_{\max} used in stage 2. In BREMS, a conservative estimate of the mentioned relative change of the PW DCS is obtained by multiplying the previously-mentioned estimate by the correction factor equal to

$$\max(1, 0.5 \times (\max|\kappa_1| + \max|\kappa_2| - l_{\max}) / |\Delta l_{\max}|), \quad (6.16.1a)$$

where Δl_{\max} is the reduction of l_{\max} used for calculating the mentioned “test” set of cross sections, and l_{\max} is the value used for calculating the “original” set of cross sections. Although this estimate of the relative uncertainty caused by the reduced value of l_{\max} (in comparison with the theoretical maximum $\max|\kappa_1| + \max|\kappa_2|$) is calculated using the PW DCS (i.e., before the extrapolation to $\kappa_{\max} \rightarrow \infty$), it is “carried over” to the final κ_{\max} -fitted DCS.

A more reliable estimate (which is more applicable to the final κ_{\max} -fitted (D)CS) is obtained by redoing stage 3 with the “test” cross sections (stored in the “..._test2.txt” files) as the input data, and then calculating the difference between the values of the κ_{\max} -fitted (D)CS corresponding to the “test” cross sections and the original cross sections. After that, this difference is multiplied by the same correction factor (6.16.1a) and added in quadrature to the other terms (including the previously mentioned term reflecting the relative change of the PW DCS).

A similar approach is applied in order to take into account the effect of the uncertainties of S integrals (see also Section 1.4). The relative deviation of the PW DCS stored in the “..._test.txt” files (which were obtained using the “test” set of S integrals) from the original PW DCS is added in quadrature to the other mentioned terms. In addition, stage 3 is redone using the mentioned set of “test” PW cross sections as the input data, and then the relative change of the κ_{\max} -fitted (D)CS caused by using this set of cross sections is added in quadrature to the other mentioned terms. In this case, no additional correction factor is needed.

Normally, the values of $\max|\kappa_1| + \max|\kappa_2|$, l_{\max} and Δl_{\max} in expression (6.16.1a) should be the same as those used in stage 2. However, if the input data files for stage 3 were created by a version of BREMS older than v1.5.6.7, then those files do not contain the mentioned values. Consequently, there are three parameters that are used to specify the mentioned three values. The names of those three parameters are “Kmax12”, “lmax3” and “lmax_decr3”, respectively. By replacing the notations “ $\max|\kappa_1| + \max|\kappa_2|$ ”, “ l_{\max} ” and “ Δl_{\max} ” with the names of the corresponding parameters, the expression of the correction factor (6.16.1a) may be written as follows:

$$\max(1, 0.5 \times (\text{Kmax12} - \text{lmax3}) / |\text{lmax_decr3}|). \quad (6.16.1b)$$

The values of parameters “Kmax12”, “lmax3” and “lmax_decr3” may be either specified explicitly, or set to the values of parameters Kmax1 + Kmax2 (No. 1.3.2 and No. 1.3.5), lmax2 (No. 2.2.13) and lmax_decr (No. 2.2.19), respectively, or read from the file “CS.txt” or (starting with BREMS v1.5.6.7) from the file “DCS_..._test2.txt” created in stage 2 (the formats of the latter files are described in Section 5.8). **Note:** In the case “firstStage=3”, reading those values from files is more reliable, because the values of Kmax1, Kmax2, lmax and lmax_decr may have been reduced in stages 1 and 2, and this reduction may be unknown if firstStage=3.

3.16.1. “fit_test” is a “switch” (1 or 0) indicating if stage 3 must be redone using the two “test” sets of PW cross sections (stored in files “..._test.txt” and “..._test2.txt”, whose format is described in Section 5.8). If this parameter is non-zero, then the relative deviations of the corresponding κ_{\max} -fitted (D)CS from the original κ_{\max} -fitted (D)CS will be added in quadrature to the other terms composing the total uncertainty of the κ_{\max} -fitted (D)CS. If this parameter is equal to 0, then the mentioned two additional terms will not be included (only the terms reflecting the relative change of the PW DCS will be included, as explained at the beginning of this section). In the case “fit_test=1”, the duration of stage 3 is longer by a factor of approximately 3 than in the case “fit_test=0”. The default value of parameter “fit_test” is equal to 1.

- 3.16.2. “**lmax3**” is the value of the variable lmax3 to be used for calculation of the correction factor (6.16.1b). If lmax3=-1, then Kmax12 and lmax3 are set equal to the default or user-specified values of parameters Kmax1+Kmax2 (No. 1.3.2 and No. 1.3.5) and lmax2 (No. 2.2.13), respectively (if firstStage < 3, then the additional reduction of Kmax1, Kmax2 and lmax2, which is possible in stages 1 and 2, is also taken into account automatically when lmax3 = -1). If lmax3=0, then the correction factor is not applied (i.e., the correction factor is equal to 1). The default value of parameter “lmax3” is equal to -1.
- 3.16.3. “**lmax_decr3**” is the value of the variable lmax_decr3 to be used for calculation of the correction factor (6.16.1b). If lmax_decr3=1, then lmax_decr3 is set equal to the default or user-specified value of parameter No. 2.2.19 “lmax_decr” (if firstStage < 3, then the additional reduction of lmax_decr, which is possible in stage 2, is also taken into account automatically when lmax_decr3 = 1). If lmax_decr3=0, then the correction factor is not applied (i.e., the correction factor is equal to 1). The default value of parameter “lmax_decr3” is equal to 1.
- 3.16.4. “**Kmax12**” is the value of the variable Kmax12 to be used for calculation of the correction factor (6.16.1b). This parameter is used only when parameter “lmax3” is positive and parameter “lmax_decr3” is non-zero (see the descriptions of parameters No. 3.16.2 and No. 3.16.3). The default value of parameter Kmax12 is equal to 0.
- 3.16.5. “**fn_lmax3**” is the name of the file where the values of the variables lmax3, lmax_decr3 and Kmax12 in Eq. (6.16.1b) are stored. This file must have the same format as the file “CS.txt” created in stage 2 (the format of this file is described in Section 5.8). If parameter “fn_lmax3” is not the empty string or the period “.”, then the mentioned parameters “lmax3” (No. 3.16.2) and “lmax_decr3” (No. 3.16.3) will be ignored and the program will attempt to open the specified file and find the last line corresponding to the specified values of Z , T_1 and k in it. The lines with nCyc=1 (in column No. 7) are ignored. If the required line is found, then the values of Kmax1, Kmax2, lmax3 and lmax_decr3 will be read from columns with headers “kmax1”, “kmax2”, “lmax2”, and “test”, respectively (more precisely, the value of lmax_decr3 is equal to the difference of the latter two values). If the required line is not found or a read error occurs, then the program will quit with an error message. This will also happen if parameter No. 3.19.3 (“checkTabPos”) is equal to 1 and the program determines that tab positions are different in different lines of the file. If fn_lmax3 is equal to the period “.”, then the same four values will be read from the first four lines of the file “DCS_..._test2.txt” created in stage 2, unless the mentioned file was created by a version of BREMS older than 1.5.6.7 (without the additional four lines at the beginning), in which case the default or user-specified values of parameters No. 3.16.2–4 (“lmax3”, “lmax_decr3” and “Kmax12”) will be used. The default value of parameter “fn_lmax3” is the period “.”.
- 3.16.6. “**folder_CS**” indicates the folder where the file defined by parameter “fn_lmax3” is located. If parameter “folder_CS” is equal to the period “.” (the default value), then the folder name will be obtained by removing the part of parameter “prefix_fit_CS” (No. 3.15.1) following the last slash, and if the string defined by the latter parameter does not contain a slash, then parameter “folder_CS” will be set to the empty string (i.e., the current folder).
- 3.16.7–8. “**theorSD_CS**” and “**theorSD_DCS**” (alias “theorSD” for both) is a “switch” (1 or 0) indicating if the value of the “theoretical” uncertainty (i.e., the estimate of the uncertainty of parameter c in Eq. (1.5.1) or Eq. (1.5.10), calculated according to Eq. (1.6.2b)) must be taken into account when calculating the final estimate of the uncertainty (or “standard deviation”, indicated by the subscript “SD” in the headers of the corresponding columns of the output files) of the κ_{\max} -fitted (and optionally spline-fitted) CS or DCS, respectively. In the case “theorSD_(D)CS=1”, the mentioned theoretical uncertainty will be added in quadrature to the “empirical” standard deviation calculated over multiple fitting intervals (see also Section 1.6). In the case “theorSD_(D)CS=0”, the final estimate of the uncertainty will be purely empirical (see the descriptions of parameters No. 3.17.3–11), i.e., it will

reflect only the magnitude of variation of (D)CS among the different fitting intervals (for example, in the case of a single fitting interval it will be equal to zero). Specifically, if `wt_avg_DCS=1` (see the description of parameters No. 3.17.3–4), the final estimate of the uncertainty of the DCS will be calculated as the square root of the ratio of the sum of squared deviations from the arithmetic average, and the number of included “shifts” reduced by 1 (i.e., the number of degrees of freedom, which is equal to the number of observations minus 1). In such a case, it is possible to obtain the estimate of the uncertainty of the mentioned average value: one has to divide the estimate of the SD contained in the output file by the square root of the number of included shifts (which is also output) and to multiply by the critical value of the t statistic corresponding to the current number of degrees of freedom (such calculation is based on the assumption that the errors are distributed normally and that their statistical average is equal to zero). The default value of parameters “`theorSD_CS`” and “`theorSD_DCS`” is 1.

Note: If the angular spline fitting and extrapolation of the κ_{\max} -fitted DCS is performed, then the theoretical uncertainties for individual shifts, calculated using the results of the linear regression (least squares optimization of the spline values at a fixed set of knots) as described in Section 1.7.1, replace the theoretical uncertainties calculated during the preceding nonlinear κ_{\max} -fitting as described in Section 1.6.

3.16.9. “`err_corr_ratio`” is the fraction of the absolute correction of the partial-wave (D)CS due to κ_{\max} -fitting by Eq. (1.5.1) or Eq. (1.5.10) that must be added in quadrature to the initial estimate of the uncertainty (standard error) of the (D)CS. The default value of this parameter is equal to 0.1 (i.e., if the (D)CS is calculated by least squares fitting by Eq. (1.5.1) or Eq. (1.5.10), then the standard error of the (D)CS is by default calculated according to Eq. (1.6.2b)).

6.17. Parameters defining weight factors for averaging κ_{\max} -fitting results over different intervals

3.17.1–2. “`wt_Nfit_CS`” and “`wt_Nfit_DCS`” (alias “`wt_Nfit`” for both) specify the weighting method when averaging the fitting results over the two alternative widths of the κ_{\max} -fitting interval in the case “`fitRange_(D)CS=3`” (see the description of parameters No. 3.2.3–4). `wt_Nfit_(D)CS=1` indicates that equal weights must be assigned to both fitting intervals. `wt_Nfit_(D)CS=2` indicates weighting by inverse squared uncertainties. The default value of parameters “`wt_Nfit_CS`” and “`wt_Nfit_DCS`” is 1.

3.17.3–4. “`wt_avg_CS`” and “`wt_avg_DCS`” (alias “`wt_avg`” for both) is the number “1” or “2” indicating the weighting method when calculating the average and standard deviation of the κ_{\max} -fitted CS, and the κ_{\max} -fitted, spline-fitted and extrapolated DCS, respectively, over multiple “shifts”. “`wt_avg_(D)CS=1`” indicates no weighting, and “`wt_avg_(D)CS=2`” indicates weighting by inverse squared uncertainties (corresponding to either the original κ_{\max} -fitted DCS or the κ_{\max} -fitted and spline-fitted DCS, depending on the sign of parameter “`splineFit_wt`”). The default value of parameter “`wt_avg_CS`” is 1. The default value of `wt_avg_DCS` is also 1, except when $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$, in which case `wt_avg_DCS` is equal to 2 by default.

3.17.5. “`splineFit_wt`” is the number ± 1 or ± 2 , which indicates the weighting method applied during the angular spline fitting of the κ_{\max} -fitted DCS, and modifies the calculation of the weight factors during the averaging of the κ_{\max} -fitted and spline-fitted DCS over multiple shifts (when `wt_avg_DCS=2`). $|\text{splineFit_wt}|=1$ means no weighting during the linear regression when calculating the optimal values of the spline corresponding to a given set of spline knots (see also Section 1.7.1), and $|\text{splineFit_wt}|=2$ means weighting by the inverse relative uncertainties squared. The sign of this parameter indicates the weighting method used for averaging the κ_{\max} -fitted DCS and its uncertainties over multiple shifts during the optimization of the other adjustable parameters related to the spline fitting (the knot spacing

and the choice of the reference function, spline argument and the logarithm option): splineFit_wt>0 means no weighting, splineFit_wt<0 means weighting by the average value of the squared inverse relative uncertainty of the original κ_{\max} -fitted DCS (prior to the angular spline fitting). In the case splineFit_wt<0, the mentioned relative uncertainty of the κ_{\max} -fitted DCS has the same value for all values of θ , and it is calculated by integration of the uncertainties over the entire angular interval $0^\circ \leq \theta \leq 180^\circ$ with respect to the solid angle of photon emission. When splineFit_wt<0 and wt_avg_DCS=2, the same weights are also used for averaging the κ_{\max} -fitted and spline-fitted DCS over multiple shifts (conversely, when splineFit_wt>0 and wt_avg_DCS=2, the weights are calculated using the uncertainties of the spline-fitted DCS returned by the subroutine performing the mentioned linear regression). The default value of parameter “splineFit_wt” is -1, except when $T_1 > 3$ MeV and $T_2 / T_1 \leq 10^{-4}$, in which case splineFit_wt is equal to -2 by default.

The next six parameters define the rules of shift selection for the averaging of the κ_{\max} -fitted (D)CS over multiple shifts (both during the angular spline fitting and during the subsequent averaging of the spline-fitted DCS), and modify some of the weighting factors. The minimum number of included observations (shifts) of (D)CS is $nmin = \max(\mathbf{nAvg_D}CS, \mathbf{fractAvg_D}CS * ntot)$, where ntot is the total number of observations (shifts). This “minimum” set consists of nmin shifts with the smallest absolute values of the uncertainty, or “standard deviation” (SD), plus all shifts corresponding to relative range of variation less than 0.1% inside the κ_{\max} -fitting interval. All remaining shifts are excluded, unless the corresponding absolute SD exceeds the maximum absolute SD of the minimum set by a factor less than **SDratio_D**CS. In the case wt_avg_(D)CS=2, all included shifts that do not belong to the minimum set are assigned a weight equal to the inverse squared SD of the corresponding shift, whereas the weight of all shifts in the minimum set is equal to the inverse squared maximum SD among the mentioned nmin shifts (this is needed in order to avoid unrealistically small uncertainties, which could otherwise appear if one shift was accidentally assigned a very small SD). In the case wt_avg_(D)CS=1, all included shifts have equal weights.

3.17.6–7. “**nAvg_CS**” or “**nAvg_DCS**” (alias “nAvg” for both) is the first one of the two parameters defining the minimum number of “shifts” in the “minimum” set corresponding to the κ_{\max} -fitted CS or the κ_{\max} -fitted DCS, respectively (see the previous paragraph). The default value of parameters “nAvg_CS” and “nAvg_DCS” is 5.

3.17.8–9. “**fractAvg_CS**” or “**fractAvg_DCS**” (alias “fractAvg” for both) is the second one of the two parameters defining the minimum number of “shifts” in the “minimum” set corresponding to the κ_{\max} -fitted CS or the κ_{\max} -fitted DCS, respectively (see above). The default values of parameters “fractAvg_CS” and “fractAvg_DCS” are 0.25 and 0.5, respectively.

3.17.10–11. “**SDratio_CS**” and “**SDratio_DCS**” (alias “SDratio” for both) is the maximum allowed ratio of the uncertainty of a κ_{\max} -fitted value of the CS or DCS (respectively) corresponding to the given shift and the maximum uncertainty of the “minimum” set (see above). If the mentioned ratio is greater than the value of “SDratio_(D)CS”, then the corresponding shift will not be included in the average. The default value of parameters “SDratio_CS” and “SDratio_DCS” is 3.

6.18. Parameters controlling usage of the alternative κ_{\max} -fitted DCS

As mentioned in Section 1.8 and in Section 2, under conditions specified in the description of parameter No. 13 (“S_data”) of the main program, subroutine Brems_fit is called twice: first for processing the alternative set of partial-wave (PW) data, and then for processing the original dataset. This yields two angular dependences of the κ_{\max} -fitted DCS, which are then joined smoothly in the angular range where their difference is smallest. As mentioned in Section 2, the values of the alternative κ_{\max} -fitted DCS are used to modify some aspects of the calculation of the original κ_{\max} -fitted DCS. In particular, if the “ μ -correction” described in Section 1.5.4 is applied

during calculation of the original κ_{\max} -fitted DCS, then the scale factor μ is calculated as the median value of expression (1.5.25), where “DCS($\kappa_{\max} \rightarrow \infty, \theta$)” is the κ_{\max} -fitted DCS obtained from analysis of the alternative PW DCS, over the angular interval where the absolute value of the relative correction of the alternative PW DCS is less than 2 % (to ensure maximum accuracy of DCS($\kappa_{\max} \rightarrow \infty, \theta$)), whereas the absolute value of the relative correction of the original PW DCS is greater than 10 % (accuracy of the estimate of μ (1.5.25) improves with increasing relative difference of the two terms that are subtracted from each other in the numerator and denominator, i.e., with increasing relative correction).

The alternative κ_{\max} -fitted DCS is calculated when parameter No. 13 (“S_data”) of the main program is equal to 2 or 3 (in the former case, only the alternative κ_{\max} -fitted DCS is calculated, and in the latter case it is calculated together with the original κ_{\max} -fitted DCS). The alternative κ_{\max} -fitted DCS is by default calculated in the angular range $30^\circ \leq \theta \leq 180^\circ$, because at small angles the alternative κ_{\max} -fitted DCS is less accurate than the original κ_{\max} -fitted DCS (see Fig. 10b in Section 1.8). Many parameters controlling κ_{\max} -fitting of the alternative DCS are fixed and cannot be modified by the user. For example, the alternative DCS is always fitted by a superposition of a simple exponential and a constant, i.e., Eq. (1.5.1) is used with $d = 1$ and $h = 0$ (this is achieved by setting `simple_exp_DCS=3`, `d_exp_DCS1=1`, `d_exp_DCS2=1`, `simple_exp_thr_DCS1=10100`, and `simple_exp_thr_DCS2=10100`), the nonlinear fitting of the dependence of the alternative CS on κ_{\max} is skipped (`T1_CS_mode_thr=0`), but the corresponding changes of default values of several parameters controlling the angular spline fitting are not applied (see Section 6.12), the μ -correction of the alternative DCS is disabled, angular spline fitting of the alternative PW DCS is not performed, parameters “`tol_range_max`” and “`tol_range_max2`” (3.4.7–8) are both equal to 0.002, parameters “`splineFit_wt`” (No. 3.17.5), “`wt_avg_DCS`” (No. 3.17.4) and “`spline_combine`” (No. 3.8.30) are equal to -2, 2 and 2, respectively, parameter “`fitRef_extrap`” is equal to 0, etc. If the option “S_data=2” is used and the user attempts to modify any of the mentioned parameters, then a warning message will be displayed, but the calculation process will not be affected. If the option “S_data=3” is used, then changes of the mentioned parameters will affect only calculation of the original κ_{\max} -fitted DCS, but not calculation of the alternative κ_{\max} -fitted DCS. Some parameters of stage 3 are “shared” between the original and alternative DCS, i.e., their changes affect calculation of both κ_{\max} -fitted DCS.

After calculating both the original and the alternative κ_{\max} -fitted DCS, the large-angle part of the original κ_{\max} -fitted DCS is replaced by the alternative κ_{\max} -fitted DCS. Inside the entire large-angle angular range (up to 180°) where the mentioned replacement is applied, the absolute value of the relative correction of the DCS corresponding to the alternative dataset must not exceed the absolute value of the relative correction corresponding to the original dataset by a factor greater than the value of parameter “**thr_corrRatio+**” (10 by default), or at least one of the two mentioned relative corrections must be less than 0.01 in absolute value. In addition, all points that are in the first 3° (specified by parameter “**theta_width_min+**”) of this angular range must satisfy the following three requirements: (a) the relative difference of the two κ_{\max} -fitted DCS must be less than 3 % in absolute value (parameter “**thr_diff+**”), (b) the absolute values of the relative corrections of the PW DCS corresponding to the original and alternative datasets must be less than 99 % (“**thr_corr1+**”) and 3 % (“**thr_corr2+**”), respectively, (c) the relative uncertainty (standard deviation) of the alternative κ_{\max} -fitted DCS must be less than 3 % in absolute value (“**thr_reISD+**”). If no such interval is found, or if its width is less than the value of parameter “**theta_width_min+**”, then the program will quit with an error message. If such an interval is found, then the values of the original κ_{\max} -fitted DCS are replaced by a weighed average of the original and alternative κ_{\max} -fitted DCS inside the “transition interval” corresponding to the consecutive points satisfying the mentioned three constraints. At greater angles, the original κ_{\max} -fitted DCS is replaced by the alternative κ_{\max} -fitted DCS. The value of the weigh factor of the mentioned weighted average is a linear function of θ , and it is defined so as to smooth out the small discontinuity, which would otherwise exist at the end of the mentioned transition interval after the

mentioned replacement. I.e., the final κ_{\max} -fitted DCS changes smoothly from the original κ_{\max} -fitted DCS (at the point that immediately precedes the transition interval) to the alternative κ_{\max} -fitted DCS (at the endpoint of the transition interval). The maximum allowed width of the transition interval is 30° (parameter “**theta_width_max+**”). If the width of the interval satisfying the mentioned three constraints is greater than the value of parameter “**theta_width_max+**”, then a subinterval with width equal to **theta_width_max+** will be selected on the basis of the requirement of the smallest value of the ratio of the maximum relative difference between the two κ_{\max} -fitted DCS to the ratio of the maximum and minimum values of the original κ_{\max} -fitted DCS inside the mentioned subinterval. The same criterion is used for selecting an interval among several non-overlapping intervals satisfying the same constraints. The uncertainty of the final κ_{\max} -fitted DCS inside the transition interval is calculated by adding up the weighed uncertainties of the original and alternative DCS in quadrature, with the same weight factors that are used to calculate the final κ_{\max} -fitted DCS, and the weighted absolute deviations of the same two κ_{\max} -fitted DCS from the final κ_{\max} -fitted DCS.

Below is the list of all parameters that are specific to calculation of the alternative κ_{\max} -fitted DCS in stage 3, or to the method of joining the small-angle part of the original κ_{\max} -fitted DCS with the large-angle part of the alternative κ_{\max} -fitted DCS. Explanations of the role of some parameters, which were provided above, are not repeated in the descriptions of parameters presented below.

- 3.18.1. “**theta_min+**” is the starting angle (in degrees) of the angular interval where the alternative κ_{\max} -fitted DCS is defined. The default value of this parameter is equal to 30.
- 3.18.2. “**thr_corrRatio+**” is the maximum allowed value of the ratio of the absolute values of relative corrections of the alternative PW DCS and the original PW DCS in the large-angle replacement interval. The default value of this parameter is equal to 1 (that is to say, the relative correction of the alternative PW DCS must be less than the relative correction of the original PW DCS).
- 3.18.3. “**thr_diff+**” is the maximum allowed absolute value of the relative deviation of the alternative κ_{\max} -fitted DCS from the original κ_{\max} -fitted DCS inside the transition interval. The default value of this parameter is equal to 0.03.
- 3.18.4. “**thr_relSD+**” is the maximum relative uncertainty of the alternative κ_{\max} -fitted DCS inside the transition interval. The default value of this parameter is equal to 0.03.
- 3.18.5–6. “**thr_corr1+**” and “**thr_corr2+**” (alias “**thr_corr+**” for both) are the maximum allowed absolute values of the relative correction of the original PW DCS and the alternative PW DCS inside the transition interval. Parameter “**thr_corr2+**” is also used as the maximum allowed absolute value of the relative correction of the alternative PW DCS in the angular interval where the median value of the scale factor μ is calculated during the μ -correction of the original DCS (see the beginning of the current section). The default values of parameters “**thr_corr1+**” and “**thr_corr2+**” are equal to 0.99 and 0.03, respectively.
- 3.18.7. “**theta_width_min+**” is the minimum allowed width of the transition interval (in degrees). The default value of this parameter is equal to 3.
- 3.18.8. “**theta_width_max+**” is the maximum allowed width of the transition interval (in degrees). The default value of this parameter is equal to 30.
- 3.18.9. “**extrap_offset+**” is the offset (in degrees), which must be subtracted from the endpoint of the angular range (i.e., from $\max(\text{theta_max1}, \text{theta_max2})$) in order to obtain the smallest value of the endpoint of the spline-fitting interval (i.e., parameter No. 3.8.4 “**spline_theta_max_fitted1**”) for spline fitting of the angular dependence of the alternative κ_{\max} -fitted DCS (the largest value of the mentioned endpoint is always equal to $\max(\text{theta_max1}, \text{theta_max2})$). The default value of parameter “**extrap_offset+**” is equal to 20 (i.e., the default value of parameter “**spline_theta_max_fitted1**” for spline fitting of the angular dependence of the alternative κ_{\max} -fitted DCS is equal to $180^\circ - 20^\circ = 160^\circ$).

3.18.10. “**n_extrap+**” is the number of equidistant values of the endpoint of the spline-fitting interval to be tested during spline fitting of the angular dependence of the alternative κ_{\max} -fitted DCS. That is to say, parameter “n_extrap+” is the counterpart of parameter No. 3.8.6 (“n_spline_theta_max_fitted”). The default value of parameter “n_extrap+” is equal to 5 (i.e., the default set of endpoints is 160°, 165°, 170°, 175°, and 180°).

6.19. Other parameters

3.19.1. “**del_CS**” is a “switch” (0, 1, or 2) indicating if the cross section data files created in stage 2 (by the subroutine *Bremsstrahlung*), excluding the files “CS.txt” and “CS_2.txt” that were updated by appending a single line, must be deleted after a successful completion of stage 3. If del_CS=2, then only the files “CS.txt” and “CS_2.txt” will be retained. If del_CS=1, then the two files whose names start with “_CS_” or “DCS_” and do not include the suffix “_test” or “_test2” will also be retained. If del_CS=0, then none of the files created in stage 2 will be deleted. The value “1” or “2” of this parameter (indicating deletion of the cross section data files) will have an effect only if firstStage < 3. The default value of this parameter is equal to 1 (meaning that only four output files of stage 2 are not deleted by default: “CS.txt”, “CS_2.txt”, “_CS_....txt”, and “DCS_....txt”).

3.19.2. “**verbosity**” is a “switch” (1 or 0) controlling output of messages about irrecoverable κ_{\max} -fitting errors in stage 3. Allowed values: 0 – no messages about irrecoverable κ_{\max} -fitting errors, except after exceeding the maximum allowed number of such errors, 1 – only messages about irrecoverable κ_{\max} -fitting errors that occur at $\theta < 0.5 * (180^\circ + |\text{spline_theta_max_thr}|)$, 2 – messages about all irrecoverable κ_{\max} -fitting errors. The default value of this parameter is equal to 0.

3.19.3. “**checkTabPos**” is a “switch” (1 or 0) indicating if the format of file “CS_fitted.txt”, which belongs to the first group of files described in Section 6.20, must be checked for consistency. If this parameter is equal to 1, then the program will compare tab positions and length of the first and last lines of the file (this check is performed after appending the line with the results of the current run). If a discrepancy is found, then a warning will be displayed (however, execution of the program will not be stopped). If this parameter is equal to 0, then the mentioned check will not be performed. The default value of this parameter is equal to 1.

Note: Parameter “checkTabPos” is also used in stage 2 by subroutine “*Bremsstrahlung*”, for checking the files “CS.txt” and “CS_2.txt”, and by subroutine “*Born_SM_appr*” (for checking the file “CS_Born_SM.txt”). In the case “checkTabPos=1”, a similar check of input files is also performed when generating the grid data for the cubic-spline fitting and interpolation of the logarithm of the scaled SDCS with respect to the logarithm of the incident electron energy (see Section 9). However, in the latter case, *all* lines are checked, and a change of tab positions is treated as a terminal error (i.e., the program then exits with an error message).

6.20. Output data of stage 3 (subroutine “*Brems_fit*”)

Brems_fit creates or updates up to 14 ASCII (human-readable) files. Each file starts with a header line, which is followed by multiple columns of numbers of fixed width. It is convenient to define five groups of the output files of “*Brems_fit*” according to their purpose and format:

- I. Three files with the values of the CS and the DCS extrapolated to $\kappa_{\max} \rightarrow \infty$ (i.e., the values of the parameter c in Eq. (1.5.1) or Eq. (1.5.10) returned by the fitting procedure), and the corresponding values of the shape function (defined as the ratio DCS/CS). The name of the file with the fitted CS data is “CS_fitted.txt”. The names of the other two files start with the string “DCS_fitted_” and “ShapeFn_fitted_”, respectively, followed by the name of the input file with the cross section data. If the file “CS_fitted.txt” already exists, then a line will be

appended to it. The other two files are overwritten after each fitting. The “ShapeFn_fitted_...” file is created only when the starting angle (specified by parameter “theta_min”) is equal to 0.

- II. Two files with the parameters of the fitting function (1.5.1) or (1.5.10) obtained after fitting the CS and the DCS for each value of θ . The name of the file with the CS fitting parameters is “**CS_parms.txt**”. A line of text is appended to this file after each fitting. In addition to the values of parameters c , a , b , d , and h in Eq. (1.5.1), or c , c_1 , c_2 , ..., c_M in Eq. (1.5.10) obtained by fitting the dependence of the CS on κ_{\max} , the file “CS_parms.txt” contains several parameters pertaining to the angular dependence of the fitted DCS. The name of the file with the DCS fitting parameters starts with the string “**DCS_parms_**” and includes the input file name. This file is overwritten after each fitting.
- III. The file “**Errors.txt**”. This file is created for the purpose of the future statistical analysis with the aim of determining the degree of correlation between several quantities related to the accuracy of the fitting (see also the description of parameter No. 3.2.12). Several lines of text are appended to this file after each error testing. Each line has 24 entries and corresponds to one of the intervals of κ_{\max} where the fitting is performed (in decreasing order of the endpoints of these intervals). Each set of results contained in a single line of this file is obtained by complete processing of the data corresponding to a particular maximum value of κ_{\max} , including the averaging of the results corresponding to the fitting intervals shifted by up to $\text{shift_k_max_}(D)CS$ relative to the original interval (see the description of parameters No. 3.2.7–8).
- IV. Five files with intermediate data of the angular spline fitting and extrapolation. The first two of these files contain the results of the angular spline fitting and extrapolation of the original PW DCS (prior to the subsequent κ_{\max} -fitting) for all angles and all values of κ_{\max} . The names of those two files are formed from the name of the input file with the PW DCS data by inserting the suffix specified by one of parameters “suffix_spline” or “suffix_extrap” (see the description of parameters No. 3.15.5–6). If the angular spline fitting of the PW DCS is not performed, then those two files are not created. If only the spline fitting in the entire angular range $0^\circ \leq \theta \leq 180^\circ$ is performed (without the angular extrapolation), then only the first one of those two files is created (with the suffix specified by parameter “suffix_spline”). If the angular extrapolation of the PW DCS is performed, then both those files are created (if they already exist, then they will be overwritten). The third one of the files of this group contains the results of κ_{\max} -fitting of the spline-fitted and extrapolated PW DCS (prior to the subsequent angular spline fitting and extrapolation of the κ_{\max} -fitted DCS) for all angles and all “shifts” where the κ_{\max} -fitting has been completed successfully. The name of this file starts with the string “**DCS_interm0_**” and includes the input file name. This file is also overwritten after each fitting. The fourth one of these files contains the results of the angular spline fitting and extrapolation of the κ_{\max} -fitted DCS for all angles and all “shifts” where the κ_{\max} -fitting has been completed successfully. The name of this file starts with the string “**DCS_interm1_**” and includes the input file name. This file is also overwritten after each fitting. The fifth one of these files contains a short summary of the results (i.e., values of the main parameters) of angular spline fitting and extrapolation of the κ_{\max} -fitted DCS corresponding to each “shift” where the κ_{\max} -fitting has been completed successfully. The name of this file is “**Data_interm1.txt**”. Several lines of text (one line per shift) are appended to the file “Data_interm1.txt” after each fitting.
- V. Two files with the data of the μ -corrected DCS (see Section 1.5.4) corresponding to the maximum value of κ_{\max} in the analyzed dataset, and a file with the μ -fitting data for each “shift”. The first two mentioned files are updated only when parameter No. 3.10.5 “output_mu” is equal to ± 1 , or 2, and the third mentioned file is updated only when parameter “output_mu” is equal to 2. The first one of those two files (“**mu_range.txt**”) contains the limits

of the angular range corresponding to constant scale factor μ in Eq. (1.5.12a), the limits of the angular range of the polynomial fitting of the μ -corrected DCS (see Section 1.5.4), the values of the normalized differential of the function $\text{DCS}(\kappa_{\max})$, the optimal value of μ , and the corresponding rms values of the relative deviation of the μ -corrected DCS (and of its polynomial approximation) from the reference function defined by parameter “compRef_mu” (No. 3.6.35). A line of text is appended to the file “mu_range.txt” after each μ -fitting. The name of the second file of this group starts with the string “DCS_mu_”, followed by the name of the input file with the cross section data. This file contains the values of the μ -corrected DCS and of its polynomial approximation for each value of the photon emission angle θ . This file is overwritten after each μ -fitting. The format of the third mentioned file (“mu.txt”) is similar to the format of the first mentioned file (“mu_range.txt”), and the main difference between these two file is that the file “mu_range.txt” contains the data only for the maximum value of κ_{\max} in the analyzed dataset (i.e., for “shift 0”), whereas the file “mu.txt” contains the data for each shift. Several lines of text (one line for each shift) are appended to the file “mu.txt” after each run where the μ -fitting was performed.

In the case “S_data=2” (see Section 6.18 and the description of parameter No. 13 of the main program at the end of Section 2), the names of all mentioned files will have the plus sign ‘+’ inserted at the end of the file name. In the names of the files that are re-created in each run of BREMS (rather than updated by adding a line or several lines), the plus sign is inserted immediately before the suffix defined by parameter 2.5.3 (“suffix2_CS”) or No. 2.5.4 (“suffix2_DCS”), or immediately after the suffix defined by parameter No. 1.9.2 (“suffix”). In the names of the files that are updated in each run of BREMS by adding a line or several lines, the plus sign is inserted immediately before the extension “.txt”. In the case “S_data=3”, the files with the additional ‘+’ in the name will not be updated (and if they were created, then they will be deleted automatically), except for the file “Data_interm1+.txt”. In the case of a failure to join the small-angle part of the original κ_{\max} -fitted DCS with the large-angle part of the alternative κ_{\max} -fitted DCS, the files “DCS_fitted_...+.txt” and “DCS_parms_...+.txt” (with the results of κ_{\max} -fitting of the alternative partial-wave DCS) will not be deleted.

In order to avoid a crash when two or more instances of BREMS attempt to update the same file simultaneously, a temporary read-only file with the name “write_lock3” is opened in the current folder just before updating the mentioned files (the number “3” in the mentioned file name indicates that this file was created in stage 3 of the current run of BREMS). If another instance of the program attempts to update the same files, it will first check for existence of the mentioned temporary file, and then attempt to delete it if it exists. If the file exists and the delete attempt is not successful, then the program will wait until the mentioned file is deleted by the instance that created it.

Each line written to the file “CS_fitted.txt” contains 74 entries, which have the following meaning:

- (1) the atomic number of the target material (column header “Z”),
- (2) the kinetic energy of the incident electron in MeV (“T1(MeV)”)
- (3) the energy of the bremsstrahlung photon in MeV (“Ep(MeV)”)
- (4) the original value of K defined by Eq. (1.5.3) (“kmax0”),
- (5) the value of K after the possible reduction on the basis of the restrictions on the maximum relative error (“kmax”); see the descriptions of parameters No. 3.14.1–2,
- (6) the value of parameter No. 3.11.25 (“vary_h_CS”),
- (7) the value of parameter No. 3.11.26 (“vary_h_DCS”),
- (8) the final value of parameter No. 3.2.7, taking into account parameter No. 3.2.9 (column header “shift_CS”),
- (9) the final value of parameter No. 3.2.8, taking into account parameter No. 3.2.9 (column header “shift_DCS”)

- (10) the number of observations of the fitted CS used for averaging and calculation of its standard deviation (“**nObs**”). If no “shifts” were excluded, then this number is equal to $\text{shift_k_max}+1$. If some shifts were excluded, then this number will be smaller,
- (11) the number “1” or “2” indicating one of the two possible widths of the fitting interval corresponding to a successful fitting of the dependence of CS on κ_{max} in shift 0 (see the description of parameters No. 3.2.3–4). If the option “fitRange_CS=3” is used and the fitting succeeds in both fitting intervals, then this entry is equal to 3 (“**fitRange_CS**”),
- (12) same as above for the DCS (“**fitRange_DCS**”),
- (13) the tolerance for the relative error caused by uncertainties of the S integrals (“**maxRelErr**”),
- (14) the tolerance for the relative error caused by truncation of the sum (1.1.10) with respect to l (“**maxRelErr2**”).

The next ten entries specify the values of the adjustable spline-fitting parameters during the angular spline fitting of the partial-wave (PW) DCS, as described in Section 1.7.1:

- (15) the starting angle of the angular fitting range (θ_{min} , using the notations of Section 1.7) for the spline fitting and extrapolation of the angular dependence of the partial-wave (PW) DCS, or the number -1 if the mentioned fitting has not been performed (“**splThetaMin**”),
- (16) the value of the ending angle of the angular spline-fitting range (θ_{max} , using the notations of Section 1.7) for the spline fitting and extrapolation of the angular dependence of the PW DCS, or the number -1 if the mentioned angular spline fitting has not been performed (“**splThetaMax**”),
- (17) the number of spline knots in the angular fitting range for the spline fitting and extrapolation of the angular dependence of the PW DCS, or the number -1 if the mentioned angular fitting has not been performed. In the case of the linear or quadratic angular fitting (see the note at the end of Section 1.7.1), this entry is equal to 0 or 1, respectively (although the actual number of knots is 2). The header of this column is “**nKnots**”,
- (18) the final value of the first knot-density parameter (denoted ε_1 in Section 1.7) for the spline fitting and extrapolation of the angular dependence of the PW DCS, or the number 0 if the mentioned angular spline fitting has not been performed or if the number of knots is equal to 2 (“**splIntRatio_1**”),
- (19) the final value of the second knot-density parameter (denoted ε_2 in Section 1.7) for the spline fitting and extrapolation of the angular dependence of the PW DCS, or the number 0 if the parameter ε_2 has not been used (“**splIntRatio_2**”),
- (20) the minimum width of the inter-knot interval for the spline fitting and extrapolation of the angular dependence of the PW DCS, or the number 0 if the mentioned angular spline fitting has not been performed (“**minSplIntWth**”),
- (21) the maximum width of the inter-knot interval for the spline fitting and extrapolation of the angular dependence of the PW DCS, or the number 0 if the mentioned angular spline fitting has not been performed (“**maxSplIntWth**”),
- (22) the number 0, 1 or 2 identifying the reference function used for the spline fitting and extrapolation of the angular dependence of the PW DCS, or the number -1 if the mentioned angular spline fitting has not been performed (“**splRef**”). The meanings of the mentioned numbers are the following:
 - 0 – no division by a reference function (or the reference function equal to 1),
 - 1 – reference DCS No. 1 as defined by parameters No. 3.5.1–20,
 - 2 – reference DCS No. 2 as defined by parameters No. 3.5.1–20,
- (23) the number 1, 2 or 3 identifying the spline argument used for the spline fitting and extrapolation of the angular dependence of the PW DCS, or the number 0 if the

mentioned angular spline fitting has not been performed (“**splArg**”). The meanings of the mentioned numbers are the following:

- 1 – spline argument is equal to the angle θ ,
 - 2 – spline argument is equal to $-\cos \theta$,
 - 3 – spline argument is equal to $\ln[(1 - \cos \theta) / 2]$,
- (24) the number 1 or 0 indicating if the original function has been replaced by its logarithm or not (respectively) during the spline fitting and extrapolation of the angular dependence of the PW DCS (“**splLog**”).

The next ten entries specify the values of the adjustable spline-fitting parameters during the angular spline fitting of the κ_{\max} -fitted DCS. If two or more κ_{\max} -fitting intervals (“shifts”) have been used and the angular spline fitting has been performed for each shift separately (i.e., if the option “spline_combine=0” or “spline_combine=1” has been used), then these ten entries correspond to the final spline smoothing of the spline-fitted and extrapolated DCS, averaged over all shifts. As mentioned at the end of Section 1.7.2, this spline fitting is always performed over the entire angular range, hence parameters θ_{\min} and θ_{\max} are in this case equal to 0° and 180° , respectively (the parameters of the spline fitting of the κ_{\max} -fitted DCS corresponding to individual shifts can be found in the file “Data_interm1.txt”, which belongs to the fourth group of files created or updated in stage 3). If there is only one “shift”, or if the option “spline_combine=2” has been used, then these ten entries correspond to the first angular spline fitting of the κ_{\max} -fitted DCS (not the subsequent spline smoothing), and they coincide with the corresponding ten entries in the file “Data_interm1.txt”. The meanings of these ten entries are identical to the meanings of the previous ten entries, and the column headers differ from the corresponding headers of the previous ten columns only by the additional subscript “2”:

- (25) the starting angle of the angular fitting range (θ_{\min} , using the notations of Section 1.7) for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number -1 if the mentioned fitting has not been performed (“**splThetaMin2**”),
- (26) the value of the ending angle of the angular spline-fitting range (θ_{\max} , using the notations of Section 1.7) for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number -1 if the mentioned angular spline fitting has not been performed (“**splThetaMax2**”),
- (27) the number of spline knots in the angular fitting range for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number -1 if the mentioned angular fitting has not been performed. In the case of the linear or quadratic angular fitting (see the note at the end of Section 1.7.1), this entry is equal to 0 or 1, respectively. The header of this column is “**nKnots2**”,
- (28) the final value of the first knot-density parameter (denoted ε_1 in Section 1.7) for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number 0 if the mentioned angular spline fitting has not been performed or if the number of knots is equal to 2 (“**splIntRatio2_1**”),
- (29) the final value of the second knot-density parameter (denoted ε_2 in Section 1.7) for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number 0 if the parameter ε_2 has not been used (“**splIntRatio2_2**”),
- (30) the minimum width of the inter-knot interval for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number 0 if the mentioned angular spline fitting has not been performed (“**minSplIntWth2**”),
- (31) the maximum width of the inter-knot interval for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number 0 if the mentioned angular spline fitting has not been performed (“**maxSplIntWth2**”),

- (32) the number 0, 1 or 2 identifying the reference function used for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number -1 if the mentioned angular spline fitting has not been performed (“**splRef2**”). The meanings of the mentioned numbers are the following:
- 0 – no division by a reference function (or the reference function equal to 1),
 - 1 – reference DCS No. 1 as defined by parameters No. 3.5.1–20,
 - 2 – reference DCS No. 2 as defined by parameters No. 3.5.1–20,
- (33) the number 1, 2 or 3 identifying the spline argument used for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number 0 if the mentioned angular spline fitting has not been performed (“**splArg2**”). The meanings of the mentioned numbers are the following:
- 1 – spline argument is equal to the angle θ ,
 - 2 – spline argument is equal to $-\cos \theta$,
 - 3 – spline argument is equal to $\ln[(1 - \cos \theta) / 2]$,
- (34) the number 1 or 0 indicating if the original function has been replaced by its logarithm or not (respectively) during the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS (“**splLog2**”),
- (35) the total number of values of θ where an irrecoverable error occurred when fitting the dependence of the DCS on κ_{\max} in the case of zero shift of the fitting interval (“**nErrTot**”),
- (36) the maximum number of consecutive values of θ where an irrecoverable error occurred when fitting the dependence of the DCS on κ_{\max} in the case of zero shift of the fitting interval (“**nErr**”),
- (37) the original (unfitted) value of the PW CS calculated by Bremsstrahlung for $\kappa_{\max} = K$ and smoothed by replacing it with a moving average (MA) as explained in Section 1.5.3 (“**CS_MA[kmax]**”),
- (38) the value of the “reference CS”, which was used to calculate the term δ_{CS} in the definition of the objective function (6.8.1a) or (6.8.1b) for the angular spline fitting and extrapolation of the κ_{\max} -fitted DCS (see also the description of parameter No. 3.8.41) (“**CS_ref_spline**”),
- (39) the value of c (“**CS_fitted[k->Inf]**”), averaged over all fitting intervals as explained in the description of parameters No. 3.2.7–8,
- (40) the estimate of the CS obtained by integrating the fitted DCS numerically with respect to $\cos(\theta)$ and multiplying by 2π (and averaging over all fitting intervals as explained in the description of parameters No. 3.2.7–8). This integration is performed using the 10th order Newton-Cotes formula, and the bounds of this integral are equal to parameters No. 3.3.1 and No. 3.3.2 (or No. 3.3.1 and No. 3.3.4) described above. If the DCS is not fitted (i.e., if parameter No. 3.2.13 is zero), then this integral is set to zero. The header of this column is “**DCSint(10th_orderNC)**”,
- (41) the relative difference of the previous two values, i.e., the relative deviation of the numerical integral of the fitted DCS from the final κ_{\max} -fitted value of c (“**rel_diff**”). *Note:* If the entry in column “DCSint(10th_orderNC)” is zero (i.e., if fitMode = 0) and CS_ref_spline > 0, then the entry in column “rel_diff” is equal to the relative difference of the entries in columns “CS_fitted[k->Inf]” and “CS_ref_spline”,
- (42) value of reference CS No. 1 (it is equal to the integral of reference DCS No. 1 with respect to the solid angle of photon emission), or the number 0 if reference DCS No. 1 is not used (“**ref1_CS**”),
- (43) value of reference CS No. 2 (it is equal to the integral of reference DCS No. 2 with respect to the solid angle of photon emission), or the number 0 if reference DCS No. 2 is not used (“**ref2_CS**”),

- (44) the starting point of the angular transition interval between the small-angle part of the original κ_{\max} -fitted DCS and the large-angle part of the alternative κ_{\max} -fitted DCS (see Section 6.18), or zero if the alternative DCS was not used (“**theta1+**”),
- (45) the endpoint of the angular transition interval between the small-angle part of the original κ_{\max} -fitted DCS and the large-angle part of the alternative κ_{\max} -fitted DCS (see Section 6.18), or zero if the alternative DCS was not used (“**theta2+**”),
- (46) the maximum relative deviation of the alternative κ_{\max} -fitted DCS from the original κ_{\max} -fitted DCS inside the angular transition interval (see Section 6.18), or zero if the alternative DCS was not used (“**maxRelDif+**”).

The next five entries specify the corrections of the original PW CS, PW DCS, and PW shape function (replaced with a moving average over the last several values of κ_{\max}) due to the angular spline fitting and extrapolation, and the subsequent κ_{\max} -fitting. When calculating the “scaled” corrections, the product of $\sin(\theta)$ and the correction of the fitted DCS or fitted shape function is divided by the maximum value of the product of $\sin(\theta)$ and the original (unfitted) PW DCS or shape function. Thus, the scaled correction is the correction of the probability density function of θ , expressed in terms of the fraction of the maximum value of the original (unfitted) probability density function:

- (47) relative correction of the CS (“**CS_relCorr**”),
- (48) maximum relative correction of the DCS (“**DCS_maxRelCorr**”),
- (49) maximum scaled absolute correction of the DCS (“**DCS_maxScCorr**”),
- (50) maximum relative correction of the shape function (“**SF_maxRelCorr**”),
- (51) maximum scaled absolute correction of the shape function (“**SF_maxScCorr**”).

The next four entries specify the corrections of the spline-fitted and extrapolated PW DCS (see Section 1.7.1) and of the corresponding shape function due to the κ_{\max} -fitting. They should be interpreted in the same way as the previous four entries (if the angular spline fitting and extrapolation of the PW DCS has not been performed, then these four entries are equal to the previous four entries):

- (52) maximum relative correction of the DCS (“**DCS_maxRelC_ext**”),
- (53) maximum scaled absolute correction of the DCS (“**DCS_maxScC_ext**”),
- (54) maximum relative correction of the shape function (“**SF_maxRelC_ext**”),
- (55) maximum scaled absolute correction of the shape function (“**SF_maxScC_ext**”).

The next five entries specify the standard deviations (SD) of the CS, DCS, and shape function, reflecting the differences of the fitting results for different fitting intervals (see the descriptions of parameters No. 3.2.7–8 and No. 3.17.3–11), as well as the uncertainty of the parameter c associated with each shift (see the description of parameters No. 3.16.7–8). When calculating the “scaled” SD, the product of $\sin(\theta)$ and the absolute SD of the fitted DCS or fitted shape function is divided by the maximum value of the product of $\sin(\theta)$ and the same DCS or fitted shape function. Thus, the scaled SD is the absolute SD of the probability density function of θ , expressed in terms of the fraction of the maximum value of the same probability density function:

- (56) relative standard deviation of the CS (“**CS_fitted_relSD**”),
- (57) maximum relative standard deviation of the DCS (“**DCS_maxRelSD**”),
- (58) maximum scaled standard deviation of the DCS (“**DCS_maxScaledSD**”),
- (59) maximum relative standard deviation of the shape function (“**SF_maxRelSD**”),
- (60) maximum scaled standard deviation of the shape function (“**SF_maxScaledSD**”).

If the relative range of variation of the CS or DCS for “shift 0” is less than 0.001 (and the angular spline fitting of the κ_{\max} -fitted DCS is not performed), then the final value of the corresponding SD is set equal to the range of variation of the CS or DCS in the fitting interval

corresponding to shift 0. As an indication of this special case, the value of the mentioned SD is output with the minus sign.

The next six entries specify the deviations of the final fitted CS, DCS and SF from the corresponding reference values defined by the reference DCS No. 1 (it is calculated using the Born approximation by default) and No. 2 (it is calculated using the Sommerfeld-Maue approximation with the next-to-leading order correction by default):

- (61) relative deviation of the final fitted CS from reference CS No. 1 (“**CS_ref1_relDiff**”),
- (62) maximum relative deviation of the final fitted DCS from reference DCS No. 1 over all angles (“**DCS_ref1_maxRelD**”),
- (63) maximum relative deviation of the final fitted SF from reference SF No. 1 over all angles (“**SF_ref1_maxRelD**”),
- (64) relative deviation of the final fitted CS from reference CS No. 2 (“**CS_ref2_relDiff**”),
- (65) maximum relative deviation of the final fitted DCS from reference DCS No. 2 over all angles (“**DCS_ref2_maxRelD**”),
- (66) maximum relative deviation of the final fitted SF from reference SF No. 2 over all angles (“**SF_ref2_maxRelD**”).

The last eight entries specify the time of calculation, BREMS version number, and timestamps of various files used for the current run or created during it:

- (67) the total duration of stage 3 in seconds (“**time**”),
- (68) the total duration of the current run of BREMS in seconds (“**total_time**”),
- (69) the version number of the program used for the calculations (“**BREMS_ver**”). The version number is written as an integer number obtained by concatenating all four components of the version number, with the last three components having two digits each (the first of these two digits may be zero). For example, BREMS v1.5.7.0 would be indicated by “1050700”.
- (70) the timestamp (i.e., last modification time) of the executable file used for the calculations (“**exe_timestamp**”). The timestamp is written as a 14-digit integer number, whose first eight digits indicate the date using the format YYYYMMDD, and the last six digits indicate the time using the format HHMMSS. For example, the timestamp “20230527132051” indicates the time 13:20:51 on May 27, 2023,
- (71) the timestamp of the file with the data of reference DCS No. 1, or “0” if this reference DCS was not used (“**ref1_timestamp**”),
- (72) the timestamp of the file with the data of reference DCS No. 2, or “0” if this reference DCS was not used (“**ref2_timestamp**”),
- (73) the timestamp of one of the files belonging to the first group of files created in stage 2, which was used as input for stage 3 in the current run. This is the file whose name starts with “_CS_” and does not include the suffix “_test” or “_test2” (see Section 5.8). The header of this column is “**_CS_timestamp**”,
- (74) the timestamp of the file whose name starts with “DCS_fitted_”, which was created during the current run, or “0” if this file was not created (“**DCS_timestamp**”).

Each line written to the “**DCS_fitted_**” file contains 22 entries, which have the following meaning:

- (1) the value of θ in degrees (column header “**theta**”),
- (2) the spline-fitted value of the PW DCS (without the angular extrapolation), or the moving average of the PW DCS if the angular spline fitting of the PW DCS has not been performed (“**DCS_smoothed[kmax]**”). If the angular spline fitting of the PW DCS has been performed, then the values in this column are the same as in the last column of the “_spline” file belonging to the fourth group of files created in stage 3,
- (3) the value of the DCS obtained by angular spline extrapolation of the PW DCS as described in Section 1.7.1 and in the descriptions of parameters No. 3.7.1–38 (“**DCS_extrap[kmax]**”). If the angular spline extrapolation has not been performed,

- then the value in this column is equal to the value in the previous column. Otherwise, the values in this column are the same as in the last column of the “_spline_extrap” file belonging to the fourth group of files created in stage 3,
- (4) the κ_{\max} -fitted value of the DCS after the optional angular spline fitting and extrapolation described in Section 1.7.2 and in the descriptions of parameters No. 3.8.1–47 (“**DCS_fitted**”),
 - (5) the value of the reference DCS No. 1 defined by parameters No. 3.5.1–20, or the number 0 if reference DCS No. 1 is not used (“**DCS_ref1**”),
 - (6) the value of the reference DCS No. 2 defined by parameters No. 3.5.1–20, or the number 0 if reference DCS No. 2 is not used (“**DCS_ref2**”),
 - (7) the product of $\sin \theta$ and the κ_{\max} -fitted DCS (“**sin(theta)*DCS_fitted**”). If the angular distribution of bremsstrahlung photons is strongly peaked in the forward direction, then the angular range contributing the most to the value of the SDCS is located near the maximum of this product (and the errors of the κ_{\max} -fitted DCS in this angular range contribute the most to the errors of the final SDCS),
 - (8) the number “1” or “2” indicating the type of the PW data used for the κ_{\max} -fitting (see the description of parameter No. 3.2.11). “1” indicates that the PW shape function (SF) has been fitted by the function (1.5.1) or (1.5.10), and the corresponding κ_{\max} -fitted DCS has been calculated by multiplying the κ_{\max} -fitted SF by the κ_{\max} -fitted CS. “2” indicates that PW DCS has been fitted by the function (1.5.1) or (1.5.10), and the corresponding SF has been calculated by dividing the κ_{\max} -fitted DCS by the κ_{\max} -fitted CS. The header of this column is “**data**”,
 - (9) relative correction of the PW DCS due to the initial angular spline fitting and extrapolation, κ_{\max} -fitting and the subsequent angular spline fitting and extrapolation of the κ_{\max} -fitted DCS (“**DCS_relCorr**”),
 - (10) “scaled” absolute correction of the PW DCS due to the initial angular spline fitting and extrapolation, κ_{\max} -fitting and the subsequent angular spline fitting and extrapolation of the κ_{\max} -fitted DCS (“**DCS_scaledAbsCorr**”), calculated as explained above in the description of the corresponding entries of the file “CS_fitted.txt”,
 - (11) relative correction of the spline-fitted and extrapolated PW DCS due to the κ_{\max} -fitting and the subsequent angular spline fitting and extrapolation of the κ_{\max} -fitted DCS (“**DCS_relCorr_extrap**”),
 - (12) scaled absolute correction of the spline-fitted and extrapolated PW DCS due to the κ_{\max} -fitting and the subsequent angular spline fitting and extrapolation of the κ_{\max} -fitted DCS (“**DCSscaledAbsCorExt**”),
 - (13) relative deviation of the final value of the κ_{\max} -fitted DCS from reference DCS No. 1 (it is calculated using the Born approximation by default), or the number 0 if reference DCS No. 1 is not used (“**DCS_ref1_relDiff**”),
 - (14) relative deviation of the final value of the κ_{\max} -fitted DCS from reference DCS No. 2 (it is calculated using the Sommerfeld-Maue approximation with the next-to-leading order correction by default), or the number 0 if reference DCS No. 2 is not used (“**DCS_ref2_relDiff**”),
 - (15) relative change of the DCS after replacing the original S integrals with the “test” values, i.e., using the files with the additional suffix “_test” created in stage 2 (see also Sections 1.4, 5.8, and 6.16). The header of this column is “**relDiff_S_int**”,
 - (16) relative change of the DCS caused by the reduction of the value of l_{\max} in the sum of Eq. (1.1.10), after the correction by the factor (6.16.1b) (see Section 6.16). The header of this column is “**relDiff_lmax**”,
 - (17) number of observations (“shifts”) used for the final angular spline fitting, extrapolation and averaging of the κ_{\max} -fitted data, as well as for calculation of the standard deviation (“**nObs**”),

- (18) relative standard deviation (SD) of the κ_{\max} -fitted DCS (“**DCS_relSD**”), reflecting both the differences between the results for the different fitting intervals (see the descriptions of parameters No. 3.2.7–8 and No. 3.17.3–11) and the uncertainties of the value of parameter c associated with each fitting interval (see also the description of parameters No. 3.16.7–8). If the relative range of variation of the CS or DCS for “shift 0” is less than 0.001 and the angular spline fitting of the κ_{\max} -fitted DCS is not performed, then the value of the corresponding SD is set equal to the relative range of variation of the DCS in the fitting interval corresponding to shift 0. As an indication of this special case, the value of the mentioned SD is output with the minus sign,
- (19) “scaled” absolute standard deviation of the κ_{\max} -fitted DCS (“**DCS_scaledAbsSD**”), calculated using the value in the previous column as explained above in the description of the corresponding entries of the file “CS_fitted.txt”,
- (20) the number of values of the endpoint θ' of the polynomial fitting interval used for optimization of the scale factor μ and of the degree of the fitting polynomial, as well as for the choice of the reference function used for the mentioned fitting (see also Section 1.5.4), or the number 0 if the current value of θ is less than the starting angle θ_{start} of the range of angle-independence of the scale factor μ in Eq. (1.5.12a) when the PW DCS is a decreasing function of κ_{\max} , or greater than the ending angle θ_{end} of the same range when the PW DCS is an increasing function of κ_{\max} (“**n_mu**”),
- (21) the total relative standard deviation (i.e., total relative uncertainty) of the κ_{\max} -fitted DCS (“**DCS_relSD_tot**”), which is obtained by combining in quadrature four relative uncertainties: **(a)** the relative change of the DCS caused by the replacement of the original S integrals with the “test” values, which is given in column “relDiff_S_int” (see also Sections 1.4 and 6.16), **(b)** the uncertainty of the DCS due to the reduction of l_{\max} , which is given in column “relDiff_lmax” (see also Sections 1.3.2 and 6.16), **(c)** the relative standard deviation reflecting the differences between the results for the different “shifts”, i.e., for the different κ_{\max} -fitting intervals, which is given in column “DCS_relSD” (see also Section 1.6), and **(d)** the relative standard deviation reflecting the differences between the values of the μ -corrected DCS corresponding to different endpoints of the polynomial fitting interval at the maximum value of κ_{\max} (i.e., for “shift 0”), using the optimal degree (or user-specified) of the fitting polynomial and the optimal (or user-specified) choice of the reference function (see also Section 1.5.4). The first two mentioned components (“a”) and “b”) of the total relative uncertainty are usually much less than the remaining components,
- (22) “scaled” absolute total standard deviation of the κ_{\max} -fitted DCS (“**DCS_scAbsSD_tot**”), calculated using the value in the previous column as explained above in the description of the corresponding entries of the file “CS_fitted.txt”.

Note: If the alternative DCS has been used (see Section 6.18), then the part of the “DCS_fitted_” file starting with the endpoint of the transition interval (indicated in column “theta2+” of file “CS_fitted.txt”) is replaced with the results of κ_{\max} -fitting of the alternative DCS. I.e., this part of the output data is copied from the “DCS_fitted_” file that would be created using the option “S_data=2” (see the description of parameter No. 13 of the main program).

Each line of text written to the “ShapeFn_fitted_” file contains 22 entries, whose meaning is the same as the meaning of the corresponding entries in the “DCS_fitted_” file, except that in this case the functions whose values or differences are output have the meaning of shape functions rather than DCS. The values of the standard deviations in the last two columns are the same as in the corresponding “DCS_fitted_” file. The headers of the corresponding columns in the two files differ only by the prefix: in the “ShapeFn_fitted_”, the prefix is “ShapeFn” or “SF”, whereas in the “DCS_fitted_” file, it is “DCS” (see the description of the “DCS_fitted_” file above).

Each line of text written to the “CS_parms.txt” file contains the following 61 entries:

- (1) – (5) same as columns No. 1 – 5 in the file “CS_fitted.txt” described above,
- (6) – (9) same as columns No. 11 – 14 in the file “CS_fitted.txt” described above,
- (10) – (11) same as columns No. 37 and No. 39 in the file “CS_fitted.txt” described above,
- (12) the final value of the variable “tol_range” (see the descriptions of parameters No. 3.4.7–8),

The next 23 entries in the file “CS_parms.txt” are related to the angular spline fitting and extrapolation:

- (13) the value of parameter No. 3.17.5 “splineFit_wt” (the header is “splFitWt”),
- (14) – (33) same as columns No. 15 – 34 in the file “CS_fitted.txt” described above,
- (34) the fraction of the total angular integral of the final κ_{\max} -fitted DCS with respect to the solid angle of photon emission contained inside the angular range from 0° to θ_x , where θ_x is the smallest value of the angle from the set defined by parameters No. 3.3.1–5, defined so as to ensure that the mentioned fraction is greater than or equal to the value of parameter No. 3.8.40. This fraction is either equal to or slightly greater than the value of the mentioned parameter. The header of this column is “smallAngleFraction_final”,
- (35) the value of the angle θ_x defined above (“smallAngleFractEndpoint”),

All subsequent entries in the file “CS_parms.txt” correspond to “shift 0”, i.e., to the κ_{\max} -fitting interval with the maximum value of the upper endpoint:

- (36) the value of θ corresponding to the last occurrence of the shape function (SF) with sign +1 (the meaning of the term “sign” used here is explained after the description of parameter No. 3.4.8). If there are no values of θ corresponding to the SF with sign +1, then the corresponding entry is –1, and if the SF data has not been analyzed, then it is equal to –2. The header of this column is “SF_theta_limit_1”,
- (37) the value of θ corresponding to the first occurrence of the SF with sign –1 (the meaning of the term “sign” used here is explained after the description of parameter No. 3.4.8). If there are no values of θ corresponding to the DCS with sign –1, then the corresponding entry is –1, and if the SF data has not been analyzed, then it is equal to –2. The header of this column is “SF_theta_limit_2”,
- (38) the value of θ corresponding to the last occurrence of the DCS with sign +1 (the meaning of the term “sign” used here is explained after the description of parameter No. 3.4.8). If there are no values of θ corresponding to the DCS with sign +1, then the corresponding entry is –1, and if the DCS data has not been analyzed, then it is equal to –2. The header of this column is “DCS_theta_limit_1”,
- (39) the value of θ corresponding to the first occurrence of the DCS with sign –1 (the meaning of the term “sign” used here is explained after the description of parameter No. 3.4.8). If there are no values of θ corresponding to the DCS with sign –1, then the corresponding entry is –1, and if the DCS data has not been analyzed, then it is equal to –2. The header of this column is “DCS_theta_limit_2”,
- (40) – (41) same as columns No. 35 – 36 in the file “CS_fitted.txt” described above.
- (42) the starting point of the range of κ_{\max} (“kStart”),
- (43) the endpoint of the range of κ_{\max} (“kEnd”),
- (44) the number of values of κ_{\max} in the κ_{\max} -fitting interval (“Nfit”),
- (45) the moving average interval used when processing the CS data (“nAvg”),
- (46) the timestamp of one of the files belonging to the first group of files created in stage 2, which was used as input for stage 3 in the current run. This is the file whose name starts with “_CS_” and does not include the suffix “_test” or “_test2” (see Section 5.8). The header of this column is “_CS_timestamp”,

- (47) the timestamp of the file whose name starts with “DCS_fitted_”, which was created during the current run, or “0” if this file was not created (“**DCS_timestamp**”),
- (48) the rms value of the residual of the κ_{\max} -fitting of the CS (“**rmsResidual**”),
- (49) the relative uncertainty of parameter c in Eq. (1.5.1) or (1.5.10), calculated using Eq. (1.6.2b) (“**c_relErr**”),
- (50) the “sign” of the dependence of the κ_{\max} -fitted CS on κ_{\max} as defined after the description of parameter No. 3.4.8 (if the fitting has not been performed, then this entry is zero). The header of this column is “**sign**”,
- (51) the optimal degree of the approximating polynomial (1.5.10) if the polynomial fitting of the CS has been performed, or the opposite of the absolute value of parameter No. 3.11.25 “vary_h_CS” if the five-parameter fitting using the stretched exponential (1.5.1) has been performed. If parameter h in Eq. (1.5.1) has been fixed at 0, or if the fitting has not been performed, then this entry is 0. The header of this column is “**degree**”,
- (52) – (61) the optimal values of the five coefficients $c, a, b, d,$ and h in (1.5.1), or of the coefficients $c, c_1, b, d, h, c_2, c_3, \dots, c_6$ in (1.5.10) and (1.5.8) (in the same order). If the fitting has not been performed, then c is equal to the original (unfitted) value of the PW CS, and the subsequent entries are empty. If the fitting has been performed using the approximation (1.5.6), then $b = -1$. The headers of these ten columns are “**c**”, “**a(c1)**”, “**b**”, “**d**”, “**h**”, “**c2**”, “**c3**”, “**c4**”, “**c5**”, “**c6**”. If the polynomial approximation (1.5.10) has been used and the degree M is less than 6, then the last $6 - M$ entries are empty. If the stretched exponential approximation (1.5.1) has been used, then the last five entries are empty.

Each line of text written to the “DCS_parms_” file contains 24 entries with the fitting results in the case of zero shift of the fitting interval:

- (1) the value of θ (“**theta**”),
- (2) the starting point of the range of κ_{\max} (“**kStart**”). A zero value of this entry indicates that the fitting has been terminated due to an unrecoverable error, and the corresponding value in the column “**c**” is either the value of the original DCS, or the value obtained by interpolation (see the description of parameter No. 3.14.3),
- (3) the endpoint of the range of κ_{\max} (“**kEnd**”),
- (4) the number of values of κ_{\max} in the κ_{\max} -fitting interval (“**Nfit**”),
- (5) the moving average interval when processing the DCS data (“**nAvg**”),
- (6) the type of the data processed (see also the description of parameter No. 3.2.11). This entry is equal to 1 if the κ_{\max} -fitting has been performed using the PW shape function data, and to 2 if the κ_{\max} -fitting has been performed using the PW DCS data. The header of this column is “**data**”,
- (7) the root mean square value of the residual of the κ_{\max} -fitting (“**rmsResidual**”),
- (8) the relative uncertainty of parameter c in Eq. (1.5.1) or Eq. (1.5.10), calculated using Eq. (1.6.2b) (“**c_relErr**”),
- (9) the “sign” of the dependence of the κ_{\max} -fitted DCS on κ_{\max} as defined after the description of parameter No. 3.4.8. This number indicates the direction of change of the DCS as a function of κ_{\max} . If the fitting has not been performed, then this entry is zero. The header of this column is “**sign**”,
- (10) the optimal degree of the approximating polynomial (1.5.10) if the polynomial fitting of the DCS has been performed, or the opposite of the absolute value of parameter No. 3.11.26 “vary_h_DCS” if the five-parameter fitting using the stretched exponential (1.5.1) has been performed. If parameter h in (1.5.1) has been fixed at 0, or if the fitting has not been performed, then this entry is 0. The header of this column is “**degree**”,
- (11) – (24) the optimal values of the five coefficients $c, a, b, d,$ and h in (1.5.1), or of the coefficients $c, c_1, b, d, h, c_2, c_3, \dots, c_{10}$ in (1.5.10) and (1.5.8) (in the same order). If the

fitting has not been performed, then c is equal to the original (unfitted) value of the PW DCS, and the subsequent entries are empty. If the fitting has been performed using the approximation (1.5.6), then $b = -1$. The headers of these 14 columns are “c”, “a(c1)”, “b”, “d”, “h”, “c2”, “c3”, “c4”, “c5”, “c6”, “c7”, “c8”, “c9”, “c10”. If the polynomial approximation (1.5.10) has been used and the degree M is less than 10, then the last $10 - M$ entries are empty. If the stretched exponential approximation (1.5.1) has been used, then the last nine entries are empty.

Note: If the alternative DCS has been used (see Section 6.18), then the part of the “DCS_parms_” file starting with the endpoint of the transition interval (indicated in column “theta2+” of file “CS_fitted.txt”) is replaced with the results of κ_{\max} -fitting of the alternative DCS. I.e., this part of the output data is copied from the “DCS_parms_” file that would be created using the option “S_data=2” (see the description of parameter No. 13 of the main program).

The meanings of all 24 entries in the file “**Errors.txt**” are explained below:

- (1) the atomic number of the target material (column header “Z”),
- (2) the kinetic energy of the incident electron in MeV (“T1(MeV)”)
- (3) the energy of the bremsstrahlung photon in MeV (“Ep(MeV)”)
- (4) the endpoint of the interval of κ_{\max} where the fitting has been performed (“kmax”),
- (5) the number 1 or 2 indicating one of the two possible widths of the fitting interval corresponding to a successful fitting of the dependence of CS on κ_{\max} in shift 0 (see the description of parameters No. 3.2.3–4). If the option “fitRange_CS=3” is used and the fitting is successful for both fitting intervals, then the value of this entry is 3. The header of this column is “fitRange_CS”;
- (6) same as above for the DCS (“fitRange_DCS”),
- (7) the value of parameter No. 3.2.12, i.e., the maximum allowed relative correction of the CS due to the κ_{\max} -fitting for the error test to be performed (“tol_err_test”),
- (8) the original (unfitted) value of the PW CS calculated by Bremsstrahlung for the current value of the endpoint of the range of κ_{\max} and smoothed by replacing it with a moving average (MA) as explained in Section 1.5.3 (“CS_MA[kmax]”),
- (9) the value of c obtained by extrapolation to $\kappa_{\max} \rightarrow \infty$ at the current value of the endpoint of the range of κ_{\max} (“CS[k->Inf]”),
- (10) the value of the angular integral of the κ_{\max} -fitted DCS, obtained by numerical quadrature using the 10th order Newton-Cotes formula (“DCS_integral”),
- (11) the relative difference of the κ_{\max} -fitted and unfitted CS, i.e., the opposite of the relative deviation of “CS_MA[kmax]” from “CS[k->Inf]” (“1-CS_MA[kmax]/CS[k->Inf]”),
- (12) the opposite of the relative deviation of the value of the numerical integral of the fitted DCS corresponding to the current value of the endpoint of the range of κ_{\max} from the value of c obtained by the κ_{\max} -fitting at that endpoint. If the DCS is not fitted (i.e., if parameter No. 3.2.13 is zero), then this entry is equal to 1. The header of this column is “1-DCS_integral/CS[k->Inf]”,
- (13) the relative deviation of the value of the unfitted CS corresponding to the current value of the endpoint of the range of κ_{\max} from the value of c obtained by the κ_{\max} -fitting at the maximum (original) value of that endpoint (i.e., at the “optimal” fitting conditions) (“CS_MA[kmax]/CS_fit_opt-1”),
- (14) the relative deviation of the value of c obtained by nonlinear fitting at the current value of the endpoint of the range of κ_{\max} , and the value of c obtained by nonlinear fitting at the maximum (original) value of that endpoint (i.e., at the “optimal” fitting conditions) (“CS[k->Inf]/CS_fit_opt-1”),
- (15) the relative deviation of the value of the angular integral of the fitted DCS corresponding to the current value of the endpoint of the range of κ_{\max} , and the value of

the fitted DCS integral corresponding to the maximum (original) value of that endpoint (i.e., to the “optimal” fitting conditions) (“DCS_int/DCS_int_fit_opt-1”),

The next four entries indicate the maximum differences between the fitted DCS or fitted shape function corresponding to the current value of the endpoint of the range of κ_{\max} , and the same function corresponding to the maximum (original) value of that endpoint (i.e., to the “optimal” fitting conditions):

- (16) maximum relative difference of the fitted DCS (“DCS_maxRelDiff”),
- (17) maximum scaled absolute difference of the fitted DCS (“DCS_maxScaledDiff”),
- (18) maximum relative difference of the fitted shape function (“SF_maxRelDiff”),
- (19) maximum scaled difference of the fitted shape function (“SF_maxScaledDiff”).

Note: When calculating the “scaled” differences, the product of $\sin(\theta)$ and the difference of the κ_{\max} -fitted DCS or κ_{\max} -fitted shape function corresponding to the current value of the endpoint of the range of κ_{\max} is divided by the maximum value of the product of $\sin(\theta)$ and the κ_{\max} -fitted DCS or κ_{\max} -fitted shape function corresponding to the maximum (original) value of that endpoint. Thus, the scaled differences are the differences of the probability density functions of θ , expressed in terms of the fraction of the maximum value of the κ_{\max} -fitted probability density function corresponding to the maximum (original) value of the endpoint of the range of κ_{\max} .

The last five entries are equal to the standard deviations of the CS, DCS and shape function, reflecting the differences of the fitting results for different fitting intervals (see the description of parameters No. 3.2.7–8):

- (20) relative standard deviation of the CS (“CS_fitted_relSD”),
- (21) maximum relative standard deviation of the DCS (“DCS_maxRelSD”),
- (22) maximum scaled standard deviation of the DCS (“DCS_maxScaledSD”),
- (23) maximum relative standard deviation of the shape function (“SF_maxRelSD”),
- (24) maximum scaled standard deviation of the shape function (“SF_maxScaledSD”).

The first of the lines appended to the file “Errors.txt” after the κ_{\max} -fitting corresponds to the absolute maximum of κ_{\max} , i.e., to the optimal fitting conditions. Consequently, the six entries in columns No. 14 – 19 (“CS[k->Inf]/CS_fit_opt-1” to “SF_maxScaledDiff”) in this line are always zero, and the entry in column No. 13 (“CS_MA[kmax]/CS_fit_opt-1”) is an exact opposite of the entry in column No. 11 (“1-CS_MA[kmax]/CS[k->Inf]”).

As mentioned in the description of parameter No. 3.2.12, existence of correlation between the values of the relative differences in columns No.11 and No.14 (“1-CS_MA[kmax]/CS[k->Inf]” and “CS[k->Inf]/CS_fit_opt-1”, respectively) would be useful for defining a rule of estimating the upper bound of the relative uncertainty of the final estimate of the CS obtained by the extrapolation to $\kappa_{\max} \rightarrow \infty$, given the magnitude of the relative correction of the CS due to the κ_{\max} -fitting (the entry in column No. 11).

If the κ_{\max} -fitting has not been performed at a particular value of the endpoint of the range of κ_{\max} due to insufficient variation of the CS in that range, then the value of the relative difference in column No. 11 corresponding to that endpoint is zero (clearly, such cases cannot be used for estimating the mentioned correlation).

It should be noted that in the case when the partial-wave (PW) interpolation is applied at the maximum (optimum) value of κ_{\max} (which will be denoted K), it will also be applied at all smaller (“test”) values of κ_{\max} that are greater than the starting point of the interpolation range (i.e., greater than the value of parameter “k2_breakpoint1”, which is described in Section 4.3). It is possible that some of those values of κ_{\max} are too small for the PW interpolation to be effective, so that the corresponding cross sections may be too inaccurate. In the case of the default values of parameters that specify the conditions for the PW interpolation (parameters No. 1.3.8–10 in Section 4.3), it is recommended to ignore the results corresponding to

$30 < \kappa_{\max} < 80$ when $|\kappa_2|_{\max} \geq 80$ and the photon energy is non-zero, and the results corresponding to $30 < \kappa_{\max} < 120$ when $|\kappa_2|_{\max} \geq 120$ and the photon energy is zero.

Each line of text written to the two files with the results of the angular spline fitting and extrapolation of the partial-wave (PW) DCS (further called the “**spline**” and “**spline_extrap**” files, because their names are formed using the suffix “_spline” or “_spline_extrap” by default, as mentioned in the descriptions of parameters No. 3.15.5–6) begins with a value of the angle (column header “theta”), which is followed by the values of the spline-fitted DCS corresponding to that angle and to all values of κ_{\max} starting with 1. The value of κ_{\max} is indicated in the header of all columns starting from the third one (which corresponds to $\kappa_{\max}=2$). Since those results are obtained by spline-fitting the moving average (MA) of the PW DCS (see Section 1.5.3), the corresponding values of κ_{\max} in the fitting equation (1.5.1) or (1.5.10) are less by 0.5 times the MA average interval reduced by 1. The value of κ_{\max} indicated in the header of column No. 2 is equal to $1 - \text{offset}$, where “offset” is equal to half the reduced MA interval. For example, if the MA interval is 5, then the header of column No. 2 is “kmax=-1”, and if the MA interval is 10, then the header of column No. 2 is “kmax=-3.5”. If this file is subsequently used as input for stage 3, then the program will calculate the mentioned offset from the header of column No. 2.

Each line of text written to the “**DCS_interm0_**” file begins with a value of the angle (column header “**theta**”). The number of remaining entries in each line is greater than the number of “valid” shifts by a factor of 4, i.e., four entries for each fitting interval where the κ_{\max} -fitting was successful. The sequence number of each shift (a negative number or zero) is indicated in parentheses at the end of the header of each column. The descriptions of each of the mentioned four entries are below:

- the value of the κ_{\max} -fitted DCS (the header of this column starts with “**fitted**”),
- the estimate of the absolute uncertainty (“**err**”),
- the relative correction of the original partial-wave DCS due to the initial angular spline fitting and the subsequent κ_{\max} -fitting (“**relCorr**”). This correction may be either relative to the moving average of the original PW DCS, or relative to the spline approximation of it, depending on the sign of parameter No. 3.8.8 (“relCorr_thr”): the moving average of the original PW DCS will be used as the “base” value if relCorr_thr \geq 0, and the spline approximation of the PW DCS will be used if relCorr_thr $<$ 0. Negative values of this relative correction are defined as explained after the description of parameters No. 3.8.37–39,
- the number “0”, “ ± 1 ” or “2” indicating the type of the κ_{\max} -fitting error (“**t**”). “0” indicates that there has been no fitting error in the current shift at the current value of θ . “1” indicates that the κ_{\max} -fitting could not be performed because the dependence of DCS on κ_{\max} at the current angle is not suitable for fitting, i.e., non-monotonous or with a wrong curvature, or out-of-sequence with respect to the one corresponding to the previous value of θ (see also the paragraph after the description of parameter No. 3.4.8). “2” indicates that the fitted value has been rejected (i.e., it is on the wrong side of the range of variation of the PW DCS as a function of κ_{\max} inside the fitting interval, or negative, or exceeds the original value of the PW DCS by a factor greater than 20, or differs from the original value by more than 200 widths of the range of variation of the PW DCS as a function of κ_{\max} inside the fitting interval). In the case of a κ_{\max} -fitting error, the fitted value of the DCS is replaced as explained in the description of parameter No. 3.14.3 (the column “fitted” contains the replacement value). If there has been no error during the κ_{\max} -fitting, but the data point has been excluded for other reasons, then the corresponding entry in this column is equal to -1.

Each line of text written to the “**DCS_interm1_**” file begins with a value of the angle (column header “**theta**”). The number of remaining entries in each line is greater than the number of “valid”

shifts by a factor of 2, i.e., two entries for each fitting interval where the κ_{\max} -fitting was successful. The sequence number of each shift (a negative number or zero) is indicated in parentheses at the end of the header of each column. The descriptions of each of the mentioned two entries are below:

- the value of the κ_{\max} -fitted, spline-fitted and extrapolated DCS (the header of this column starts with “**fitted**”),
- the estimate of the absolute uncertainty after the angular spline fitting and extrapolation of the κ_{\max} -fitted DCS (“**err**”).

After each κ_{\max} -fitting and the angular spline fitting and extrapolation of the κ_{\max} -fitted DCS, the values of the main spline-fitting parameters corresponding to each κ_{\max} -fitting interval (“shift”) where the κ_{\max} -fitting was successful are written to the file “**Data_intern1.txt**”. Each line appended to this file contains the parameters corresponding to one shift, except in the case “spline_combine=2”, when all the entries pertain to the final fitted DCS (in this case, only one line is appended to this file after each run of BREMS). The meanings of all 31 entries in the file “Data_intern1.txt” are explained below.

- (1) the atomic number of the target material (column header “**Z**”),
- (2) the kinetic energy of the incident electron in MeV (“**T1(MeV)**”),
- (3) the energy of the bremsstrahlung photon in MeV (“**Ep(MeV)**”),
- (4) the sequence number of a shift (“**shift**”),
- (5) the value of the starting angle of the angular spline-fitting range (θ_{\min} , using the notations of Section 1.7) for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS (“**spline_theta_min**”),
- (6) the value of the ending angle of the angular spline-fitting range (θ_{\max} , using the notations of Section 1.7) for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS (“**spline_theta_max**”),
- (7) the number of spline knots in the angular spline-fitting range for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS. In the case of the linear or quadratic angular fitting (see the note at the end of Section 1.7.1), this entry is equal to 0 or 1, respectively (although the actual number of knots is 2). The header of this column is “**nKnots**”,
- (8) the final value of the first knot-density parameter (denoted ε_1 in Section 1.7) for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number 0 if the number of knots is equal to 2 (“**splIntRatio_1**”),
- (9) the final value of the second knot-density parameter (denoted ε_2 in Section 1.7) for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS, or the number 0 if the parameter ε_2 has not been used (“**splIntRatio_2**”),
- (10) the minimum width of the inter-knot interval for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS (“**minSplIntWidth**”),
- (11) the maximum width of the inter-knot interval for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS (“**maxSplIntWidth**”),
- (12) the number 0, 1 or 2 identifying the reference function used for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS (“**splRef**”). The meanings of the mentioned numbers are the following:
 - 0 – no division by a reference function (or the reference function equal to 1),
 - 1 – reference DCS No. 1 as defined by parameters No. 3.5.1–20
 - 2 – reference DCS No. 2 as defined by parameters No. 3.5.1–20,
- (13) the number 1, 2 or 3 identifying the spline argument used for the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS (“**splArg**”). The meanings of the mentioned numbers are the following:
 - 1 – spline argument is equal to the angle θ ,
 - 2 – spline argument is equal to $-\cos \theta$,

- 3 – spline argument is equal to $\ln[(1 - \cos \theta) / 2]$,
- (14) the number 1 or 0 indicating if the original function has been replaced by its logarithm or not (respectively) during the spline fitting and extrapolation of the angular dependence of the κ_{\max} -fitted DCS (“**splLog**”),
 - (15) the value of the term δ_{diff} in Eq. (6.8.1a,b) (“**err1_rms**”). This entry is non-zero only in the case “spline_combine=1”, when the number of shifts is greater than 1. Since this term reflects the differences between the different shifts, it cannot be defined for each shift separately, hence the same overall value of δ_{diff} is specified for all shifts,
 - (16) the value of the term δ_{unc} in Eq. (6.8.1a,b) for the current shift (“**err2_rms**”),
 - (17) the value of the term δ_{res} in Eq. (6.8.1a,b) for the current shift (“**err3_rms**”). If a distortion (a minimum or an extra inflection point) has been found in the large-angle extrapolation range (such as illustrated in Fig. 8b), and if the spline-extrapolated angular dependence is greater than the original function in a part of the large-angle extrapolation range, then this entry is output with the minus sign in order to indicate an abnormal extrapolated dependence in the large-angle extrapolation range (the correct extrapolated angular dependence should be below the original one in the entire large-angle extrapolation range, as shown in Fig. 8b),
 - (18) the value of the term δ_{CS} in Eq. (6.8.1a,b) for the current shift, i.e., the absolute value of the relative difference between the κ_{\max} -fitted CS and the angular integral of the fitted DCS corresponding to the current shift, or the number 0 if the fourth coefficient (a_{CS}) of the objective function (6.8.1a,b) is equal to zero (“**err4_rms**”),
 - (19) the value of the term δ_{SF} in Eq. (6.8.1a,b) for the current shift, i.e., the rms value of the relative deviation of the κ_{\max} -fitted shape function (SF) from the reference SF, calculated over the entire angular range $0^\circ \leq \theta \leq 180^\circ$, or the number 0 if the fifth coefficient (a_{SF}) of the objective function (6.8.1a,b) is equal to zero (“**err5_rms**”),
 - (20) the maximum value of the relative deviation of a value of the κ_{\max} -fitted DCS from the average κ_{\max} -fitted DCS (“**err1_max**”). Since this value reflects the differences between the different shifts, it cannot be defined for each shift separately, hence the same overall value is specified for all shifts. In the case of a single shift, or in the case “spline_combine=2”, the corresponding entry is equal to zero,
 - (21) the maximum relative uncertainty of the spline fitting over the entire angular range $0^\circ \leq \theta \leq 180^\circ$ for the current shift (“**err2_max**”),
 - (22) the maximum relative residual of the spline fitting inside the interval $\theta_{\min} \leq \theta \leq \theta_{\max}$ for the current shift (“**err3_max**”),
 - (23) the relative difference between the κ_{\max} -fitted CS and the angular integral of the fitted DCS corresponding to the current shift, or the number 0 if the fourth coefficient (a_{CS}) of the objective function (6.8.1a,b) is equal to zero (“**err4_max**”),
 - (24) the maximum relative deviation of the κ_{\max} -fitted shape function (SF) from the reference SF for the current shift, or the number 0 if the fifth coefficient (a_{SF}) of the objective function (6.8.1a,b) is equal to zero (“**err5_max**”),
 - (25) the square root of the objective function (6.8.1a,b) for the current shift, using the values in the columns No. (15) – (19) (“**err_tot**”),
 - (26) the value of the κ_{\max} -fitted, spline-fitted and extrapolated DCS at $\theta = 0^\circ$ (“**DCS_first**”),
 - (27) the estimate of the relative uncertainty of the κ_{\max} -fitted and spline-fitted DCS at $\theta = 0^\circ$ (“**relErr_first**”),
 - (28) the value of the κ_{\max} -fitted and spline-fitted DCS at $\theta = 180^\circ$ (“**DCS_last**”),
 - (29) the estimate of the relative uncertainty of the κ_{\max} -fitted and spline-fitted DCS at $\theta = 180^\circ$ (“**relErr_last**”).
 - (30) the timestamp of one of the files belonging to the first group of files created in stage 2, which was used as input for stage 3 in the current run. This is the file whose name starts

- with “_CS_” and does not include the suffix “_test” or “_test2” (see Section 5.8). The header of this column is “_CS_timestamp”,
- (31) the timestamp of the file whose name starts with “DCS_fitted_”, which was created during the current run (“DCS_timestamp”).

Each line of text written to the file “mu_range.txt” file contains the following 71 entries:

- (1) the atomic number of the target material (column header “Z”),
- (2) the kinetic energy of the incident electron in MeV (“T1(MeV)”)
- (3) the energy of the bremsstrahlung photon in MeV (“Ep(MeV)”)
- (4) the value of K' in Eq. (1.5.12a) (“K”),
- (5) the value of K'' in Eq. (1.5.12b) (“K”)
- (6) the value of K in Eq. (1.5.12a,b), i.e., maximum κ_{\max} in the analyzed data (“K”),
- (7) the moving average period used for calculation of the normalized differential of the partial-wave DCS as a function of κ_{\max} (the term “normalized differential” is defined at the end of Section 1.5.4). The header of this column is “MA_period”,
- (8) the starting angle (in degrees) of the angular interval where the test for constant value of the scale factor μ in Eq. (1.5.12a) is performed (“start_angle_mu”). This angle may be either specified explicitly using parameter No. 3.6.8 “start_angle_mu”, or optimized using the values of parameters “the_range_mu[1,2]” (No. 3.6.12–13) and “tol_mu[1,2]” (No. 3.6.14–15) as explained in the description of parameters No. 3.6.14–15,
- (9) the ending angle (in degrees) of the angular interval where the test for constant value of the scale factor μ in Eq. (1.5.12a) is performed (“end_angle_mu”). This angle may be either specified by the user explicitly using parameter No. 3.6.9 “end_angle_mu”, or optimized using the values of parameters “the_range_mu[1,2]” (No. 3.6.12–13) and “tol_mu[1,2]” (No. 3.6.14–15) as explained in the description of parameters No. 3.6.14–15,
- (10) the difference of the previous two angles in degrees (“angular_width_mu”),
- (11) the starting angle (in degrees) of the angular interval where the polynomial fitting of the μ -corrected DCS is performed (“fitStart_mu”),
- (12) the minimum ending angle (in degrees) of the angular interval where the polynomial fitting of the μ -corrected DCS is performed (“fitEnd_mu_min”),
- (13) the maximum ending angle (in degrees) of the angular interval where the polynomial fitting of the μ -corrected DCS is performed (“fitEnd_mu_max”),
- (14) the minimum width of the polynomial fitting interval in degrees (“fit_width_mu”),
- (15) the number of values of the endpoint of the polynomial fitting interval (“nTries_mu”),
- (16) the angle of the first irregularity (a minimum or an extra inflection point) in the angular dependence of the PW DCS corresponding to $\kappa_{\max} = K'$ (“infl_angle_K”),
- (17) the angle of the first irregularity (a minimum or an extra inflection point) in the angular dependence of the PW DCS corresponding to $\kappa_{\max} = K$ (“infl_angle_K”),
- (18) the maximum range of variation (i.e., the maximum difference of the maximum and minimum values) of the normalized differential of the PW DCS as a function of κ_{\max} , calculated over all values of κ_{\max} in the interval $K' \leq \kappa_{\max} \leq K$. For each κ_{\max} , the range of variation is calculated over all θ in the interval $\text{start_angle_mu} \leq \theta \leq \text{end_angle_mu}$. The header of this column is “mu_range_normalized”. The sign of this entry indicates the direction of variation of the PW DCS with increasing κ_{\max} (if DCS is a decreasing function of κ_{\max} , then the mentioned range of variation is output with the minus sign),
- (19) the optimal or user-specified value of the scale factor μ in Eq. (1.5.12b), where K'' is defined according to Eq. (1.5.31), and N_{fit} is calculated according to Eq. (1.5.11a). In the case of multiple polynomial fitting intervals (when the entry in the column “nTries” is greater than 1), the average value of μ over all fitting intervals is given. The header of this column is “mu_opt_avg”,

- (20) the standard deviation of the scale factor μ in Eq. (1.5.12b) over all fitting intervals (“**mu_opt_SD**”),
- (21) the sequence number of the reference function used as the divisor when calculating the dependent variable of the angular polynomial fitting of the μ -corrected DCS (see Section 1.5.4) (“**fitRef_mu**”),
- (22) number of 1 or 0 indicating if the logarithm of the μ -corrected DCS was used during the polynomial fitting (“**fitLog_mu**”),
- (23) the (optimal) degree of the polynomial used for the angular polynomial fitting of the μ -corrected DCS (see Section 1.5.4) (“**fitDegree_mu**”),
- (24) the sequence number of the reference function used for the comparison with the μ -corrected DCS or with its polynomial approximation (“**compRef_mu**”). If such comparison has not been requested, then this entry is equal to zero.

The next 45 columns contain the results of comparison of the μ -corrected DCS or of its polynomial approximation with the reference function indicated by the number in column “**compRef_mu**”, as well as the values of the maximum relative difference of the μ -corrected DCS and the PW DCS corresponding to $\kappa_{\max} = K$. The mentioned comparison is performed in various angular intervals. Each of those angular intervals is represented by five entries: the root-mean-square (rms) value of the relative deviation of the μ -corrected DCS or of its polynomial approximation from the reference DCS, the maximum value of the same relative deviation, the maximum relative deviation of the μ -corrected DCS from the PW DCS corresponding to $\kappa_{\max} = K$ (when the mentioned relative deviations are negative, they are replaced by the opposite of the relative deviation of the larger value from the smaller value), the maximum value of the relative standard deviation, calculated over all fitting intervals (i.e., first this standard deviation is calculated for each angle, and then the maximum is found), and the number of points in that angular interval (in the same order):

- (25) – (29) the interval starting at 0° and ending just before “**fitStart_mu**” (when the PW DCS increases with κ_{\max}), or starting just after “**fitEnd_mu**” and ending at 180° (when the PW DCS decreases with κ_{\max}), using the original (unfitted) μ -corrected DCS for the comparison (column headers “**rmsRelDev1**”, “**maxRelDev1**”, “**maxRelCorr1**”, “**maxRelSD1**”, “**n1**”),
- (30) – (34) the interval starting at “**fitStart_mu**” and ending at “**fitEnd_mu**”, using the original (unfitted) μ -corrected DCS for the comparison (column headers “**rmsRelDev2**”, “**maxRelDev2**”, “**maxRelCorr2**”, “**maxRelSD2**”, “**n2**”),
- (35) – (39) the interval starting just after “**fitEnd_mu**” and ending at “**end_angle_mu**” (when the PW DCS increases with κ_{\max}), or starting at “**start_angle_mu**” and ending just before “**fitStart_mu**” (when the PW DCS decreases with κ_{\max}), using the original (unfitted) μ -corrected DCS for the comparison (column headers “**rmsRelDev3**”, “**maxRelDev3**”, “**maxRelCorr3**”, “**maxRelSD3**”, “**n3**”),
- (40) – (44) the interval starting just after “**end_angle_mu**” and ending at 180° (when the PW DCS increases with κ_{\max}), or starting at 0° and ending just before “**start_angle_mu**” (when the PW DCS decreases with κ_{\max}), using the original (unfitted) μ -corrected DCS for the comparison (column headers “**rmsRelDev4**”, “**maxRelDev4**”, “**maxRelCorr4**”, “**maxRelSD4**”, “**n4**”),
- (45) – (49) the interval starting at 0° and ending just before “**fitStart_mu**” (when the PW DCS increases with κ_{\max}), or starting just after “**fitEnd_mu**” and ending at 180° (when the PW DCS decreases with κ_{\max}), using the polynomial approximation of the μ -corrected DCS for the comparison (column headers “**rmsRelDevFit1**”, “**maxRelDevFit1**”, “**maxRelCorrFit1**”, “**maxRelSDfit1**”, “**nFit1**”),
- (50) – (54) the interval starting at “**fitStart_mu**” and ending at “**fitEnd_mu**”, using the polynomial approximation of the μ -corrected DCS for the comparison (column headers

- “**rmsRelDevFit2**”, “**maxRelDevFit2**”, “**maxRelCorrFit2**”, “**maxRelSDfit2**”, “**nFit2**”),
- (55) – (59) the interval starting just after “fitEnd_mu” and ending at 180° (when the PW DCS increases with κ_{\max}), or starting at 0° and ending just before “fitStart_mu” (when the PW DCS decreases with κ_{\max}), using the polynomial approximation of the μ -corrected DCS for the comparison (column headers “**rmsRelDevFit3**”, “**maxRelDevFit3**”, “**maxRelCorrFit3**”, “**maxRelSDfit3**”, “**nFit3**”),
- (60) – (64) the interval starting at 0° and ending at “end_angle_mu” (when the PW DCS increases with κ_{\max}), or starting at “start_angle_mu” and ending at 180° (when the PW DCS decreases with κ_{\max}), using a “combined” function equal to the original (unfitted) μ -corrected DCS at angles $\theta \geq \text{fitStart_mu}$ (when the PW DCS increases with κ_{\max}) or at $\theta \leq \text{fitEnd_mu}$ (when the PW DCS decreases with κ_{\max}), and equal to the polynomial approximation of the μ -corrected DCS elsewhere (column headers “**rmsRelDevComb1**”, “**maxRelDevComb1**”, “**maxRelCorrComb1**”, “**maxRelSDcomb1**”, “**nComb1**”),
- (65) – (69) the interval starting at 0° and ending at “end_angle_mu” (when the PW DCS increases with κ_{\max}), or starting at “start_angle_mu” and ending at 180° (when the PW DCS decreases with κ_{\max}), using a “combined” function equal to the original (unfitted) μ -corrected DCS at angles $\theta \geq \text{fitEnd_mu}$ (when the PW DCS increases with κ_{\max}) or at $\theta \leq \text{fitStart_mu}$ (when the PW DCS decreases with κ_{\max}), and equal to the polynomial approximation of the μ -corrected DCS elsewhere (column headers “**rmsRelDevComb2**”, “**maxRelDevComb2**”, “**maxRelCorrComb2**”, “**maxRelSDcomb2**”, “**nComb2**”),
- (70) the timestamp of one of the files belonging to the first group of files created in stage 2, which was used as input for stage 3 in the current run. This is the file whose name starts with “_CS_” and does not include the suffix “_test” or “_test2” (see Section 5.8). The header of this column is “**_CS_timestamp**”,
- (71) the timestamp of the file whose name starts with “DCS_fitted_”, which was created during the current run (“**DCS_timestamp**”).

In the file “mu_range.txt”, a failure of μ -fitting is indicated by zero or negative entries in columns where the values should normally be positive (for example, “start_angle_mu”, “end_angle_mu”, “mu_opt_avg”, “rmsRelDev<...>”).

Each line of text written to the file “mu.txt” file contains 71 entries, whose meanings and column headers are identical to those in the file “mu_range.txt”, with one exception: column No. 18 (“mu_range_normalized”) of the file “mu_range.txt” is replaced in the file “mu.txt” with column “**maxDev_mu**”, which has the meaning of the maximum absolute deviation of the empirical scale ratio $\mu = (\text{DCS}(\kappa_{\max \rightarrow \infty}, \theta) - \text{DCS}(K', \theta)) / (\text{DCS}(K, \theta) - \text{DCS}(K', \theta))$ from 1, calculated inside the angular interval where the absolute value of the relative correction of the DCS due to the κ_{\max} -fitting is between the values specified using parameters No. 3.6.2 (“maxCorr_mu”) and No. 3.6.3 (“thrCorr_mu”). If no such angular interval exists, or if it is too narrow (as defined by parameters No. 3.6.5 “minWidth_mu” and No. 3.6.6 “minPoints_mu”), or if parameter No. 3.6.1 (“mode_mu”) is equal to 1, then the entry in this column is equal to 0.

Each line of text written to the “DCS_mu_” file contains the following fourteen entries:

- (1) the value of θ (column header “**theta**”),
- (2) the value of the μ -corrected DCS (1.5.12b) corresponding to the optimal value of μ , averaged over multiple angular intervals used for the polynomial fitting (“**DCS_mu**”),

- (3) the standard deviation of the μ -corrected DCS (1.5.12b) over multiple angular intervals used for the polynomial fitting (“DCS_mu_SD”),
- (4) the value of the polynomial approximation of the μ -corrected DCS, averaged over multiple polynomial fitting intervals (“DCS_mu_polynomial”),
- (5) the standard deviation of the polynomial approximation of the μ -corrected DCS over multiple angular intervals used for the polynomial fitting (“DCS_mu_polyn_SD”),
- (6) the value of the “type 1 combined” DCS, which is equal to the original (unfitted) μ -corrected DCS at angles $\theta \geq \text{fitStart_mu}$ (when the PW DCS increases with κ_{max}) or at $\theta \leq \text{fitEnd_mu_min}$ (when the PW DCS decreases with κ_{max}), where “fitEnd_mu_min” is the minimum ending angle of the angular interval where the polynomial fitting of the μ -corrected DCS is performed, and equal to the polynomial approximation of the μ -corrected DCS elsewhere (“DCS_mu_combined1”),
- (7) the standard deviation of the “type 1 combined” DCS over multiple angular intervals used for the polynomial fitting (“DCS_mu_comb1_SD”),
- (8) the value of the “type 2 combined” DCS, which is equal to the original (unfitted) μ -corrected DCS at angles $\theta \geq \text{fitEnd_mu}$ (when the PW DCS increases with κ_{max}) or at $\theta \leq \text{fitStart_mu}$ (when the PW DCS decreases with κ_{max}), and equal to the polynomial approximation of the μ -corrected DCS elsewhere (“DCS_mu_combined2”),
- (9) the standard deviation of the “type 2 combined” DCS over multiple angular intervals used for the polynomial fitting (“DCS_mu_comb2_SD”),
- (10) the value of reference function No. 1, or zero if reference function No. 1 is not used (“DCS_ref1”),
- (11) the value of reference function No. 2, or zero if reference function No. 2 is not used (“DCS_ref2”),
- (12) – (14) the values of the partial-wave DCS corresponding to $\kappa_{\text{max}} = K'$ (using the notations of Eq. (1.5.12a)), $\kappa_{\text{max}} = K''$ (using the notations of Eq. (1.5.12b)), and to the maximum value of κ_{max} in the analyzed data ($\kappa_{\text{max}} = K$, using the notations of Eq. (1.5.12a,b)). The column headers are “PW_DCS(K)”, “PW_DCS(K'”) and “PW_DCS(K)”, respectively.

At the start of the calculation, Brems_fit displays the original value of the scaled CS (1.1.5) corresponding to the last (greatest) value of κ_{max} (i.e., to $\kappa_{\text{max}} = K$). After performing the initial κ_{max} -fitting, the program displays the final value of the “tol_range” variable mentioned in the descriptions of parameters No. 3.4.7–8, the values of θ corresponding to the change of the “sign” from 1 to 0 and from 0 to -1 (“theta_limits”; see also the descriptions of columns No. 36–39 in the file “CS_parms.txt” described above), the κ_{max} -fitted value of the scaled CS, and the relative difference between the fitted CS and the unfitted CS. In addition, if the error test mentioned in the description of parameter No. 3.2.12 has been performed, then some of the information pertaining to each of the tested values of the endpoint of the κ_{max} -fitting range is displayed, too.

7. Calculating the DCS and CS according to the Born and Sommerfeld-Maue approximations

One of the special modes of operation of BREMS is calculation of the angular dependence of the DCS and of the corresponding CS (the angular integral of the DCS with respect to the solid angle of photon emission) using one of the analytical approximations described in Sections 1.1.2 and 1.1.3. This mode is activated only in the case “firstStage=1”, when parameter “appr” is equal to 0, -1 or -2 . If the user does not specify the value of “appr” explicitly, then this mode is used by default if the atomic number (parameter “Z”) is sufficiently small ($Z \leq 2$, controlled by parameter “Z_max_Born”) and the final kinetic energy of the electron (parameter “T2”, or the difference of “T1” and “Ep”) is sufficiently large ($T_2 \geq 0.5$ MeV, controlled by parameter “T2_min_Born”). Below are the descriptions of the parameters used in this special mode of operation.

7.1. Physical parameters and parameters defining the point-nucleus screening function

4.1.1–7. The names, meanings and default values of parameters No. 4.1.1–7 are the same as the names, meanings and default values of parameters No. 1.1.1–7. The only exception is the default value of parameter No. 4.1.5 (“IV”): it is equal to 2 in this case. In this special mode, parameter “IV” is not allowed to be equal to 3. If the user specifies “IV=3”, then the program will reset it to 2 with a warning message.

4.1.8. “Z_V” is the same as parameter No. 1.1.9.

4.1.9. “Zi” is the same as parameter No. 1.1.10, i.e., it is used to specify the ion charge.

4.1.10. “appr” is used as a “switch”, whose negative or zero value indicates that one of the analytical approximations must be used, and specifies the type of the approximation to be applied. The presence or absence of screening is indicated independently by the value of parameter “IV” (2 or 1, respectively). In order to use one of the approximations described in Sections 1.1.2 and 1.1.3, parameter “appr” must be equal to 0, –1 or –2:

“appr=0” indicates that the Born approximation with or without screening must be used. In this case, the DCS is calculated either by evaluating the exact analytical expression (1.1.36) or (1.1.32) (if parameter “nd_DCS” is non-zero), or by the double angular numerical integration of the corresponding TDCS (1.1.28) according to Eq. (1.1.31a) (if parameter “nd_DCS” is zero), and the CS is calculated by numerical integration of the DCS (the single integral with respect to θ_1 in Eq. (1.1.31b)) or of the TDCS (the triple integral in Eq. (1.1.31b)),

“appr=-1” indicates that the leading-order (LO) Sommerfeld-Maue (SM) approximation with or without screening correction must be used. In this case, the DCS is calculated by numerical angular integration of the analytical expression of the TDCS (1.1.40) according to Eq. (1.1.31a), and the CS is calculated by numerical integration of the DCS or of the TDCS (the single or triple angular integral in Eq. (1.1.31b)). The screening correction is calculated using the Born approximation, as an additive term in the analytical expression of the DCS (see Eq. (1.1.46)),

“appr=-2” indicates that the next-to-leading-order (NLO) Sommerfeld-Maue (SM) approximation with or without screening correction must be used. This case differs from the case “appr=-1” only by the additional term (1.1.44) in the analytical expression of the TDCS.

If parameter “appr” is not specified by the user explicitly, then its default value is determined by comparing the values of Z and T_2 with the corresponding threshold values “Z_max_Born” and “T2_min_Born” (parameters No. 5–6 of the main program, described in Section 2). If $Z \leq Z_{\text{max_Born}}$ and $T_2 \geq T2_{\text{min_Born}}$ (MeV), then $\text{appr}=0$ by default. If $Z > Z_{\text{max_Born}}$ or $T_2 < T2_{\text{min_Born}}$ (MeV), then the default value of “appr” depends on the value of parameter “IV”: if $IV=1$, then $\text{appr}=1$; if $IV=2$, then $\text{appr}=2$; if $IV=3$, then appr is not used (see also the description of parameter No. 1.1.8 in Section 4.1).

4.1.11–24. The names, meanings and default values of parameters No. 4.1.11–24 are the same as the names, meanings and default values of parameters No. 1.1.11–24.

4.1.25. The name, meaning and default value of parameter No. 4.1.25 is the same as the name, meaning and default value of parameter No. 1.1.29.

7.2. Parameters defining the finite-nucleus correction of the screening function

4.2.1–6. The names, meanings and default values of parameters No. 4.2.1–6 are the same as the names, meanings and default values of parameters No. 1.2.1–6.

7.3. Parameters controlling the accuracy and the choice of the calculation method

- 4.3.1. “**relErr_tol**” (alias “rel_err_tol”) is the maximum relative error of the numerical integration when calculating the DCS or SDCS as the double or triple angular integral of the TDCS (1.1.31a) or (1.1.31b) using the method of adaptive multidimensional quadrature. The default value of this parameter is equal to 10^{-5} .
- 4.3.2. “**T1_scrCorr_mode_thr**” is the value of T_1 (in MeV) corresponding to the transition between two methods of calculating the screening correction of the Sommerfeld-Maue DDCS or SDCS. The screening correction of the DDCS is defined as the value of the expression in brackets in Eq. (1.1.46), i.e., as the difference of the screened and unscreened Born-approximation DDCS. However, it can also be calculated as the double angular integral of the difference of the screened and unscreened Born TDCS. Although both methods are mathematically equivalent, the former method (the “first” one) is typically more efficient at low energies (when $T_1 < 10$ keV), whereas the latter method (the “second” one) is typically more accurate at higher energies. If $T_1 < T1_scrCorr_mode_thr$, then the first method will be used, and if $T_1 \geq T1_scrCorr_mode_thr$, then the second method will be used. The default value of parameter “**T1_scrCorr_mode_thr**” is equal to 10^{-2} . I.e., the first method is applied by default only when $T_1 < 10$ keV.
- 4.3.3. “**nd_DCS**” (alias “nd”) is the approximate number of significant digits to be used in the case of the screened Born approximation (“appr=0 IV=2”) when calculating the approximate DCS according to its analytical expression (1.1.36). In the case of the unscreened Born approximation (“appr=0 IV=1”), a non-zero value of this parameter indicates that the approximate DCS must be calculated using its analytical expression (1.1.32) (this expression is always evaluated at double precision, regardless of the value of parameter “nd_DCS”). A zero value of this parameter indicates that the DCS corresponding to the Born approximation must be calculated by numerical integration of the analytical TDCS (1.1.28) according to Eq. (1.1.31a). In the case of the Sommerfeld-Maue approximation (appr<0), this parameter is not used. The default value of this parameter is equal to 200.
- 4.3.4. “**nd_F**” (alias “nd”) is the approximate number of significant digits to be used when calculating the atomic form factor (1.1.35), which is needed when screening of the nuclear charge by the electron cloud is taken into account and the DCS is calculated by numerical integration of one of the analytical expressions of the TDCS presented in Sections 1.1.2 and 1.1.3 according to Eq. (1.1.31a). The default value of this parameter is equal to 30 (this value corresponds to quadruple precision).
- 4.3.5. “**nd_HG**” (alias “nd”) is the approximate minimum number of significant digits to be used when calculating the hypergeometric function, which is used in Eqs. (1.1.42i) and (1.1.42j), in the case of the Sommerfeld-Maue approximation. In the case of the Born approximation (appr=0), this parameter is not used. The option “nd_HG=15” corresponds to double precision (the lowest possible precision level), the values from 16 to 30 correspond to quadruple precision, which is the second lowest possible precision level (these 15 values are equivalent), and the values greater than 30 correspond to multiple precision. The default value of this parameter is equal to 15.

Note: After assigning a value less than 15 to any one of parameters “nd_DCS”, “nd_F” or “nd_HG”, it will be reset to the default value.

- 4.3.6–8. “**nTries_max_HG**”, “**tol_change_HG**”, and “**err_test_int_HG**” are the maximum number of consecutive precision levels to be tried when calculating the hypergeometric (HG) function (used in Eqs. (1.1.42i) and (1.1.42j)), the maximum allowed relative change of the HG function corresponding to two consecutive precision levels, and the period of the error checking, respectively (these parameters are used only in the case of the SM approximation, i.e., when appr<0). The initial precision level is specified by the value of parameter “nd_HG” (see the description of parameter No. 4.3.5). If nTries_max_HG > 1 and

$\text{tol_change_HG} > 0$, then a sequence of up to nTries_max_HG or $\text{nTries_max_HG}-1$ consecutive precision levels will be tried during each calculation of the HG function until the relative difference of the estimates of the HG function corresponding to the last two precision levels becomes less than tol_change_HG . The maximum number of precision levels (i.e., nTries_max_HG) will be used every $|\text{err_test_int_HG}|$ evaluations of the HG function (starting from evaluation No. 1), and if the relative difference of the estimates of the HG function corresponding to the last two precision levels (No. $\text{nTries_max_HG}-1$ and No. nTries_max_HG) is greater than tol_change_HG , then the program will either terminate the calculation of the DDCS or SDCS with an error message (when $\text{err_test_in_HG} > 0$) or display a warning message (when $\text{err_test_in_HG} < 0$). During the other evaluations (whose sequence numbers are not equal to $1 + n * |\text{err_test_int_HG}|$, where n is an integer number), up to $\text{nTries_max_HG}-1$ consecutive precision levels will be tried, and if the relative difference of the estimates of the HG series corresponding to the last two precision levels is greater than tol_change_HG , then the estimate of the HG series corresponding to the last precision level (No. $\text{nTries_max_HG}-1$) will be used, without any additional actions or messages. Each multiple-precision level differs from the previous precision level by 16 to 25 additional significant digits. For example, if $\text{nd_HG}=15$, then the third precision level to be tried corresponds to 43–50 significant digits, and the fourth precision level corresponds to 65–75 significant digits. If $\text{nTries_max_HG} = 1$ or $\text{tol_change_HG} = 0$, then no error checking is performed, and the values of these three parameters are not used. The default values of parameters “ nTries_max_HG ”, “ tol_change_HG ”, and “ err_test_int_HG ” are 4, 10^{-9} , and 11, respectively.

- 4.3.9. “**x_HG_transform_thr**” is the threshold value of the argument x (defined by Eq. (1.1.42k)) of the hypergeometric (HG) function used in Eq. (1.1.42i) and Eq. (1.1.42j), which must be exceeded in order to apply the transformation formula (1.1.43). The default value of this parameter is equal to 0.7.

Note: The mentioned transformation formula is not applied if the absolute value of the resulting estimate of the HG function is less than the absolute value of each of the two terms on the right-hand side of the transformation formula by a factor greater than 10^8 . This condition eliminates the cancellation errors, which could have a significant influence on the values of the Sommerfeld-Maue DDCS and on the duration of angular integration of the Sommerfeld-Maue TDCS, especially at low energies.

- 4.3.10–11. “**adapt_theta_min1**” and “**adapt_theta_min2**” (aliases “**adapt_theta_min**” and “**theta0**” for both) are the two values of the lower bound of the integral with respect to the photon emission angle θ when calculating the CS by adaptive numerical integration of the analytical expression of the DCS or TDCS according to Eq. (1.1.31b) (where the angle θ is denoted θ_1) in the case of the Born approximation ($\text{appr}=0$) or the SM approximation ($\text{appr}<0$), respectively. Although the value of this integration bound should be theoretically equal to 0 (as in Eq. (1.1.31b)), it may be necessary to set this bound to a small positive value in order to avoid numerical difficulties when using the SM approximation ($\text{appr}<0$). If this parameter is set equal to a negative number, then the CS will not be calculated by adaptive quadrature. Instead, it will be calculated by integration of the tabular DCS data using the 10th order Newton-Cotes formula. The default values of parameters “**adapt_theta_min1**” and “**adapt_theta_min2**” are equal to 0 and -1 , respectively (i.e., the method of adaptive multidimensional quadrature will be applied for calculation of the integrals in Eq. (1.1.31b) only in the case of the Born approximation).

- 4.3.12–13. “**Elwert1**” and “**Elwert2**” (alias “**Elwert**” for both) are the two “switches” (1 or 0) indicating whether the DCS calculated according to the Born approximation must be modified by the Elwert factor (1.1.47) in the case $\text{appr}=0$ and $\text{appr}<0$, respectively (in the latter case, this factor can be applied only to the additive screening correction, which is equal to the expression in brackets in Eq. (1.1.46)). The default value of those two

parameters is equal to 1 (i.e., the Elwert factor is applied, except in the case “appr=-1 IV=1” or “appr=-2 IV=1”, when this factor is not applicable).

7.4. Parameters defining the set of angles

4.4.1–5. The names, meanings and default values of parameters No. 4.4.1–5 are the same as the names, meanings and default values of parameters No. 2.3.1–5 of Bremsstrahlung (see Section 5.3), i.e., they specify the limits of variation of the photon emission angle θ and the number of values of θ .

7.5. Parameters defining the cutoff radius of the interaction potential

The “cutoff radius” of the interaction potential is the value of the radial coordinate $r = R_a$ such that $V(r) \equiv 0$ when $r > R_a$. The expression of the atomic form factor (AFF) (1.1.35) corresponds to the exact (non-truncated) interaction potential (the corresponding screening function is defined by Eqs. (1.1.34a,b)). When the DCS is calculated using one of the analytical approximations described in Sections 1.1.2 and 1.1.3, truncation of the interaction potential is not recommended, because it is unphysical and because it complicates the numerical integration of TDCS according to Eqs. (1.1.31a,b) (due to the highly oscillatory character of the resulting AFF as a function of the momentum transfer q). However, such truncation may be necessary in special cases, e.g., in order to evaluate its effect on the results of partial-wave calculations, where truncation of the interaction potential is necessary for improving the performance (see Section 1.3.5). Consequently, BREMS includes an option to use a truncated interaction potential when calculating the approximate DCS according to one of the analytical approximations described in Sections 1.1.2 and 1.1.3. Truncation of the interaction potential affects only the calculation of the AFF, causing the following two changes in the expression of the AFF (1.1.30a):

- 1) the upper bound of the integral in Eq. (1.1.30a) is replaced by R_a ,
- 2) an additional term appears in the expression of the AFF. In the case of a screened potential (“IV=2”), this term is equal to $(Z'/Z) (\sin qR_a) / (qR_a)$, where Z' is the average number of electrons in the radial range $r > R_a$. In the case of a pure Coulomb potential (“IV=1”), the mentioned additional term (and the total AFF) is equal to $(\sin qR_a) / (qR_a)$.

The two parameters defining the cutoff radius R_a are described below:

- 4.5.1. “R_atom” is used to specify the cutoff radius (R_a) defined above (the name and meaning of this parameter are the same as the name and meaning of parameter No. 1.5.4). Two methods of specifying R_a are possible, depending on the sign of this parameter. When R_atom>0, it is interpreted as the value of R_a in relativistic units. When R_atom<0, it is interpreted as the opposite of the factor that must be used for multiplying the inverse minimum momentum transfer ($1 / q_{\min}$) in order to calculate the value of R_a (see also Section 1.3.5). In this case, the final value of R_a will not be allowed to become less than $\max(800, 126/p_2)$ (when $T_1 \leq 3$ MeV) or less than $\max(1200, 126/p_2)$ (when $T_1 > 3$ MeV), and it may be increased additionally, depending on the value of parameter “pr_transition2” (No. 4.5.2). When R_atom=0 (the default), the interaction potential is not truncated.
- 4.5.2. “pr_transition2” is used only when R_atom<0, in order to specify the minimum allowed value of R_a , which is further denoted $R_{a,\min}$ (the name and meaning of this parameter are the same as the name and meaning of parameter No. 1.5.3). Two methods of specifying $R_{a,\min}$ are possible, depending on the sign of this parameter. When pr_transition2<0, it is interpreted as the opposite of the value of $R_{a,\min}$ in relativistic units. When pr_transition2>0, it is interpreted as the product $p_2 R_{a,\min}$, where p_2 is the modulus of the momentum of the outgoing electron (also in relativistic units). If R_atom<0 and the value of $R_{a,\min}$ specified by this parameter is greater than the value of R_a specified by parameter R_atom, then R_a will be set equal to $R_{a,\min}$. When pr_transition2=0 (the default), this parameter is not used.

7.6. Parameters defining the names of output files, and the conditions for overwriting

- 4.6.1–2. “prefix” and “suffix” are, respectively, the character strings that must be inserted at the beginning and at the end of the name of the output files with the DCS and shape function data. They are used similarly to the parameters No. 1.9.1–2 described in Section 4.9. The file name prefix may include the folder name (folder names must be terminated with the slash ‘/’). If parameter No. 4.6.1 is the empty string (specified by writing a space after “prefix=”) then no prefix will be used, and the mentioned output files will be created in the current folder. If parameter No. 4.6.2 is the empty string, then no suffix will be used. In order to specify an arbitrary name, parameter No. 4.6.1 must be the period ‘.’, and parameter No. 4.6.2 must be the “root” of the output file name (without the additional output prefix, which is denoted “prefix2” in Section 7.8, and without the file name extension, which is always “.txt”). If the specified file name includes the folder name, then the additional output prefixes (for example, “DCS_Born_” and “ShapeFn_Born_”) will be added to the folder name (the corresponding folders must exist), otherwise all output files will be placed in the current folder. If parameter No. 4.6.1 is not the period ‘.’, then the default name (with the specified prefix and suffix) will be used (the default format of the output file names is described in Section 7.8). The default value of parameters “prefix” and “suffix” is equal to the empty string.
- 4.6.3. “overwrite” has the same name and meaning as parameter No. 4 of the main program (see Section 2), i.e., it is a “switch” (1 or 0), indicating whether the existing files with the DCS and shape function data must be overwritten or not. The default value of this parameter is equal to 1.

7.7. Other parameters

- 4.7.1. “checkTabPos” is a “switch” (1 or 0) indicating if the format of file “CS_Born_SM.txt”, which is described in Section 7.8, must be checked for consistency. If this parameter is equal to 1, then the program will compare tab positions and length of the first and last lines of the file (this check is performed after appending the line with the results of the current run). If a discrepancy is found, then a warning will be displayed (however, execution of the program will not be stopped). If this parameter is equal to 0, then the mentioned check will not be performed. The default value of this parameter is equal to 1.

Note: Parameter “checkTabPos” is also used in stage 2 (by subroutine “Bremsstrahlung”) for checking the files “CS.txt” and “CS_2.txt”, and in stage 3 (by subroutine “Brems_fit”) for checking the file “CS_fitted.txt”. In the case “checkTabPos=1”, a similar check of input files is also performed when generating the grid data for the cubic-spline fitting and interpolation of the logarithm of the scaled SDCS with respect to the logarithm of the incident electron energy (see Section 9). However, in the latter case, *all* lines are checked, and a change of tab positions is treated as a terminal error (i.e., the program then exits with an error message).

7.8. Output data of subroutine “Born_SM_appr”

In the case “appr≤0”, BREMS creates or updates three files: the file “CS_Born_SM.txt” with the values of the CS, physical parameters and control parameters, and two files whose names start with “DCS_” and “ShapeFn_”, respectively, containing the values of the DCS and the shape function for all angles. All these files contain two or more columns of numbers with fixed width and with a header above each column. The values of the CS and DCS in the output data are equal to the single- or double differential cross sections multiplied by k/Z^2 (the units are mb and mb/sr, respectively). Below are the detailed descriptions of the format of these files.

Every calculation of the approximate DCS and CS ends by appending a line of text to the file “CS_Born_SM.txt”. The entries in each line of this file have the following meaning:

- (1) the atomic number of the target material (column header “**Z**”),
- (2) the kinetic energy of the incident electron in MeV (“**T1(MeV)**”),
- (3) the energy of the bremsstrahlung photon in MeV (“**Ep(MeV)**”),
- (4) the cutoff radius of the interaction potential in relativistic units, or the number 0 if the interaction potential has not been truncated (“**R_atom**”),
- (5) the number “1” or “2” indicating the type of the interaction potential – pure Coulomb or screened, respectively (“**IV**”),
- (6) the ion charge, in units of the elementary charge (“**Zi**”),
- (7) the type of the nuclear charge distribution, which is specified by parameter No. 4.2.1 (“**nuclear_model**”),
- (8) the mean nuclear radius in fm (“**Rn(fm)**”),
- (9) the number “0”, “-1” or “-2” indicating the type of the approximation used, i.e., the value of parameter No. 4.1.10 (“**appr**”),
- (10) the number of values of angle θ (“**nPoints**”),
- (11) the maximum relative difference between the values of the hypergeometric function in Eqs. (1.1.42i) and (1.1.42j) corresponding to the two highest precision levels in all cases when it was possible to determine if precision level No. nTries_max_HG–1 was sufficient to achieve the relative accuracy specified by parameter “tol_change_HG” (see also the description of parameters No. 4.3.6–8). If the hypergeometric function has not been used (Born approximation), or if the precision level has not been varied, then this number is equal to 0. The header of this column is “**relChangeHG_max**”,
- (12) the approximate number of significant digits used when calculating the atomic form factor (1.1.35), or a negative number opposite to the approximate number of significant digits used when calculating the analytical expression of the DDCS (1.1.36) or (1.1.32) (the header of this column is “**nDig_F**”). Double precision is always indicated by “±15”, and quadruple precision is always indicated by “±30”. If the DCS has been calculated for the case of a pure Coulomb potential (“IV=1”) by numerical integration of the TDCS according to Eq. (1.1.31a), then this number is equal to 0,
- (13) the approximate initial number of significant digits used when calculating the hypergeometric function in Eqs. (1.1.42i) and (1.1.42j), or the number “0” if the hypergeometric function has not been calculated (“**nDig_HG**”). Double precision is always indicated by “15”, and quadruple precision is always indicated by “30”,
- (14) the estimate of the maximum relative error of the DCS (over all angles) calculated by adaptive numerical integration of the TDCS according to Eq. (1.1.31a), or the number 0 if the DCS was calculated by evaluating the analytical expression (1.1.36) or (1.1.32). The header of this column is “**relErr_DCS_max**”,
- (15) the total number of evaluations of the integrand function (TDCS) during the adaptive numerical integration of the TDCS according to Eq. (1.1.31a), summed over all angles (“**nEval_DCS**”),
- (16) the integral of the tabular DCS data, using the 10th-order Newton-Cotes formula (“**DCS_integral**”),
- (17) the value of the CS obtained by single adaptive integration of the DCS or triple adaptive integration of the TDCS according to Eq. (1.1.31b), or the same number as in the previous column if the method of adaptive multidimensional quadrature was not applied for calculation of the CS (“**CS**”),
- (18) the relative difference of the previous two values (“**DCS_int/CS-1**”),
- (19) the estimate of the relative error of the CS calculated by single adaptive integration of the DCS or triple adaptive integration of the TDCS according to Eq. (1.1.31b), or the number 0 if the method of adaptive multidimensional quadrature was not applied for calculation of the CS (“**relErr_CS**”),
- (20) the number of evaluations of the integrand function (DCS or TDCS) when calculating the CS by single adaptive integration of the DCS or triple adaptive integration of the TDCS

- according to Eq. (1.1.31b), or the number 0 if the method of adaptive multidimensional quadrature was not applied for calculation of the CS (“**nEval_CS**”),
- (21) the value of the product $Z\alpha$, where Z is the atomic number, and α is the fine-structure constant (“**Z_alpha**”),
 - (22) the value of the expression $Z\alpha / \beta_1$, where β_1 is the ratio of the initial speed of the electron and the speed of light (“**Z_alpha_beta1**”),
 - (23) the value of the expression $Z\alpha / \beta_2$, where β_2 is the ratio of the final speed of the electron and the speed of light (“**Z_alpha_beta2**”),
 - (24) the value of the Elwert factor (1.1.47), or the number 1 if the application of the Elwert factor has been “switched off” by the user, i.e., if parameter No. 4.3.12 or No. 4.3.13 (“Elwert1” or “Elwert2”, respectively) has been set to 0 (the header of this column is “**Born_DCS_factor**”),
 - (25) the processing time in seconds (“**time(s)**”).
 - (26) the version number of the program used for the calculations (“**BREMS_ver**”). The version number is written as an integer number obtained by concatenating all four components of the version number, with the last three components having two digits each (the first of these two digits may be zero). For example, BREMS v1.5.7.0 would be indicated by “1050700”,
 - (27) the timestamp (i.e., last modification time) of the executable file used for the calculations (“**exe_timestamp**”). The timestamp is written as a 14-digit integer number, whose first eight digits indicate the date using the format YYYYMMDD, and the last six digits indicate the time using the format HHMMSS. For example, the timestamp “20230527132051” indicates the time 13:20:51 on May 27, 2023,
 - (28) the timestamp of the DCS data file created in the current run (“**DCS_timestamp**”).
- The last seven entries are present only in the case of a screened interaction potential (“IV=2”):
- (29) The number of exponential terms in the analytical expression of the point-nucleus screening function (1.1.34a) (“**nexp**”),
 - (30) the first preexponential factor (a_1) in Eq. (1.1.34a) (“**factor1**”),
 - (31) the first exponent (b_1) in Eq. (1.1.34a) (“**exp1**”),
 - (32) the second preexponential factor (a_2) in Eq. (1.1.34a) (“**factor2**”),
 - (33) the second exponent (b_2) in Eq. (1.1.34a) (“**exp2**”),
 - (34) the third preexponential factor (a_3) in Eq. (1.1.34a) (“**factor3**”),
 - (35) the third exponent (b_3) in Eq. (1.1.34a) (“**exp3**”).

In addition to updating the file “CS_Born_SM.txt”, the subroutine “Born_SM_appr” creates two files with the values of the DCS and the shape function for all angles. The default names of those two files have the following format:

⟨prefix⟩⟨prefix2⟩Z_T.TE±XX_k.kkkE±YY⟨suffix⟩.txt,

where “Z” is the atomic number consisting of 1, 2 or 3 digits, “T.TE±XX” is the kinetic energy of the incident electron (MeV) rounded to 2 significant digits in scientific notation, “k.kkkE±YY” is the energy of the bremsstrahlung photon (MeV) rounded to 4 significant digits in scientific notation (“E±XX” and “E±YY” are the respective decimal exponents), “prefix” and “suffix” are defined by parameters No. 4.6.1–2, and “prefix2” is an additional output prefix consisting of three components, which are concatenated with each other:

- “**DCS**” or “**ShapeFn**” for the DCS and shape function data, respectively,
- “_Born_”, “_SM_LO_” or “_SM_NLO_” indicating the approximation used (Born, leading-order Sommerfeld-Maue, or next-to-leading order Sommerfeld-Maue, respectively),
- “screened_”, which is included only when screening of the nuclear charge by the electron cloud is taken into account.

The “DCS_” file has four or two columns, depending on whether the DCS has been calculated by double adaptive integration of the TDCS according to Eq. (1.1.31a), or by evaluation of the analytical expression (1.1.36) or (1.1.32). The “ShapeFn_” file always has two columns. The first

column (“**theta**”) in both of these files contains the values of the angle in degrees, and the second column contains the corresponding values of the DCS or the shape function (which is equal to the ratio DCS/CS). The header of the second column is the same as “prefix2” in the above description of the corresponding file name format (without the trailing underscore). The third and fourth columns in the “DCS_” file are present only when the DCS has been calculated by double adaptive integration of the TDCS according to Eq. (1.1.31a). The third column (“**relErr**”) contains the estimates of the relative error of the DCS for each angle, and the fourth column (“**nEval**”) contains the corresponding numbers of evaluations of the integrand function (TDCS).

8. Fitting an arbitrary point-nucleus screening function by a superposition of exponentials

Another special mode of operation of BREMS is fitting of an arbitrary tabular point-nucleus screening function by a linear combination of exponentials (1.1.34a) by the method described in Section 1.9. Below are the descriptions of the corresponding parameters of BREMS. In those descriptions, the term “screening function” and notation $\tilde{V}(r)$ always indicate the normalized *variable* part of the *point-nucleus* screening function (it is denoted $\tilde{V}_p(r)$ in Eqs. (1.2.4a–c)). In the case of an ion, the constant term (denoted i in Eq. (1.2.4b)) is not represented in the output data.

8.1. Parameters defining the tabular screening function data

- 5.1.1. “Z” is the atomic number of the target material with the minus sign (this parameter has the same name and meaning as parameter No. 1.1.1, but its value is opposite to the latter). The minus sign indicates that the program must enter the special mode of operation described in this section. The program will subsequently load the tabular interaction data from the text file corresponding to the absolute value of this parameter, or from the file specified by parameter No. 5.1.3 (“fn_V”).
- 5.1.2. “dirV” is the same as parameter No. 1.1.6.
- 5.1.3. “fn_V” is the same as parameter No. 1.1.7.
- 5.1.4. “Z_V” is the same as parameter No. 1.1.9.
- 5.1.5. “Zi_V” is the same as parameter No. 1.1.11, i.e., it is used to specify the ion charge corresponding to the input interaction potential data.
- 5.1.6–9. These parameters are the same as parameters No. 1.1.26–29, respectively. Their only purpose is defining the “reference” value of the radial coordinate, which will be used to calculate the “reference” value of the final approximate screening function (see the description of parameter No. 1.1.26).
- 5.1.10. “**R_atom_max**” is the endpoint of the radial fitting range. If the last radial breakpoint in the tabular $V(r)$ data is less than R_atom_max, then up to 100 equally-spaced breakpoints will be inserted between the last breakpoint and R_atom_max. Values of the original screening function $\tilde{V}(r)$ at the new breakpoints are calculated using the results of the exponential extrapolation at large r (see Section 12). If the value of this parameter is between 0 and 1, then it is interpreted as the maximum allowed value of $\tilde{V}(r)$ at the endpoint of the radial fitting range (\tilde{V}_{\max}). In such a case, the program will first attempt to find the smallest radial breakpoint such that $\tilde{V} < \tilde{V}_{\max}$. If such a breakpoint is found, then R_atom_max will be reset to the value obtained by exponential interpolation. If no such breakpoint is found (i.e., if $\tilde{V}(r) \geq \tilde{V}_{\max}$ in the entire dataset), then the value of R_atom_max will be calculated by exponential extrapolation of $\tilde{V}(r)$ to \tilde{V}_{\max} . The default value of this parameter is equal to 10^{-6} (i.e., R_atom_max will be reset to the value of the radial coordinate where the screening function is equal to 10^{-6}).

8.2. Adjustable parameters of the analytical screening function

- 5.2.1–2. “**nexp_min**” and “**nexp_max**” are the minimum and maximum values of the number of exponential terms in the analytical expression of the screening function (1.1.34a), respectively. The default values of these two parameters are equal to 2 and 50, respectively.
- 5.2.3–5. “**rmax_R_atom_ratio_min**”, “**rmax_R_atom_ratio_max**” and “**nTries_rmax**” are the minimum and maximum values of the ratio ρ_{\max}/r_{\max} , where ρ_{\max} is the largest of the “characteristic radii” ρ_i ($i = 1, 2, \dots, N$) used for defining the b -coefficients (see Eq. (1.9.1a,b)), and the number of the equidistant values of the same ratio, respectively (r_{\max} is the value of parameter “**R_atom_max**”). The default values of these parameters are the following: **rmax_R_atom_ratio_min**=0.02, **rmax_R_atom_ratio_max**=0.1, **nTries_rmax**=81.
- 5.2.6. “**V_max_large_r_max_ratio**” is the maximum allowed value of the ratio $\tilde{V}_{\text{appr}}(r)/\tilde{V}(r_{\max})$ in the range $r_{\max} < r < 10r_{\max}$, where $\tilde{V}_{\text{appr}}(r)$ is the approximate analytical screening function and $\tilde{V}(r_{\max})$ is the value of the original tabular screening function at $r = r_{\max}$ (see the paragraph after Eq. (1.9.1b)). The default value of this parameter is equal to 10.

8.3. Other parameters

- 5.3.1. “**nTaylorCoefs_max**” is the maximum degree of the truncated Taylor series expansion of the final approximate screening function at small values of the radial coordinate r . The default value of this parameter is equal to 200.

8.4. Output data of subroutine “FitExp”

After the fitting of the tabular screening function data by the linear combination of exponentials (1.1.34a), BREMS creates or updates six files: the file “FitData_all.txt” with the summary of the results, the files “FitData.txt” and “FitData_lo.txt” with the “high” and “low” parts of the calculated quadruple-precision values of the a - and b -coefficients in Eq. (1.1.34a), the file “FittingResults.txt” with the double-precision values of the a -coefficients and the optimum set of the “characteristic radii” ρ_i ($i = 1, 2, \dots, N$) in Eq. (1.9.1a), the file “TaylorCoefs.txt” with the coefficients of the Taylor series expansion of the analytical screening function (1.1.34a) in the vicinity of $r = 0$, and the file “⟨Z⟩.txt” with the values of the interaction potential and the screening function corresponding to all radial breakpoints (“⟨Z⟩” is the atomic number). Below are the detailed descriptions of the format of these files.

After every calculation of the a - and b -coefficients in Eq. (1.1.34a), BREMS appends a line of text to the file “FitData_all.txt”. This file contains the values of the mentioned adjustable parameters (the number of exponentials N and the maximum characteristic radius ρ_{\max}), the optimum values of the a - and b -coefficients, and the root-mean-square (rms) and maximum values of relative residuals. The fitting is performed using quadruple precision (QP) arithmetic in order to reduce the effects of rounding errors (see Section 1.9). However, in order to provide feedback regarding the magnitude of the rounding errors, BREMS also calculates the final values of the mentioned residuals using double precision (DP) and outputs the absolute deviation of the DP value from the QP value. The columns containing values obtained using QP are indicated by the suffix “_QP” in the column header, and the columns containing the difference of the two values corresponding to DP and QP are indicated by the suffix “_diff”. The entries in each line of this file have the following meaning:

- (1) the atomic number (column header “**Z**”),
- (2) the number of exponentials in Eq. (1.1.34a) (“**N**”),
- (3) the optimum value of the ratio ρ_{\max}/r_{\max} , where ρ_{\max} is the largest of the “characteristic radii” ρ_i ($i = 1, 2, \dots, N$) used for defining the b -coefficients (see Eq. (1.9.1a,b)), and

- r_{\max} is the value of parameter “R_atom_max” (the header of this column is “**r_char_max/R_atom_max**”),
- (4) the value of parameter “**R_atom_max**”,
 - (5) the root-mean-square (rms) value of the relative residual (i.e., the relative deviation of the value of the analytical approximation (1.1.34a) from the corresponding original value of the tabular screening function), calculated using QP (“**rmsDev_QP**”),
 - (6) the difference of the DP and QP values of the rms relative residual (“**rmsDev_diff**”),
 - (7) the value of the original tabulated screening function at the last radial breakpoint (i.e., at the last tabulated value of r belonging to the interval $0 < r \leq r_{\max}$) (“**V_last**”),
 - (8) the value of the last radial breakpoint (i.e., the last tabulated value of r belonging to the interval $0 < r \leq r_{\max}$) (“**r_last**”),
 - (9) the number of radial breakpoints in the interval $0 < r \leq r_{\max}$ (“**nPnt**”),
 - (10) the maximum absolute value of the approximate analytical screening function (1.1.34a) in the range $r_{\max} < r < 10r_{\max}$ (“**V_max_large_r**”). This value is calculated using DP,
 - (11) the difference of the value given in the previous column and the corresponding value obtained using QP (“**V_max_l_r_diff**”),
 - (12) the sum of the a -coefficients in Eq. (1.1.34a), calculated using QP, before the normalization to 1 (“**sum_fact_QP**”). The absolute value of the deviation of this value from 1 is equal to the maximum possible additional increase of the relative residuals after the normalization of the a -coefficients,
 - (13) the sum of the final a -coefficients (normalized to 1 using QP), calculated using DP (“**sum_fact**”). The deviation of this value from 1 is an indicator of the magnitude of rounding errors in the case of DP (the QP value of the same sum is exactly equal to 1 after conversion to DP),
 - (14) the sum of the a -coefficients, calculated after the second normalization to 1 using DP (“**sum_fact_norm**”). The relative deviation of this value from the previous number (in column “sum_fact”) is typically much less than its deviation from 1. This indicates that the latter deviation is caused not so much by inaccuracy of the DP values of the a -coefficients, as by accumulation of rounding errors during the summation of the a -coefficients,

The next six entries characterize the maximum relative residual:

- (15) the maximum relative residual in the range $0 < r \leq r_{\max}$, calculated using QP (“**MaxRelDev_QP**”),
- (16) the difference of the DP and QP values of the maximum relative residual (“**MaxRelDev_diff**”),
- (17) the value of the tabulated screening function corresponding to the radial breakpoint where the maximum relative residual is obtained using DP (“**V[maxRelDev]**”),
- (18) the radial breakpoint where the maximum relative residual is obtained using DP (“**r[maxRelDev]**”),
- (19) the sequence number of the radial breakpoint where the maximum relative residual is obtained using DP (“**n[maxRel]**”),
- (20) the deviation of the sequence number given in the previous column from the analogous value obtained using QP (“**n_diff**”).

The next six entries characterize the maximum absolute residual:

- (21) the maximum absolute residual in the range $0 < r \leq r_{\max}$, calculated using QP (“**MaxAbsDev_QP**”),
- (22) the difference of the DP and QP values of the maximum absolute residual (“**MaxAbsDev_diff**”),
- (23) the value of the tabulated screening function corresponding to the radial breakpoint where the maximum absolute residual is obtained using DP (“**V[maxAbsDev]**”),

- (24) the radial breakpoint where the maximum absolute residual is obtained using DP (“**r[maxAbsDev]**”),
- (25) the sequence number of the radial breakpoint where the maximum absolute residual is obtained using DP (“**n[maxAbs]**”),
- (26) the deviation of the sequence number given in the previous column from the analogous value obtained using QP (“**n_diff**”).

The remaining entries are the values of the a - and b -coefficients in Eq. (1.1.34a), arranged in pairs “ $a_i b_i$ ” ($i = 1, 2, \dots, N$). The corresponding column headers are “**factor*i*** **exp*i***”, respectively, where “ $\langle i \rangle$ ” is the sequence number of the corresponding exponential term (the value of the subscript i).

After every calculation of the a - and b -coefficients in Eq. (1.1.34a), BREMS appends a line of text to the files “**FitData.txt**” and “**FitData_lo.txt**” with the “high” and “low” parts of QP values of the a - and b -coefficients in Eq. (1.1.34a). The formats of these two files are identical. The first and second columns contain the values of the atomic number (column header “**Z**”) and the number of exponentials (“**N**”), respectively. The remaining columns contain the values of the coefficients, arranged in pairs “ $a_i b_i$ ” ($i = 1, 2, \dots, N$). The corresponding column headers are “**factor*i*** **exp*i***”, respectively, where “ $\langle i \rangle$ ” is the sequence number of the corresponding exponential term (the value of the subscript i). The file “FitData.txt” contains the “high” parts of the a - and b -coefficients, and the file “FitData_lo.txt” contains the corresponding “low” parts.

The file “**FittingResults.txt**” is overwritten after each fitting. This file contains the values of the a -coefficients (rounded to double precision) and of the “characteristic radii” ρ_i ($i = 1, 2, \dots, N$), which are used to calculate the b -coefficients according to Eq. (1.9.1a). Thus, this file does not provide any additional information in comparison with the file “FitData_all.txt”. The main difference is in the format: in the file “FittingResults.txt”, these numbers are arranged in two columns (not in a single line as in the file “FitData_all.txt”). The first line of the file “FittingResults.txt” contains a single number, which is equal to the number of exponential terms (N) in Eq. (1.1.34a). The remainder of this file consists of three columns of numbers: values of the sequence number i (from 1 to N), the corresponding values of a_i , and the corresponding values of ρ_i ($i = 1, 2, \dots, N$).

After every calculation of the a - and b -coefficients in Eq. (1.1.34a), BREMS appends a line of text to the file “**TaylorCoefs.txt**” with the values of the coefficients of the Taylor series expansion of the analytical approximation of the screening function (1.1.34a) at $r = 0$. These coefficients are calculated using quadruple precision. This file contains their values rounded to double precision. The first column of this file contains the values of the atomic number (column header “**Z**”). The second entry in each line (column header “**r_ref**”) is the “reference” value of the radial coordinate, which coincides with one of the radial breakpoints in the tabular $V(r)$ data (the mentioned breakpoint is specified using parameters No. 5.1.6–9, which are the same as parameters No. 1.1.26–29 described in Section 4.1). The third entry (“**V_ref**”) contains the value of expression (1.1.34a) at the mentioned “reference” value of r , when the a - and b -coefficients are equal to their optimal values. The fourth entry (“**nterms**”) is equal to the degree of the last term of the truncated Taylor series. The remaining columns contain the values of the coefficients of the Taylor series, starting with the term of degree 0 (the corresponding coefficient is always exactly equal to 1).

The file “**<Z>.txt**”, where “ $\langle Z \rangle$ ” is a one-, two- or three-digit atomic number, is overwritten after each fitting. This file contains three columns of numbers: values of the radial breakpoints in column 1 (column header “**r**”), values of the approximate (analytical) interaction potential in relativistic units in column 2 (“**-Z*alpha*V/r**”), and values of the corresponding screening function calculated according to Eq. (1.1.34a) in column 3 (“**V**”). The interaction potential is negative.

9. Spline fitting and interpolation of single differential cross sections of bremsstrahlung

Another special mode of operation of BREMS is cubic spline fitting and interpolation of the logarithm of the scaled single differential cross sections (SDCS or “CS”) with respect to the logarithm of the kinetic energy of the incident electron (T_1) for a given atomic number Z and for a fixed value of the ratio k/T_1 , where k is the energy of the bremsstrahlung photon, as well as creating the input “grid” data files used for the mentioned spline fitting, which contain values of CS and their relative uncertainties on a two-dimensional grid defined by a set of values of T_1 and k/T_1 . Below are the descriptions of the corresponding parameters of BREMS.

9.1. Parameters specifying the atomic number, the energies, and the extent of calculations

6.1.1–4. These four parameters are the same as parameters No. 1.1.1–4 of `S_integrals` (see Section 4.1), i.e., they specify the atomic number, initial electron energy, final electron energy, and photon energy, respectively.

6.1.5. “`CS_int`” is an integer number equal to 0, ± 1 , ± 2 , ± 3 , or ± 4 , which specifies the extent of the calculations in this special mode of operation, and which indicates if a successful spline fitting and interpolation must be followed by a “normal” run of BREMS, using the interpolated value of the CS instead of parameter “`CS_ref_spline`” (see the description of parameter No. 3.8.41). The latter case corresponds to a value of `CS_int` greater than 1 (i.e., 2, 3, or 4). Then the default or user-specified value of `CS_ref_spline` is ignored (a warning is displayed). The allowed values of parameter “`CS_int`” are the following:

- 0 – no interpolation (then this special mode of operation is not applied, and all parameters whose name starts with “`CS_int_`” are ignored),
- ± 1 – only create the list of grid points for the spline fitting and write them to the file whose name is defined by parameters “`CS_int_grid_fn_prefix`” (No. 6.2.5) and “`CS_int_grid_fn_suffix`” (No. 6.2.6),
- ± 2 – read the spline-fitting grid data from the file whose name is defined by parameters “`CS_int_grid_fn_prefix`” and “`CS_int_grid_fn_suffix`” (No. 6.2.5–6) or create the latter file (if it does not exist), then calculate the interpolated value, write it to the file whose name is defined by parameter “`CS_int_fn`” (No. 6.4.12), and then either quit (when `CS_int` = -2) or use the interpolated value in place of `CS_ref_spline` (when `CS_int` = 2),
- ± 3 – read the interpolated value from the file whose name is defined by parameter “`CS_int_fn`” (No. 6.4.12) and then either use it in place of `CS_ref_spline` (when `CS_int` = 3) or quit (when `CS_int` = -3), and if the read attempt fails, then read the spline-fitting grid data from the file whose name is defined by parameters “`CS_int_grid_fn_prefix`” and “`CS_int_grid_fn_suffix`” (if it does not exist, then quit with an error message), then calculate the interpolated value, write it to the file whose name is defined by parameter “`CS_int_fn`” (No. 6.4.12), and then either quit (when `CS_int` = -3) or use the interpolated value in place of `CS_ref_spline` (when `CS_int` = 3),
- ± 4 – attempt to read the interpolated value from the file whose name is defined by parameter “`CS_int_fn`” (No. 6.4.12), and if the read attempt fails, then quit with an error message (if the read is successful, then the behavior is the same as in the case “`CS_int`= ± 3 ”).

The default value of parameter “`CS_int`” is 0 (i.e., the spline fitting and interpolation of the SDCS is not performed, and the spline grid data file is not created).

9.2. Parameters defining the spline-fitting grid and the name of the grid data file

- 6.2.1. “CS_int_T1_fn” is the name of the file with the list of the grid values of T_1 (in MeV). There must be one value per line (empty lines are ignored). The default name of this file is “CS_int_T1.txt” (there is a file with such a name in the distribution package of BREMS).
- 6.2.2. “CS_int_Ep_T1_fn” is the name of the file with the list of the grid values of the ratio k / T_1 . There must be one value per line (empty lines are ignored). If this parameter is equal to the empty string, then the default list of values will be used. The default list consists of 11 values: 10 equidistant values from 0 to 0.9, and 0.95. The default value of this parameter is equal to the empty string.
- 6.2.3–4. “CS_int_Ep_T1_min” and “CS_int_Ep_T1_max” (alias “CS_int_Ep_T1” for both) are the minimum and maximum values of the ratio k / T_1 to be used for creating the grid data file when $|\text{CS_int}| \leq 2$. If $\text{CS_int_Ep_T1_min} = \text{CS_int_Ep_T1_max}$, then the mentioned list of values of k / T_1 (either the default one or loaded from the file defined by parameter No. 6.2.2 “CS_int_Ep_T1_fn”) will not be used. If $\text{CS_int_Ep_T1_min} < \text{CS_int_Ep_T1_max}$, then the program will use the values of k / T_1 that simultaneously belong to the mentioned list and to the interval starting with CS_int_Ep_T1_min and ending with CS_int_Ep_T1_max (if there are no such values, then the program will quit with an error message). These two parameters may also be set equal to the special value -1, which indicates that they both must be replaced with the “current” value of k / T_1 , which is equal to the ratio of the two physical parameters “Ep” and “T1”. The default values of these two parameters are 0.1 and 0.95, respectively.
- 6.2.5–6. “CS_int_grid_fn_prefix” and “CS_int_grid_fn_suffix” are, respectively, the prefix and suffix to be used in the name of the grid data file. If parameter “CS_int_grid_fn_prefix” is not the period “.”, then these two strings will be added to the file name “root”, which is the one-, two- or three-digit value of the atomic number (specified by parameter “Z”). The file name extension is always “.txt” (it must not be included in the mentioned suffix). Thus, the grid file name by default has the following format:

$$\langle \text{CS_int_grid_fn_prefix} \rangle \langle Z \rangle \langle \text{CS_int_grid_fn_suffix} \rangle . \text{txt}$$

If parameter “CS_int_grid_fn_prefix” is equal to the period “.”, then parameter “CS_int_grid_fn_suffix” must specify the complete name of the grid file (without the extension “.txt”). If the file name includes a folder name, then this folder must exist (otherwise a write error would occur). The default value of parameter “CS_int_grid_fn_prefix” is “CS_int/CS_int_”. This means that the grid file is by default located in subfolder “CS_int” of the current folder, and the file name by default starts with characters “CS_int_”. The default value of parameter “CS_int_grid_fn_suffix” is the empty string (i.e., no additional suffix is used).

9.3. Parameters defining the input files with the values of the spline grid data points

- 6.3.1–2. “CS_int_T1_low_max1” (alias “CS_int_T1_low_max”) and “CS_int_T1_high_min1” (alias “CS_int_T1_high_min”) are, respectively, the lower and upper endpoints of the “intermediate” energy range (in MeV). In conjunction with the energy values loaded from the file defined by parameter “CS_int_T1_fn”, these two parameters make it possible to split the entire interval of T_1 into three parts: low-energy, intermediate-energy, and high-energy (in order to achieve this aim, the values of those two parameters must be between the smallest and greatest values in the mentioned file). The grid data corresponding to each of these three energy intervals may be loaded from different input files, which are defined using parameters described below. The values of these two parameters are excluded from the intermediate-energy range, but included in the low- and high-energy intervals (i.e., these two parameters could be defined more precisely as the upper endpoint of the low-energy range

and the lower endpoint of the high-energy range, respectively). The default values of these two parameters are 10 and 50.

The next nineteen parameters are used to define the input datasets for each of the three intervals of T_1 (see also the description of parameters No. 6.3.1–2), and to apply filtering of the data according to the magnitude of the relative uncertainty. Those datasets may be defined differently for zero and non-zero photon energy. Thus, for each interval of T_1 , two different input datasets may be defined (one for zero photon energy and one for non-zero photon energy). Since the complete definition of the input dataset requires specifying three parameters (the file name and two parameters defining the subset of data that must be read from it), there are 18 parameters of this type in total ($6 \times 3 = 18$). In addition, there is a parameter that allows excluding the data points with unacceptably large uncertainties.

6.3.3–5. “CS_int_fn_low”, “CS_int_fn_high”, and “CS_int_fn_interm” (alias “CS_int_input_fn” for all three) are the input file names for each of the three intervals of T_1 (low-energy, high-energy and intermediate-energy, respectively), when the photon energy is non-zero. The default values of these three parameters are “CS_fitted.txt”, “CS_Born_SM.txt”, and “CS_fitted.txt”, respectively.

6.3.6–8. “CS_int_appr_low”, “CS_int_appr_high”, and “CS_int_appr_interm” (alias “CS_int_appr” for all three) are the indicators of the file format for each of the three intervals of T_1 (low-energy, high-energy and intermediate-energy, respectively), when the photon energy is non-zero. Two file formats are allowed: the format of the file “CS_fitted.txt” described in Section 6.20 (the corresponding indicator is equal to 1), and the format of the file “CS_Born_SM.txt” described in Section 7.8 (the corresponding indicator is equal to 0, -1, or -2). In the latter case, the value of this parameter has the same meaning as the value in the column “appr” of the file “CS_Born_SM.txt”, and the lines with another value in this column will be ignored. The default values of these three parameters are 1, -2, and 1, respectively.

6.3.9–11. “CS_int_IV_low”, “CS_int_IV_high”, and “CS_int_IV_interm” (alias “CS_int_IV” for all three) are the indicators of the potential type for each of the three intervals of T_1 (low-energy, high-energy and intermediate-energy, respectively), when the photon energy is non-zero. Each of these parameters is used only when the corresponding “CS_int_appr” indicator is zero or negative (see the description of parameters No. 6.3.6–8), and its value has the same meaning as the value in the column “IV” of the file “CS_Born_SM.txt” described in Section 7.8 (the lines with another value in this column will be ignored). The default values of these three parameters are 0, 2, and 0, respectively.

6.3.12–14. “CS_int_fn_low_0”, “CS_int_fn_high_0”, and “CS_int_fn_interm_0” (alias “CS_int_input_fn_0” for all three) are the input file names for each of the three intervals of T_1 (low-energy, high-energy and intermediate-energy, respectively), when the photon energy is zero. If any of these parameters is equal to the empty string, then the corresponding file name and the two associated indicators (parameters No. 6.3.15–20) will be assumed to coincide with the corresponding value pertaining to non-zero photon energy (parameters No. 6.3.3–11). The default value of these three parameters is equal to the empty string.

6.3.15–17. “CS_int_appr_low_0”, “CS_int_appr_high_0”, and “CS_int_appr_interm_0” (alias “CS_int_appr_0” for all three) are the indicators of the file format for each of the three intervals of T_1 (low-energy, high-energy and intermediate-energy, respectively), when the photon energy is zero. In addition to the two file formats mentioned in the description of parameters No. 6.3.6–8, another file format (corresponding to the output file of a different program, which calculates the scaled soft-photon cross sections using an alternative method mentioned in Section 1.1.1, after Eq. (1.1.20)) is also allowed (the corresponding indicator is equal to 2, and the corresponding file format is described in the description of parameters No. 6.3.22–23). The default value of these three parameters is equal to 2.

- 6.3.18–20. “CS_int_IV_low_0”, “CS_int_IV_high_0”, and “CS_int_IV_interm_0” (alias “CS_int_IV_0” for all three) are the indicators of the potential type for each of the three intervals of T_1 (low-energy, high-energy and intermediate-energy, respectively), when the photon energy is zero. Each of these parameters is used only when the corresponding “CS_int_appr..._0” indicator is not equal to 1 (see the description of parameters No. 6.3.15–17). If the corresponding “CS_int_appr..._0” indicator is zero or negative, then the value of the CS_int_IV..._0 parameter has the same meaning as the value in the column “IV” of the file “CS_Born_SM.txt” described in Section 7.8 (the lines with another value in this column will be ignored). If the corresponding “CS_int_appr..._0” indicator is equal to 2, then the value of the CS_int_IV..._0 parameter has the same meaning as the value in the column “IV” of the output file of a different program, which calculates the scaled soft-photon cross sections using an alternative method mentioned in Section 1.1.1, after Eq. (1.1.20). The default value of these three parameters is equal to 3.
- 6.3.21. “CS_int_relErrThr1” (alias “CS_int_relErrThr”) is the maximum allowed absolute value of the relative uncertainty. The data points with greater uncertainties are excluded from the data grid (i.e., the corresponding grid point values in the output file whose name is defined by parameters “CS_int_grid_fn_prefix” and “CS_int_grid_fn_suffix” are set equal to 0). The default value of this parameter is equal to 0.05. **Note:** During the spline fitting, additional grid points may be excluded (i.e., not used for the fitting) by setting parameter “CS_int_relErrThr2” (No. 6.4.5) to a value less than CS_int_relErrThr1.
- 6.3.22. “CS_int_exclude_large_T1_T2” is a “switch” (0, 1, or 2), which indicates if the data points corresponding to $T_1 > T1_CS_mode_thr$ (parameter No. 3.12.1) and $T_2 > T2_CS_mode_thr$ (parameter No. 3.12.2) and $T_2 / T_1 > tip_thr$ (parameter No. 9 of the main program, which is described in Section 2) must be excluded from the data grid, when the corresponding “CS_int_appr...” parameter is equal to 1 (i.e., when the input data file is “CS_fitted.txt”, created by BREMS in partial-wave mode). If CS_int_exclude_large_T1_T2=2 and the mentioned three inequalities are satisfied simultaneously, then the corresponding grid point value in the output file whose name is defined by parameters “CS_int_grid_fn_prefix” and “CS_int_grid_fn_suffix” is set equal to 0 (i.e., excluded from the data grid). If CS_int_exclude_large_T1_T2=1, then an additional condition has to be satisfied in order to exclude a data point: the value in column with the header “rel_diff” must be zero (this entry is equal to the relative deviation of the numerical integral of the final κ_{max} -fitted DCS from the final value of the κ_{max} -fitted CS). A zero value of this entry indicates that the “alternative CS-fitting mode” was applied, i.e., that the nonlinear fitting of the dependence of the partial-wave CS on κ_{max} -was skipped (see also Section 6.12). The default value of this parameter is 1 (i.e., only the data points corresponding to the “normal” CS-fitting mode can be included in the data grid).

The next 15 parameters are used to specify the columns with the values of the CS and its uncertainty in the input data files. The program may locate the needed columns either by their headers, or by their sequence numbers. The method of locating the columns is specified using three parameters “CS_int_useHeaders0”, “CS_int_useHeaders1”, and “CS_int_useHeaders2”, where the number at the end of the parameter name indicates the type of the input file (see the descriptions of parameters No. 6.3.6–8 and 6.3.15–17). The three parameter names differing only by this number will be further referred to using the suffix “[0,1,2]”. If parameter “CS_int_useHeaders[0,1,2]” is positive, then the program will assume that the table with the data is preceded by the header line, whose sequence number in the corresponding file is equal to the value of the same parameter. In such a case, the columns with the needed data will be identified by reading the column headers and locating the character strings specified by parameters “CS_int_header_CS[0,1,2]” (indicating the header of the column with the values of the SDCS) and “CS_int_header_relErr[0,1,2]” (indicating the header of the column with the values of relative or absolute uncertainty of the SDCS). The column headers cannot include spaces. If parameter “CS_int_useHeaders[0,1,2]” is zero or negative,

then the program will ignore the header line (if present), and the sequence number of the first line with the numerical data will be assumed to be one greater than the absolute value of this parameter. In such a case, the column numbers specified by parameters “CS_int_colNum_CS[0,1,2]” (indicating the sequence number of the column with the values of the SDCS) and “CS_int_colNum_relErr[0,1,2]” (indicating the sequence number of the column with the values of relative or absolute uncertainty of the SDCS) will be used. If the latter column number is equal to zero, then the program will set all uncertainties to zero, and will not attempt to read them from the input file. The type of the uncertainty (absolute or relative) is indicated by the “switch” “CS_int_isAbsErr[0,1,2]”. Since the default option “CS_int_exclude_large_T1_T2=1” requires checking the values in column “rel_diff” of the files of type 1 (see the description of parameter No. 6.3.22), there are additional two parameters “CS_int_header_rel_diff1” and “CS_int_colNum_rel_diff1”, which are used to specify the header and sequence number of the mentioned column, respectively. If CS_int_exclude_large_T1_T2=1, then setting parameter “CS_int_colNum_rel_diff1” to zero would have the same effect as the option “CS_int_exclude_large_T1_T2=2”.

6.3.23–24. “CS_int_colNum_CS0” and “CS_int_colNum_relErr0” are the sequence numbers of the columns with the values of the CS and its uncertainties, respectively, in the file corresponding to the “CS_int_appr..._0” indicator equal to 2 (as mentioned in the description of parameters No. 6.3.15–17, the latter value is allowed only in the case of zero photon energy). In this case, the first and second columns of the input data file must contain the values of Z and T_1 , respectively (the energy must be specified in MeV), and the fifth column must contain the value indicating the type of the interaction potential (see the description of parameters No. 6.3.18–20). Consequently, both these parameters must be greater than 5. The default values of these two parameters are 39 and 42, respectively.

6.3.25–27. “CS_int_colNum_CS1”, “CS_int_colNum_relErr1”, “CS_int_colNum_rel_diff1” are the sequence numbers of the columns with the values of the CS, its uncertainties, and the column “rel_diff”, respectively, in the file corresponding to the “CS_int_appr” indicator equal to 1 (as mentioned in the description of parameters No. 6.3.6–8, the latter value indicates that the input file has the same format as the file “CS_fitted.txt”, which is updated in stage 3 of a run of BREMS). In this case, the first three columns of the input data file must contain the values of the atomic number Z , the incident electron energy T_1 and the photon energy k , respectively (the energies must be specified in MeV). Consequently, these three parameters must be greater than 3. The default values of these three parameters are equal to 39, 56, and 41, respectively.

6.3.28–29. “CS_int_colNum_CS2” and “CS_int_colNum_relErr2” are the sequence numbers of the columns with the values of the CS and its uncertainties, respectively, in the file corresponding to the “CS_int_appr” indicator equal to 0, -1 or -2 (as mentioned in the description of parameters No. 6.3.6–8, the latter values indicates that the input file has the same format as the file “CS_Born_SM.txt”, which is updated during the calculation of the analytical cross sections according the Born approximation or the Sommerfeld-Maue approximation). In this case, the first three columns of the input data file must contain the values of the atomic number Z , the incident electron energy T_1 and the photon energy k , respectively (the energies must be specified in MeV), the fifth column must contain the value indicating the type of the interaction potential (1 or 2), and the ninth column must contain the indicator of the approximation type (0, -1 or -2). Consequently, both these parameters must be greater than 9. The default values of these two parameters are 17 and 19, respectively.

6.3.30–32. “CS_int_useHeaders0”, “CS_int_useHeaders1”, and “CS_int_useHeaders2” (alias “CS_int_useHeaders” for all three) indicate the method of locating the needed columns and the starting line of the data table (see the paragraph preceding the description of parameter No. 6.3.23 for a more detailed explanation). The default value of these three parameters is

equal to 1 (i.e., the program will read the column headers from the first line of the file by default).

- 6.3.33–39. “CS_int_header_CS0”, “CS_int_header_relErr0”, “CS_int_header_CS1”, “CS_int_header_relErr1”, “CS_int_header_rel_diff1”, “CS_int_header_CS2”, “CS_int_header_relErr2” are the headers of columns with the value of the SDSC (specified by the three parameters with “header_CS” in their names) and with the value of the absolute or relative uncertainty (specified by the three parameters with “header_relErr” in their names) for each type of the input file (indicated by the number “0”, “1” or “2” at the end of the parameter name). The column headers cannot include spaces. The default values of these six parameters are “CS_brems”, “CS_brems_relErr”, “CS_fitted[k->Inf]”, “CS_fitted_relSD”, “rel_diff”, “CS”, and “relErr_CS”, respectively.
- 6.3.40–42. “CS_int_isAbsErr0”, “CS_int_isAbsErr1”, and “CS_int_isAbsErr2” (alias “CS_int_isAbsErr” for all three) are “switches” (1 or 0) indicating if the uncertainties stored in the file of the type indicated by the number at the end of the parameter name should be interpreted as absolute (rather than relative) uncertainties. The default value of these three parameters is equal to 0 (indicating relative uncertainties).

9.4. Parameters of the cubic spline fitting

- 6.4.1–2. “CS_int_T1_low_min” (alias “CS_int_T1_min”) and “CS_int_T1_high_max” (alias “CS_int_T1_max”) are, respectively, the lower and upper endpoints of the range of T_1 of the spline-fitting grid (in MeV). All data points that correspond to $T_1 < \text{CS_int_T1_low_min}$ or $T_1 > \text{CS_int_T1_high_max}$ are excluded from the grid. The first and last grid points inside this interval are the first and last knots of the spline function. Further on, the term “knot” will mean either a point where two cubic segments of the spline function are smoothly joined together, or one of the two endpoints, where the boundary conditions are applied (the boundary conditions include the values of the first derivative, which are also optimized during the spline fitting). The default values of these two parameters are 0.1 and 300, respectively.
- 6.4.3–4. “CS_int_T1_low_max2” (aliases “CS_int_T1_low_max” and “CS_int_T1_max”) and “CS_int_T1_high_min2” (aliases “CS_int_T1_high_min” and “CS_int_T1_min”) are, respectively, the lower and upper endpoints of the “intermediate” interval of T_1 (in MeV). All data points that correspond to values of T_1 greater than CS_int_T1_low_max2 and less than CS_int_T1_high_min2 are excluded. In this respect, the effect is the same as in the case of extremely large uncertainties (see the description of parameter No. 6.4.5 “CS_int_relErrThr2”). In addition, the program will calculate the relative deviations of the optimal spline function from the mentioned excluded data points, and the maximum relative deviation will be displayed on the screen and written to the file whose name is defined by parameter “CS_int_fn”. If $\text{CS_int_T1_low_max2} < \text{CS_int_T1_high_min2}$, or if the energy range defined by these two parameters does not overlap with the energy range defined by parameters “CS_int_T1_low_min” and “CS_int_T1_high_max” (No. 6.4.1–2), then no additional grid points will be excluded on the basis of the value of T_1 . The default value of these two parameters is equal to 0 (i.e., no intermediate energy range is used).
- 6.4.5. “CS_int_relErrThr2” (alias “CS_int_relErrThr”) is the maximum allowed absolute value of the relative uncertainty at the stage of spline fitting. The data points with greater uncertainties are excluded from the spline-fitting grid. The default value of this parameter is equal to 0.05 (since this value is the same as the default value of parameter “CS_int_relErrThr1”, no additional grid points will be excluded on the basis of the relative uncertainty at the stage of spline fitting, if the default values of CS_int_relErrThr1 and CS_int_relErrThr2 are used).
- 6.4.6–7. “CS_int_nKnots_min” and “CS_int_nKnots_max” (alias “CS_int_nKnots” for both) are the minimum and maximum number of knots, respectively. The program will start with the

maximum number of knots. If the spline fitting fails, then the number of knots will be reduced by 1. This will be repeated until the spline fitting is successful or the minimum number of knots is reached, whichever happens first. The positions of spline knots coincide with some of the grid points, and they are chosen so that the numbers of grid points in all inter-knot intervals are approximately equal (they can differ from each other by no more than ± 1). If those two parameters are specified with the minus sign, then they are interpreted as the integer part of the maximum and minimum average number of grid points inside one inter-knot interval, respectively. The default values of those two parameters are equal to -7 and -4, respectively.

- 6.4.8. “**CS_int_spline_wt_thr**” is the threshold value of the relative uncertainty of a grid point value, which must be exceeded in order to apply a weight factor less than 1 to the corresponding term in the sum of squared residuals, which is minimized during the spline fitting. The mentioned weight factor is in such a case equal to the squared ratio of **CS_int_spline_wt_thr** and the mentioned relative uncertainty. If the relative uncertainty is less than **CS_int_spline_wt_thr**, or if **CS_int_spline_wt_thr**=0, then no weighting is applied (i.e., the weight factor is equal to 1). The default value of this parameter is equal to 0.01.
- 6.4.9. “**CS_int_np**” is the number of points in the table of values of the optimal spline function (i.e., the scaled fitted SDCS), which may optionally be written to a file after the spline fitting. The argument of the spline function is the incident electron energy (T_1), and the points are equidistant on the logarithmic scale. If this parameter is zero or negative, then the mentioned file will not be created. The default value of this parameter is equal to 0.
- 6.4.10–11. “**CS_int_spline_fn_prefix**” and “**CS_int_spline_fn_suffix**” are the prefix and suffix to be used when forming the name of the spline file mentioned in the description of parameter No. 6.4.9. Those two character strings are added to the “root” of the file name, which consists of the one-, two- or three-digit value of the atomic number Z and the six-digit value of the ratio k / T_1 , where k is the photon energy (specified by parameter “**Ep**”), separated by the underscore. The suffix does not include the file name extension, which is always “.txt”. In order to use an arbitrary file name, parameter “**CS_int_spline_fn_prefix**” must be set equal to the period “.”, and parameter “**CS_int_spline_fn_suffix**” must be the full name of the file, excluding the extension “.txt”. If the file name includes a folder name, then this folder must exist (otherwise a write error would occur). The default values of these two parameters are equal to “**CS_int_**” and “**_spline**”, respectively.
- 6.4.12. “**CS_int_fn**” is the name of the file where the fitted value of the scaled single differential cross section (CS) corresponding to the current value of the ratio k / T_1 must be written after the spline fitting. If the file name includes a folder name, then this folder must exist (otherwise a write error would occur). If this parameter is the empty string, then this file will not be updated. The default value of this parameter is equal to the empty string.

9.5. Other parameters

- 6.5.1. “**checkTabPos**” is a “switch” (1 or 0) indicating if the format of the input files used for generating the grid data for the cubic-spline fitting and interpolation must be checked for consistency. If this parameter is equal to 1, then the program will check if tab positions are the same in all lines of the file. If a line with different tab positions is found, then the program will terminate with an error message. If this parameter is equal to 0, then the mentioned check will not be performed (this may speed up generation of the grid data significantly, but may cause incorrect results if the input data file is corrupted). The default value of this parameter is equal to 1.

Note: Parameter “**checkTabPos**” is also used in stage 2 by subroutine “**Bremsstrahlung**” (for checking the files “**CS.txt**” and “**CS_2.txt**”), in stage 3 by subroutine “**Brems_fit**” (for checking the file “**CS_fitted.txt**”), and by subroutine “**Born_SM_appr**” (for checking the file “**CS_Born_SM.txt**”), after updating the

mentioned output files. However, in those cases, only the first and last lines of the file are compared, and a change of tab positions is not treated as a terminal error (a warning message is displayed, but execution of the program is not stopped).

9.6. Output data of subroutine “Brems_CS_interp”

Subroutine Brems_CS_interp creates or updates up to three human-readable ASCII files. Their names end with extension “.txt”. Those files are listed below:

- I. A file with the grid values of the scaled CS and its relative uncertainties for the spline fitting. The name of this file is defined by parameters “CS_int_grid_fn_prefix” and “CS_int_grid_fn_suffix” (No. 6.2.5–6). This file can be created only when the absolute value of parameter No. 6.1.5 (“CS_int”) is equal to 1 or 2.
- II. A file with the tabulated values of the optimal spline function. Its name is defined by parameters “CS_int_spline_fn_prefix” and “CS_int_spline_fn_suffix” (No. 6.4.10–11). This file can be created only when the absolute value of parameter No. 6.1.5 (“CS_int”) is equal to 2 or 3, and parameter “CS_int_np” (No. 6.4.9) is greater than 1.
- III. A file with the fitted value of the scaled single differential cross section of bremsstrahlung (CS) corresponding to the current value of the ratio k / T_1 , where k is the photon energy (specified by parameter “Ep”) and T_1 is the incident electron energy (specified by parameter “T1”). The name of this file is specified by parameter “CS_int_fn” (No. 6.4.12). If parameter “CS_int_fn” is not the empty string, then a line of text is appended to this file after each spline fitting.

Each of those files contains several columns of numbers. The first line of the file contains the column headers. A detailed description of the format of each of those files is presented below.

The file with the spline-fitting grid values contains $1 + 2n$ columns, where “ n ” is the number of values of the ratio k / T_1 used for the grid. The value of n is determined by the values of parameters No. 6.2.2 (“CS_int_Ep_T1_fn”), No. 6.2.3 (“CS_int_Ep_T1_min”), and No. 6.2.4 (“CS_int_Ep_T1_max”). The meaning of the numbers in each column is the following:

- (No. 1) the kinetic energy of the incident electron, in MeV (column header “T1(MeV)”)
- (No. $2i$, where $i = 1, 2, \dots, n$) the value of the scaled CS for the spline fitting (the format of the column header is “CS[Ep/T1= $\langle k/T_1 \rangle$]”, where “ $\langle k/T_1 \rangle$ ” is the 14-digit value of the ratio k / T_1),
- (No. $2i + 1$, where $i = 1, 2, \dots, n$) the value of the relative uncertainty of the corresponding value of the CS (the format of the column header is “RelErr[Ep/T1= $\langle k/T_1 \rangle$]”, where “ $\langle k/T_1 \rangle$ ” is the four-digit value of the ratio k / T_1).

The missing grid point values are indicated by zeros (a grid point may be missing either because of absence of the data for a particular pair of T_1 and k / T_1 in the data files used to create the grid, or because the corresponding relative uncertainty of the CS was greater than the value of parameter No. 6.3.21 “CS_int_relErrThr1”).

The subfolder “CS_int” of the distribution package of BREMS contains 100 ASCII files with the spline-fitting grid data, which were created using the option “CS_int=1” for each value of the atomic number Z from 1 to 100. The range of values of k / T_1 in those files is from 0 to 0.95 (the values from 0 to 0.9 are equidistant, with the increment equal to 0.1), whereas the range of values of T_1 is from 0.1 MeV to 300 MeV (for $k > 0$), or from 0.1 MeV to 100 MeV (for $k = 0$). In the case of non-zero photon energy, the values of the CS were calculated by the partial-wave method at $T_1 \leq 30$ MeV, and by applying the Sommerfeld-Maue (SM) approximation with the next-to-leading order (NLO) correction and the screening correction (see Section 1.1.3) at $T_1 \geq 50$ MeV. In the case of zero photon energy, all values of the CS were calculated using the alternative method mentioned in Section 1.1.1, after Eq. (1.1.20). In all cases, the Kohn-Sham potential was (the files with the tabulated values of the Kohn-Sham potential are in subfolder “V/Kohn-Sham/”), whereas the distribution of nuclear charge was the default one (i.e., Fermi distribution when the ratio of the reduced wavelength of the incident electron to the nuclear radius is less than 40, or point nucleus otherwise).

The file with the tabulated optimal spline function contains two columns:

- (1) the kinetic energy of the incident electron, in MeV (column header “**T1(MeV)**”),
- (2) the fitted value of the scaled single differential cross section of bremsstrahlung (“**CS_spline**”).

The file with the fitted CS corresponding to the current values of parameters “Ep” and “T1” contains sixteen columns:

- (1) the atomic number of the target material (column header “**Z**”),
- (2) the kinetic energy of the incident electron in MeV (“**T1(MeV)**”),
- (3) the energy of the bremsstrahlung photon in MeV (“**Ep(MeV)**”),
- (4) the fitted value of the scaled SDCS of bremsstrahlung (“**CS_interp**”),
- (5) the value of parameter No. 6.4.5 “CS_int_relErrThr2” (column header “**relErrThr**”),
- (6) the number of grid points used for the spline fitting (this number does not include the data points that were excluded either due to a large uncertainty, or because the corresponding value of T_1 is between the values defined by parameters No. 6.4.3 “CS_int_T1_low_max2” and 6.4.4 “CS_int_T1_high_min2”); the header of this column is “**nGrid**”,
- (7) the final number of spline knots (“**nKnots**”),
- (8) the maximum relative residual over the set of grid points used for the spline fitting, i.e., the maximum relative deviation of the fitted value from the original value at the grid values of T_1 (“**maxRelDev**”),
- (9) the number of excluded grid points, which correspond to values of T_1 between the values defined by parameters No. 6.4.3 “CS_int_T1_low_max2” and 6.4.4 “CS_int_T1_high_min2” (column header “**nExcl**”). *Note:* This number does not include the grid points that were excluded only because of a large uncertainty of the CS,
- (10) the maximum relative deviation of the fitted value from the original value over the set of excluded grid points, which correspond to values of T_1 between the values defined by parameters No. 6.4.3 “CS_int_T1_low_max2” and 6.4.4 “CS_int_T1_high_min2”, or the number 0 if there are no such data points (column header “**maxRelDev_excl**”),
- (11) the value of T_1 (in MeV) corresponding to the first grid point (which is also the first knot) of the spline function (“**T1_min(MeV)**”),
- (12) the value of T_1 (in MeV) corresponding to the last grid point (which is also the last knot) of the spline function (“**T1_max(MeV)**”),

The last four entries can be non-zero only when the entry in column “nExcl” is greater than 0:

- (13) the value of T_1 (in MeV) corresponding to the last grid point in the “low-energy” range $CS_int_T1_low_min \leq T_1 \leq CS_int_T1_low_max2$, or the number 0 if there are no such grid points (“**T1_low_max(MeV)**”),
- (14) the value of T_1 (in MeV) corresponding to the first grid point in the “high-energy” range $CS_int_T1_high_min2 \leq T_1 \leq CS_int_T1_high_max$, or the number 0 if there are no such grid points (“**T1_high_max(MeV)**”),
- (15) the value of T_1 (in MeV) corresponding to the first grid point in the “intermediate-energy” range $CS_int_T1_low_max2 < T_1 < CS_int_T1_high_min2$, or the number 0 if there are no such grid points (“**T1_excl_min(MeV)**”),
- (16) the value of T_1 (in MeV) corresponding to the last grid point in the “intermediate-energy” range $CS_int_T1_low_max2 < T_1 < CS_int_T1_high_min2$, or the number 0 if there are no such grid points (“**T1_excl_max(MeV)**”).

10. List of parameter aliases used in BREMS

In the code of BREMS, some parameters are grouped into small groups consisting of 2 – 4 parameters, all of which can be assigned a value using a single directive, where the parameter name is replaced by its “alias”. For example, the alias “stage” is associated with parameters “firstStage” and “lastStage”. Consequently, specifying “stage=2” on the command line or in the parameter file

would be equivalent to two directives: “firstStage=2” and “lastStage=2”. There are 219 aliases in total. The list of all aliases and the associated parameter names is presented in the following table.

No.	Alias	I parameter	II parameter	III parameter	IV parameter
1	stage	firstStage	lastStage		
2	n_terms_max	nterms_max	nterms_max_J		
3	Kmin	Kmin1	Kmin2		
4	Kmax	Kmax1	Kmax2		
5	K1	Kmin1	Kmax1		
6	K2	Kmin2	Kmax2		
7	Km	Kmin1	Kmax1	Kmin2	Kmax2
8	isAbs_K	isAbs_K1	isAbs_K2		
9	k2_step	k2_step_first	k2_step_last		
10	l	lmin	lmax		
11	lm	lmax	lmax_MP		
12	R_a_delta	R_atom_delta	R_atom_delta+		
13	T1_mode_thr	T1_Kmax_mode_thr	T1_CS_mode_thr		
14	dir_V	dirV	dirV_aux		
15	del_S	del_S_int	del_S_int+		
16	suffix2	suffix2_CS	suffix2_DCS		
17	suffix_3	suffix3	suffix3a		
18	prefix_fit	prefix_fit_CS	prefix_fit_DCS		
19	Npasses	Npasses_CS	Npasses_DCS		
20	tol	tol1	tol2	tol3	
21	rtol	rtol1	rtol2	rtol3	
22	thr_corr+	thr_corr1+	thr_corr2+		
23	tol_spl	tol_spline	tol_spline_fitted		
24	theorSD	theorSD_CS	theorSD_DCS		
25	simple_fit	simple_fit_CS	simple_fit_DCS		
26	simple_exp	simple_exp_CS	simple_exp_DCS		
27	simple_exp_thr	simple_exp_thr_CS	simple_exp_thr_DCS1	simple_exp_thr_DCS2	
28	simple_exp_thr_DCS	simple_exp_thr_DCS1	simple_exp_thr_DCS2		
29	simple_exp_thr_incr	simple_exp_thr_CS	simple_exp_thr_DCS1		
30	d_exp	d_exp_CS	d_exp_DCS1	d_exp_DCS2	
31	d_exp_DCS	d_exp_DCS1	d_exp_DCS2		
32	d_exp_incr	d_exp_CS	d_exp_DCS1		
33	d_polyn	d_polyn_CS	d_polyn_DCS1	d_polyn_DCS2	
34	d_polyn_DCS	d_polyn_DCS1	d_polyn_DCS2		
35	d_polyn_incr	d_polyn_CS	d_polyn_DCS1		
36	d_init	d_init_CS	d_init_DCS1	d_init_DCS2	
37	d_init_DCS	d_init_DCS1	d_init_DCS2		
38	d_init_incr	d_init_CS	d_init_DCS1		
39	polyn_thr	polyn_thr_CS	polyn_thr_DCS1	polyn_thr_DCS2	
40	polyn_thr_DCS	polyn_thr_DCS1	polyn_thr_DCS2		
41	polyn_thr_incr	polyn_thr_CS	polyn_thr_DCS1		
42	thrCorr_extrap	thrCorr_extrap1	thrCorr_extrap2		
43	thrAngle_extrap	thrAngle_extrap1	thrAngle_extrap2		
44	T2_thr_mu	T2_thr_mu1	T2_thr_mu2		
45	tol_range_ratio_mu	tol_range_ratio_mu1	tol_range_ratio_mu2		
46	thr_range_mu	thr_range_mu1	thr_range_mu2		
47	tol_mu	tol_mu1	tol_mu2		
48	max_corr_mu	maxCorr_mu	maxCorr_mu2		
49	min_width_mu	minWidth_mu	minWidth_mu2		
50	fitEndOffset_mu	fitEndOffset_mu_min	fitEndOffset_mu_max		
51	fitEndOffset_mu0	fitEndOffset_mu0_min	fitEndOffset_mu0_max		
52	fit_end_offset_mu	fitEndOffset_mu_min	fitEndOffset_mu_max	fitEndOffset_mu0_min	fitEndOffset_mu0_max

No.	Alias	I parameter	II parameter	III parameter	IV parameter
53	fitRef_mu	fitRef_mu1	fitRef_mu2		
54	fitLog_mu	fitLog_mu1	fitLog_mu2		
55	ref_mu1	fitRef_mu1	compRef_mu		
56	ref_mu2	fitRef_mu2	compRef_mu		
57	ref_mu	fitRef_mu1	fitRef_mu2	compRef_mu	
58	fitDegree_mu	fitDegree_mu_min1	fitDegree_mu_max1	fitDegree_mu_min2	fitDegree_mu_max2
59	fitDegree_mu1	fitDegree_mu_min1	fitDegree_mu_max1		
60	fitDegree_mu2	fitDegree_mu_min2	fitDegree_mu_max2		
61	degree_extrap	degree_extrap_min	degree_extrap_max		
62	polyn_mode_mu	polyn_mode_mu1	polyn_mode_mu2		
63	minDeg	minDeg_CS	minDeg_DCS1	minDeg_DCS2	
64	maxDeg_DCS	maxDeg_DCS1	maxDeg_DCS2		
65	maxDeg_incr	maxDeg_CS	maxDeg_DCS1		
66	maxDeg	maxDeg_CS	maxDeg_DCS1	maxDeg_DCS2	
67	minDeg_DCS	minDeg_DCS1	minDeg_DCS2		
68	minDeg_incr	minDeg_CS	minDeg_DCS1		
69	deg_CS	minDeg_CS	maxDeg_CS		
70	deg_DCS	minDeg_DCS1	maxDeg_DCS1	minDeg_DCS2	maxDeg_DCS2
71	deg_DCS1	minDeg_DCS1	maxDeg_DCS1		
72	deg_DCS2	minDeg_DCS2	maxDeg_DCS2		
73	deg_incr	minDeg_CS	maxDeg_CS	minDeg_DCS1	maxDeg_DCS1
74	polyn_thr_mu	polyn_thr_mu1	polyn_thr_mu2		
75	minDeg_mu	minDeg_mu1	minDeg_mu2		
76	maxDeg_mu	maxDeg_mu1	maxDeg_mu2		
77	deg_mu1	minDeg_mu1	maxDeg_mu1		
78	deg_mu2	minDeg_mu2	maxDeg_mu2		
79	deg_mu	minDeg_mu1	maxDeg_mu1	minDeg_mu2	maxDeg_mu2
80	vary_h	vary_h_CS	vary_h_DCS		
81	Nfit	Nfit_CS	Nfit_DCS		
82	fitRange	fitRange_CS	fitRange_DCS		
83	fitRange2	fitRange2_CS	fitRange2_DCS		
84	tol_corr	tol_corr_CS	tol_corr_DCS		
85	shift_k_mode	shift_k_mode_CS	shift_k_mode_DCS		
86	shift_k_max	shift_k_max_CS	shift_k_max_DCS		
87	shift_k_max2	shift_k_max2_CS	shift_k_max2_DCS		
88	fitRegionRatio	fitRegionRatio_CS	fitRegionRatio_DCS		
89	maxMovingAvgErrRatio	maxMovingAvgErrRatio_CS	maxMovingAvgErrRatio_DCS		
90	shiftSelection	shiftSelection_CS	shiftSelection_DCS		
91	maxShiftErrRatio	maxShiftErrRatio_CS	maxShiftErrRatio_DCS		
92	fitFunc	fitFunc_CS	fitFunc_DCS		
93	fitFunc2	fitFunc2_CS	fitFunc2_DCS		
94	thr_ratio_h	thr_ratio_h_CS	thr_ratio_h_DCS		
95	thr_ratio_h2	thr_ratio_h2_CS	thr_ratio_h2_DCS		
96	wt_avg	wt_avg_CS	wt_avg_DCS		
97	nAvg	nAvg_CS	nAvg_DCS		
98	fractAvg	fractAvg_CS	fractAvg_DCS		
99	SDratio	SDratio_CS	SDratio_DCS		
100	wt_Nfit	wt_Nfit_CS	wt_Nfit_DCS		
101	prefix_ref_fn	prefix_ref_fn1	prefix_ref_fn2		
102	prefix_ref_pn	prefix_ref_pn1	prefix_ref_pn2		
103	prefix_ref1	prefix_ref_fn1	prefix_ref_pn1		
104	prefix_ref2	prefix_ref_fn2	prefix_ref_pn2		
105	prefix_ref	prefix_ref_fn1	prefix_ref_fn2	prefix_ref_pn1	prefix_ref_pn2
106	suffix_ref	suffix_ref1	suffix_ref2		
107	auto_naming_ref	auto_naming_ref1	auto_naming_ref2		
108	name_ref_DCS	name_ref_DCS1	name_ref_DCS2		

No.	Alias	I parameter	II parameter	III parameter	IV parameter
109	name_ref_SF	name_ref_SF1	name_ref_SF2		
110	prefix2_ref	prefix2_ref1	prefix2_ref2		
111	col_ref	col_ref1	col_ref2		
112	appr_ref	appr_ref1	appr_ref2		
113	IV_ref	IV_ref1	IV_ref2		
114	nd	nd_DCS	nd_F	nd_HG	
115	np	np1	np2		
116	theta_max	theta_max1	theta_max2		
117	theta0	theta_min	adapt_theta_min1	adapt_theta_min2	
118	splineInt	splineInt_min	splineInt_max		
119	splineInt_fitted	splineInt_min_fitted	splineInt_max_fitted		
120	splineArg	splineArg1	splineArg2		
121	splineArg_fitted	splineArg_fitted1	splineArg_fitted2		
122	spl_arg	splineArg1	splineArg2	splineArg_fitted1	splineArg_fitted2
123	spl_int_min	splineInt_min	splineInt_min_fitted		
124	spl_int_max	splineInt_max	splineInt_max_fitted		
125	spl_int	splineInt_min	splineInt_max	splineInt_min_fitted	splineInt_max_fitted
126	n_spl_knots_max	nSplineKnots_max	nSplineKnots_max_fitted		
127	splineRef	splineRef0	splineRef1	splineRef2	
128	splineRef_fitted	splineRef_fitted0	splineRef_fitted1	splineRef_fitted2	splineRef_fitted3
129	spl_log	splineLog	splineLog_fitted		
130	spline_theta_min	spline_theta_min1	spline_theta_min2		
131	spline_theta_max	spline_theta_max1	spline_theta_max2		
132	spline_int_ratio1_thr	splineIntRatio1_thr	splineIntRatio1_thr_fitted		
133	splineIntRatio_min	splineIntRatio_min1	splineIntRatio_min2		
134	splineIntRatio_max	splineIntRatio_max1	splineIntRatio_max2		
135	splineIntRatio1	splineIntRatio_min1	splineIntRatio_max1		
136	splineIntRatio2	splineIntRatio_min2	splineIntRatio_max2		
137	splineIntRatio1_thr_min	splineIntRatio1_thr	splineIntRatio_min1		
138	splineIntRatio1_thr_min_fitted	splineIntRatio1_thr_fitted	splineIntRatio_min_fitted1		
139	spline_theta_min_fitted	spline_theta_min_fitted1	spline_theta_min_fitted2		
140	spline_theta_max_fitted	spline_theta_max_fitted1	spline_theta_max_fitted2		
141	splineIntRatio_min_fitted	splineIntRatio_min_fitted1	splineIntRatio_min_fitted2		
142	splineIntRatio_max_fitted	splineIntRatio_max_fitted1	splineIntRatio_max_fitted2		
143	splineIntRatio_fitted1	splineIntRatio_min_fitted1	splineIntRatio_max_fitted1		
144	splineIntRatio_fitted2	splineIntRatio_min_fitted2	splineIntRatio_max_fitted2		
145	n_splineIntRatio	n_splineIntRatio1	n_splineIntRatio2		
146	n_splineIntRatio_fitted	n_splineIntRatio_fitted1	n_splineIntRatio_fitted2		
147	spl_lastIntRatio_thr	splineLastIntRatio_thr	splineLastIntRatio_thr_fitted		
148	spl_theta_min	spline_theta_min1	spline_theta_min2	spline_theta_min_fitted1	spline_theta_min_fitted2
149	spl_theta_max	spline_theta_max1	spline_theta_max2	spline_theta_max_fitted1	spline_theta_max_fitted2
150	spl_int_ratio1_thr_min	splineIntRatio_min1	splineIntRatio1_thr	splineIntRatio_min_fitted1	splineIntRatio1_thr_fitted
151	spl_int_ratio_min1	splineIntRatio_min1	splineIntRatio_min_fitted1		
152	spl_int_ratio_min2	splineIntRatio_min2	splineIntRatio_min_fitted2		
153	spl_int_ratio_max1	splineIntRatio_max1	splineIntRatio_max_fitted1		
154	spl_int_ratio_max2	splineIntRatio_max2	splineIntRatio_max_fitted2		
155	n_spl_int_ratio1	n_splineIntRatio1	n_splineIntRatio_fitted1		
156	n_spl_int_ratio2	n_splineIntRatio2	n_splineIntRatio_fitted2		
157	min_deg_cos	minDeg_cos	minDeg_cos_fitted		
158	max_deg_cos	maxDeg_cos	maxDeg_cos_fitted		
159	deg_cos0	minDeg_cos	maxDeg_cos		
160	deg_cos_fitted	minDeg_cos_fitted	maxDeg_cos_fitted		
161	deg_cos	minDeg_cos	maxDeg_cos	minDeg_cos_fitted	maxDeg_cos_fitted
162	spl_unc_wt	splineUnc_wt	splineUnc_wt_fitted		
163	spl_res_wt	splineRes_wt	splineRes_wt_fitted		
164	spl_CS_wt	splineCS_wt	splineCS_wt_fitted		

No.	Alias	I parameter	II parameter	III parameter	IV parameter
165	geom_avg	geomAvg	geomAvg_fitted		
166	main_dev_type	mainDevType	mainDevType_fitted		
167	dev_cap_type	devCapType	devCapType_fitted		
168	spline_theta_range	spline_theta_rangeMin	spline_theta_rangeMax		
169	relCorrRangeMax	relCorrRangeMax1	relCorrRangeMax2		
170	relSD_CS_mode_thr	relSD_CS_mode_thr1	relSD_CS_mode_thr2		
171	output_interm	output_interm0	output_interm1		
172	avg_period_min	avg_period_min_CS	avg_period_min_DCS		
173	avg_period_max	avg_period_max_CS	avg_period_max_DCS		
174	avg_period_CS	avg_period_min_CS	avg_period_max_CS		
175	avg_period_DCS	avg_period_min_DCS	avg_period_max_DCS		
176	avg_period	avg_period_min_CS	avg_period_max_CS	avg_period_min_DCS	avg_period_max_DCS
177	adapt_theta_min	adapt_theta_min1	adapt_theta_min2		
178	rel_err_tol	relErr_tol	relErr_tol_ref		
179	Elwert	Elwert1	Elwert2		
180	T1_thr1	T1_thr0_1	T1_thr_fitted_1		
181	T2_thr1	T2_thr0_1	T2_thr_fitted_1		
182	Ep_thr1	Ep_thr0_1	Ep_thr_fitted_1		
183	Z_a_thr1	Z_a_thr0_1	Z_a_thr_fitted_1		
184	Z_a_b_thr1	Z_a_b_thr0_1	Z_a_b_thr_fitted_1		
185	T1_thr2	T1_thr0_2	T1_thr_fitted_2		
186	T2_thr2	T2_thr0_2	T2_thr_fitted_2		
187	Ep_thr2	Ep_thr0_2	Ep_thr_fitted_2		
188	Z_a_thr2	Z_a_thr0_2	Z_a_thr_fitted_2		
189	Z_a_b_thr2	Z_a_b_thr0_2	Z_a_b_thr_fitted_2		
190	T1_thr0	T1_thr0_1	T1_thr0_2		
191	T2_thr0	T2_thr0_1	T2_thr0_2		
192	Ep_thr0	Ep_thr0_1	Ep_thr0_2		
193	Z_a_thr0	Z_a_thr0_1	Z_a_thr0_2		
194	Z_a_b_thr0	Z_a_b_thr0_1	Z_a_b_thr0_2		
195	T1_thr_fitted	T1_thr_fitted_1	T1_thr_fitted_2		
196	T2_thr_fitted	T2_thr_fitted_1	T2_thr_fitted_2		
197	Ep_thr_fitted	Ep_thr_fitted_1	Ep_thr_fitted_2		
198	Z_a_thr_fitted	Z_a_thr_fitted_1	Z_a_thr_fitted_2		
199	Z_a_b_thr_fitted	Z_a_b_thr_fitted_1	Z_a_b_thr_fitted_2		
200	T1_thr	T1_thr0_1	T1_thr_fitted_1	T1_thr0_2	T1_thr_fitted_2
201	T2_thr	T2_thr0_1	T2_thr_fitted_1	T2_thr0_2	T2_thr_fitted_2
202	Ep_thr	Ep_thr0_1	Ep_thr_fitted_1	Ep_thr0_2	Ep_thr_fitted_2
203	Z_a_thr	Z_a_thr0_1	Z_a_thr_fitted_1	Z_a_thr0_2	Z_a_thr_fitted_2
204	Z_a_b_thr	Z_a_b_thr0_1	Z_a_b_thr_fitted_1	Z_a_b_thr0_2	Z_a_b_thr_fitted_2
205	CS_int_useHeaders	CS_int_useHeaders0	CS_int_useHeaders1	CS_int_useHeaders2	
206	CS_int_isAbsErr	CS_int_isAbsErr0	CS_int_isAbsErr1	CS_int_isAbsErr2	
207	CS_int_T1_low_max	CS_int_T1_low_max1	CS_int_T1_low_max2		
208	CS_int_T1_high_min	CS_int_T1_high_min1	CS_int_T1_high_min2		
209	CS_int_Ep_T1	CS_int_Ep_T1_min	CS_int_Ep_T1_max		
210	CS_int_relErrThr	CS_int_relErrThr1	CS_int_relErrThr2		
211	CS_int_T1_min	CS_int_T1_low_min	CS_int_T1_high_min2		
212	CS_int_T1_max	CS_int_T1_high_max	CS_int_T1_low_max2		
213	CS_int_input_fn	CS_int_fn_low	CS_int_fn_high	CS_int_fn_interm	
214	CS_int_appr	CS_int_appr_low	CS_int_appr_high	CS_int_appr_interm	
215	CS_int_IV	CS_int_IV_low	CS_int_IV_high	CS_int_IV_interm	
216	CS_int_input_fn_0	CS_int_fn_low_0	CS_int_fn_high_0	CS_int_fn_interm_0	
217	CS_int_appr_0	CS_int_appr_low_0	CS_int_appr_high_0	CS_int_appr_interm_0	
218	CS_int_IV_0	CS_int_IV_low_0	CS_int_IV_high_0	CS_int_IV_interm_0	
219	CS_int_nKnots	CS_int_nKnots_min	CS_int_nKnots_max	CS_int_IV_interm_0	

11. Displaying the S integral data

The S integral data, the phase shifts, the normalization factors, the physical parameters and most of the control parameters used in stage 1 are stored in binary files created by the subroutine `S_integrals` (see Section 2 and Section 4). The program “`Read_S_integrals.exe`” displays some of those data on the screen. The displayed data include most of the parameters of subroutine “`S_integrals`” that were used for generating the S integral data, as well as the values of all phase shifts, all normalization factors, and S integrals for any pair of values of κ_1 and κ_2 specified by the user. The parameter values must be specified on the command line or in a parameter file in the same way as for `BREMS`, i.e., using the format “`<parameter_name>=<parameter_value>`” (there must be no spaces before or after the equality sign). The other rules of using the parameter file are the same as in the case of `Brems.exe` (see Section 2). The names, descriptions, and default values of all parameters of `Read_S_integrals.exe` are given below.

11.1. Physical parameters

- 7.1.1–4. These four parameters are the same as parameters No. 1.1.1–4 of `S_integrals` (see Section 4.1), i.e., they specify the atomic number, initial electron energy, final electron energy, and photon energy, respectively.
- 7.1.5–6. These two parameters are the same as parameters No. 1.1.5 (“IV”) and No. 1.1.10 (“Zi”) of `S_integrals`, respectively (see Section 4.1). They are used only to determine if the additional increase of the default values of `Kmax1` and `Kmax2` must be applied in the case of an ion (see also the description of parameter No. 1.3.2 “`Kmax1`” in Section 4.3).

11.2. Parameters defining the sets of S integrals and of terms of the truncated partial-wave series

- 7.2.1–3. The meanings, default values and names of these three parameters are the same as the meanings, default values and names of parameters No. 7–9 of the main program (see end of Section 2).
- 7.2.4–21. The meanings, default values, names and aliases of these 18 parameters are the same as the meanings, default values, names and aliases of parameters No. 1.3.1–18 of `S_integrals` (see Section 4.3). However, these parameters are not required to be exactly equal to the corresponding parameters of the subroutine `S_integrals`. The set of values of κ_1 , κ_2 and l defined on the command line or in the parameter file is required only to be contained inside the set of values of κ_1 , κ_2 and l corresponding to the specified files with the S integral data. If it is not so and if `Kmin1` = `Kmin2` = 1 and `isAbs_K1` = `isAbs_K2` = 1, then `Kmax1`, `Kmax2` or `lmax` will be reduced automatically to make them equal to the corresponding values of the S integral data.
- 7.2.22. “**S_data**” is an integer number equal to 1, 2, or 3, which is interpreted as follows. If `S_data`=1, then the “original” set of S integrals will be loaded (see also Section 1.8 and Section 4.4). If `S_data` = 2, then the “alternative” set of S integrals will be loaded. In the latter case, the files with the plus sign ‘+’ appended to the end of the file name will be loaded in addition to the files with original names (without the additional ‘+’). If `S_data` = 3, then only the part of the alternative dataset that is not contained in the original dataset will be loaded (i.e., only the files with ‘+’ appended to the end of the original file name will be loaded). The default value of parameter “`S_data`” is equal to 1.
- 7.2.23–27. The meanings, default values and names of these five parameters are the same as the meanings, default values and names of parameters No. 1.4.1–5 of `S_integrals` (see Section 4.4). These parameters are used to define the value of `Kmax1`⁺, i.e., the maximum value of $|\kappa_1|$ in the alternative set of S integrals.
- 7.2.28. “**accuracy_level**” has the same meaning as parameter No. 1 of the main program of `BREMS` (it is described in Section 2). When $T_1 \leq 3$ MeV, the default value of `accuracy_level` is equal to 1. When $T_1 > 3$ MeV, the default value of `accuracy_level` is equal to 2.

7.2.29. “**Z_def**” has the same meaning as parameter No. 7 of the main program of BREMS (it is described in Section 2). When $T_1 \leq 3$ MeV or when $Z \geq 7$, the default value of parameter “**Z_def**” is equal to 0. When $T_1 > 3$ MeV and $Z < 7$, the default value of parameter “**Z_def**” is equal to 7.

11.3. Parameters indicating the data to be displayed

7.3.1. “**iDelta**” is a “switch” (“0” or “1”) indicating whether the values of the phase shifts and normalization factors must be displayed. The default value of this parameter is 1.

7.3.2–3. “**k1**” and “**k2**” are the values of κ_1 and κ_2 , respectively, corresponding to the S integrals whose values must be displayed. If at least one of these two parameters is zero (the default value), then the table with the values of the S integrals will not be displayed (only the minimum and maximum values of the S integrals will be shown).

7.3.4. “**check**” is a “switch” (1 or 0) indicating if the values of the S integrals interpolated with respect to l (see Section 1.3.3) must be compared with the accurate values of the same integrals. This is possible only when the interpolation with respect to l has been requested (see the descriptions of parameters No. 1.3.15–18 in Section 4.3), and the input file contains the complete set of S integrals (including the accurate values of the S integrals that must be replaced with the interpolated values). The default value of this parameter is equal to 0.

11.4. Parameters indicating the names of the input data files

7.4.1–2. “**prefix**” and “**suffix**”, respectively, have the same meaning as parameters No. 1.9.1–2 of S _integrals (see Section 4.9), i.e., they define the names of the input files with the S integral data. For more information, see the description of parameters No. 1.9.1–2 in Section 4.9. By default, parameters “**prefix**” and “**suffix**” are equal to the empty string.

7.4.3–4. “**first**” and “**last**”, respectively, specify the first and last additional suffix in the names of the files to be loaded. The allowed values of these parameters are integer numbers from 0 to 999. “0” means no additional suffix, and a positive value means that the additional suffix is formed by concatenating the underscore and the specified number. The default value of parameter “**first**” is 0. The default value of “**last**” is 999.

11.5. Other parameters

7.5.1. “**prefix_t**” is a prefix used for creating a smaller file containing only the phase shifts and the total integrals (from 0 to ∞), without the numerical integrals and estimates of the uncertainties (its size is approximately 1/4 of the size of the complete file). The name of this file is formed by adding the specified prefix (“**prefix_t**”) and the suffix “_t” to the original file name (here, “t” stands for “total integrals only”). **prefix_t** replaces the prefix of the original file name (specified by parameter No. 7.4.1), and the suffix “_t” is appended to the suffix of the original file name (specified by parameter No. 7.4.2). The “_t” file may also be used as an input file for the second stage (i.e. for the subroutine Bremsstrahlung). If this parameter is not specified, then the “_t” file will not be created.

11.6. Information displayed on the screen by Read_S_integrals.exe

Read_S_integrals.exe attempts to read all the data corresponding to the specified limits of κ_1 , κ_2 and l from the specified files, and displays both some overall information about the loaded dataset and the data corresponding to the user-specified pair of values of κ_1 and κ_2 . The S integral data may be loaded from several files with names differing by the additional suffix “_1”, “_2”, ..., “_999” (see also the description of parameter No. 1.9.8 of S _integrals in Section 4.9).

Before displaying the data stored in the indicated binary files, Read_S_integrals.exe displays the default values of several parameters, which were not explicitly specified by the user and which are used for defining the subset of S integrals to be analyzed. All the data displayed after this

preliminary information is loaded from the files with S integral data. The list of all variables loaded from the mentioned files, whose values are displayed by Read_S_integrals.exe, is below:

- the maximum absolute values of κ_1 , κ_2 and l in all files that were loaded (“Kmax1_file”, “Kmax2_file”, “lmax_file”, respectively),
- the total number of the data files loaded;

most of the data defining the calculation parameters (i.e., the energies, numerical tolerances, precision level, etc.) from the last loaded file. The amount of this type of data in the S integral data file depends on the version number of the file (the latter number is not the same as the version number of the program). For example, most of it is absent in version 0 files (such as the “_t” files mentioned in the description of parameter No. 7.5.1). In the case of version number 26 (the maximum possible S integral data file version number at the time of this writing), this part of the displayed data consists of the following entries:

- BREMS version number used for creating the data file (if different versions of BREMS were used to calculate numerical and analytical integrals, then both version numbers are displayed),
- date and time of last modification of the executable used for creating the data file ((if different versions of the BREMS executable were used to calculate numerical and analytical integrals, then both timestamps are displayed),
- the values of parameters of S_integrals No. 1.1.1–5, 1.1.10, 1.1.12–15, 1.1.32, 1.2.1–6, 1.3.1–6, 1.3.11–12, 1.3.15–18, 1.5.1–8, 1.6.1–7, 1.7.1–12, 1.8.1. The photon energy is denoted “Ep”, and the notations of all other variables in this block of output data are the same as in the descriptions of the corresponding parameters of S_integrals (see Section 4), with the exception of “R_atom”, which in this case denotes the *final* value of the cutoff radius of the potential function (the initial value of this parameter is denoted “R_atom_init”),
- the values of three processing times (in seconds): the time of the numerical integration (from 0 to r_0) “time [0 to r0]”, the time of the analytical integration (from r_0 to ∞) “time [r0 to Inf]”, and the total duration of stage 1 (“total time”),
- the final precision level, i.e., the approximate numbers of significant digits used for calculating the analytical parts of the S integrals (“n_digits”),
- estimate of the final maximum relative error of the analytical integrals after optimization of the precision level (“maxRelErr_a”),
- the final values of the six variables corresponding to parameters No. 1.3.1–6 of S_integrals (using the same notations as in the descriptions of the corresponding parameters in Section 4.3). The final values of Kmax1 and Kmax2 may be less than their original (default or user-specified) values, because S_integrals may reduce them in some situations,
- if some of the values of κ_2 have been “skipped” (see Section 1.3.4), then the number of breakpoints of κ_2 and their values (for an example of a set of breakpoints of κ_2 , see the description of parameters No. 1.3.8–10 in Section 4.3),
- the minimum and maximum values of l for the set of calculated S_1 integrals (“lmin_1” and “lmax_1”, respectively),
- the minimum and maximum values of l for the set of calculated S_2 integrals (“lmin_2” and “lmax_2”, respectively),
- the value of the radial coordinate corresponding to the transition to analytical integration (“r0”). This variable coincides with r_0 from Section 1.2. If the numerical integration region has been extended (see the descriptions of parameters No. 1.5.8 and No. 1.7.4 of S_integrals

in Sections 4.5 and 4.7, respectively), then both the original and the “extended” values of r_0 are displayed (“r0_original” and “r0_extended”, respectively),

- the values of the two phase correction integrals at $r = r_0$ (“Q(1)” and “Q(2)”);
- the version number of the file (“version”);

the next four lines characterize the complete loaded dataset (rather than the last loaded file) and answer the following questions:

- Do all the files contain the test numerical integral data? (see also the description of parameter No. 1.8.1 of S_integrals and Section 1.4),
- Did all wave functions attain the asymptotic form?
- Do all the files contain the total integrals (from 0 to ∞)? If at least one of the files contains the numerical integrals only (from 0 to r_0), then the answer to this question is “No”,
- Do all the files contain the data needed for estimating the uncertainties of the S integrals?

The last line of text in the block specifying the calculation parameters displays the minimum version number of all loaded files with the S integral data.

The final part of the data displayed by Read_S_integrals.exe contains the values of the phase shifts, normalization factors, and S integrals, as well as their uncertainties. First, if the display of the phase shifts has been requested (see the description of parameter No. 7.3.1), then the normalization factors (“A”) and phase shifts (“delta”), well as their ranges of variation (“A_range” and “delta_range”, respectively), which are stored in the S integral data files, are displayed for each energy and each value of κ (these ranges are defined as the differences of the maximum and minimum values of the normalization factors and phase shifts, respectively, calculated over the last 10 observations of those variables during the initial numerical integration and the last 10 observations during the “test” numerical integration). The values of both $\bar{\delta}_\kappa$ (used in the asymptotic expressions of the wave functions (1.1.18)) and δ'_κ (defined by Eq. (4.11.1)) are shown (the headers of the corresponding columns are “delta” and “delta'”, respectively). If the screening function approaches zero at $r \rightarrow \infty$, then the value of $\bar{\delta}_\kappa$ approaches $\pi/2$ at large negative values of κ , whereas the value of δ'_κ approaches zero (see Eq. (4.11.1)). However, the estimate of the latter value is not affected by cancellation errors caused by calculating the difference of two very similar numbers, because δ'_κ is the primary quantity (whose values are stored in the S integral data file). I.e., the program calculates $\bar{\delta}_\kappa$ from δ'_κ rather than the other way around.

If the last loaded data file corresponds to $IV = 1$ (unscreened point-Coulomb potential) and $iExact < 2$ (numerical estimation of phase shifts), then the exact phase shifts (calculated according to Eqs. (1.1.23), (1.1.24) and (1.1.25)) are displayed in addition to the phase shifts calculated by numerical solution of the coupled radial Dirac equations. If the point-Coulomb field has been truncated ($R_{atom} \neq 0$), then the values of $\tilde{\delta}_\kappa$ stored in the S integral data files should not be expected to be close to the values given by Eq. (1.1.23)), but this difference should be approximately the same for all κ if R_{atom} is sufficiently large (see the remark after Eq. (1.2.3) in Section 1.2). The values of the latter difference are shown in the column “difference”. If $R_{atom} > 0$, then the difference obtained after the additional subtraction of the term $\nu \ln(2pR_a)$ is shown in the column “difference2” (the latter difference should approach zero when $R_a \rightarrow \infty$).

If interpolation of S integrals with respect to l has been requested (see Section 1.3.3), then the numbers of non-interpolated and interpolated S integrals are shown next. In addition, the numbers of integrals interpolated on logarithmic scale and the number of integrals interpolated on the linear scale are shown (the interpolation method is described in Section 1.3.3). If the latter number is greater than the former, this indicates that the “envelope” of the dependences $S_1(l)$ and $S_2(l)$ has mainly oscillatory character (as in Fig. 2d), otherwise this dependence is mainly

exponential (as in Fig. 2c). In the case “check=1” (see the description of parameter No. 7.3.4), the maximum absolute and relative differences of interpolated and non-interpolated S integrals are shown (“maxAbsDiff” and “maxRelDiff”, respectively), along with the corresponding values of κ_1 , κ_2 and l and the difference of the other kind (these eight values are denoted “k1_maxAbsDiff”, “k2_maxAbsDiff”, “l_maxAbsDiff”, “relDiff_maxAbsDiff”, “k1_maxRelDiff”, “k2_maxRelDiff”, “l_maxRelDiff”, “absDiff_maxRelDiff”). **Note:** A large value of the maximum relative difference does not necessarily imply large inaccuracies of the cross sections, because the largest relative errors of the interpolation with respect to l occur near the values of l where the mentioned envelope changes sign (see Fig. 2d in Section 1.3.3). Since the corresponding values of the S integrals are very small, they do not affect the cross section significantly, and the large values of their relative errors do not have any important consequences.

Next, the maximum and minimum values of the S_1 and S_2 integrals (“S1” and “S2”, respectively) are displayed along with their absolute uncertainties (“err_S1” and “err_S2”, respectively). The indices of the displayed S integrals are indicated in parentheses after “S1” and “S2” in this order: κ_1 , κ_2 , l . After that, the two phase shifts ($\bar{\delta}_\kappa$) corresponding to the values of κ_1 and κ_2 specified on the command line are displayed (“delta1” and “delta2”, respectively, followed by the values of κ_1 and κ_2 in parentheses). If $\kappa_1 < 0$ or $\kappa_2 < 0$, then the value of δ'_κ (defined by Eq. (4.11.1)) is displayed before the value of $\bar{\delta}_\kappa$ (the value of δ'_κ is denoted “delta'”). Finally, a table of values of the S_1 and S_2 integrals corresponding to the values of κ_1 and κ_2 specified on the command line and their percent uncertainties is displayed. This table consists of 7 columns:

- 1) values of l ,
- 2) values of the S_1 integrals,
- 3) absolute uncertainties of the S_1 integrals,
- 4) relative uncertainties of the S_1 integrals (in percent, i.e., multiplied by 100),
- 5) values of the S_2 integrals,
- 6) absolute uncertainties of the S_2 integrals,
- 7) relative uncertainties of the S_2 integrals (in percent, i.e., multiplied by 100).

If interpolation of S integrals with respect to l has been applied (see Section 1.3.3), then the interpolated values are indicated by the minus sign before their absolute and relative uncertainties (the absolute uncertainties of the interpolated values are calculated by linear interpolation of the absolute uncertainties of the non-interpolated S integrals, which correspond to the knots of the cubic spline). If the uncertainties cannot be estimated due to absence of the “test” integrals in the available data (see Section 1.4), then the error estimates are set to zero in the case of non-interpolated S integrals, whereas the value of -1 is displayed instead of the error estimates of interpolated S integrals. The table with the S integrals will be displayed only if both values of κ specified by parameters No. 7.3.2–3 are represented in the available data. If it is not so and if both κ_1 and κ_2 are non-zero, then a corresponding error message will be displayed at the beginning of the output data. If κ_1 or κ_2 is zero, then this error message will not be displayed.

12. Using the interaction potential data in BREMS

As mentioned in Section 1.1, the definition of the interaction potential (or the screening function) in the code of BREMS in general consists of two independent terms: the point-nucleus interaction potential (or the point-nucleus screening function) and the finite-nucleus correction. The first mentioned term includes the electron screening effects, whereas the second term includes the nuclear size effects. The finite-nucleus correction is calculated using one of three predefined analytical approximations of the nuclear charge distribution (see Section 1.1.6 and Section 4.2). The type of the point-nucleus interaction potential to be used during the calculation of the S integrals is defined by parameter No. 1.1.5 of S_integrals (see Section 4.1). The name of this parameter (and of the corresponding variable in the source code) is “IV”. Three types of the point-nucleus interaction potential are currently allowed:

- IV = 1: the point-Coulomb potential $V(r) = -\alpha Z / r$ (the unscreened nucleus),
- IV = 2: the screening function equal to a linear combination of up to 200 decaying exponentials,
- IV = 3: the Kohn-Sham (KS) potential or a user-specified potential in tabular format.

When the option “IV=3” (the default) is specified, the Kohn-Sham potential is used by default. The text files with the Kohn-Sham $V(r)$ data tables are in subfolder “V/Kohn-Sham/” of the BREMS distribution package. There is one file for each value of Z from 1 to 100 (the value of Z is indicated in the name of the corresponding file). Each of these files contains three columns of numbers with the values of the radial coordinate r , the point-nucleus interaction potential $V(r)$, and the point-nucleus screening function $\tilde{V}(r)$. Both r and V are specified in relativistic units (see Section 1.1.1). This means that r is specified in units of $\hat{\lambda}_e = 3.861592679588 \times 10^{-13}$ m, where $\hat{\lambda}_e$ is the reduced Compton wavelength of the electron, and V is specified in units of the electron rest energy $m_0 c^2 = 510.9989461$ keV. In the case “IV=3”, an arbitrary radial potential function $V(r)$ of the form $\bar{V}(r)/r$, where $\bar{V}(r)$ is any smooth negative-valued monotonous function that decays exponentially in the limit $r \rightarrow \infty$ and is equal to $-\alpha Z$ at $r = 0$, may be specified by the user in tabular format by modifying the parameters “dirV” (No. 1.1.6) and “dirV_aux” (No. 1.1.29), which are used to specify the folders with the $V(r)$ data tables. Alternatively, the source code of BREMS (specifically, the subroutine “INITIALIZE” in the file “Brems_common.f90”) could be modified to allow an additional type of the point-nucleus interaction potential (for example, corresponding to IV = 4). This would require specifying the default $V(r)$ data folder corresponding to the option “IV=4” in the source code of BREMS rather than on the command file or in the parameter file. If the format of the corresponding $V(r)$ data files is different from the format described above, then the appropriate changes in the source code should be made. The maximum allowed number of the values of r in the $V(r)$ data table (“breakpoints”) is 5000.

The value of r corresponding to the first point of the $V(r)$ data table (r_1) cannot be zero (i.e., it must be positive). r_1 should not be too small, because it is used for setting the upper limits of the increment of r for numerical quadrature and of the step size of the Hamming’s modified predictor-corrector algorithm (see the descriptions of parameters No. 1.7.3 and No. 1.7.5 of $S_{\text{integrals}}$ in Section 4.7). A very small value of r_1 may cause a decrease of the mentioned step sizes. This, in turn, would increase the calculation time.

Cubic spline interpolation of the screening function $\tilde{V}(r)$ is applied between the discrete values of r in the $V(r)$ data tables. If the input data table contains the values of the point-nucleus interaction potential or point-nucleus screening function (without the nuclear size effects), then the dependence of \tilde{V} on r in the interval $0 < r < r_1$, where r_1 is the first value of r in the $V(r)$ data table, is approximated by a Taylor series expansion, with the coefficients calculated from the approximation of the screening function by a linear combination of up to 50 decaying exponentials. This is the default behavior. There is also an option to calculate the values of $\tilde{V}(r)$ in the interval $0 < r < r_1$ using simple exponential interpolation. If the $\tilde{V}(r)$ input data table includes the nuclear size effects (which implies that the initial grid points correspond to the interior of the nucleus), then linear interpolation is applied in the interval $0 < r < r_1$, where r_1 is the first value of r in the $V(r)$ data table. Exponential extrapolation of the screening function is applied in order to estimate $V(r)$ when r is greater than the last value of r in the data table. The slope and intercept of $\ln \tilde{V}(r)$ in this range of r are determined by linear least squares fitting over a set of 10 adjacent values of r , with an additional constraint requiring the fitted value of \tilde{V} corresponding to the first point in the set to be equal to the corresponding value in the data table. The mentioned set of 10 data points is in the range containing the last 20 points of the data table, excluding the part of the data beginning with the first zero or positive value of V . 11 sets of 10 points are tried, and the one providing the best fit is chosen. After that, the first point of the chosen set of 10 values of r is treated as the last point of the data table (at greater values of r , the interaction potential is calculated using the known slope and intercept of $\ln \tilde{V}(r)$).

Any other point-nucleus interaction potential defined in tabular format may be used instead of the Kohn-Sham potential, with the condition that it is described by a positive-valued screening function, which is a monotonous function equal to 1 at $r=0$ and decaying exponentially when $r \rightarrow \infty$, and which can be approximated by a cubic spline between any two adjacent points of the data table. In addition, any point-nucleus interaction potential defined in tabular format may be fitted by a linear combination of up to 200 decaying exponentials by the method described in Section 1.9. This is a necessary first step before calculation of the atomic form factor and the approximate DCS based on the screened Born approximation using the formulas of Section 1.1.2.

By default, when the option “IV=2” is specified, the point-nucleus screening function is expressed as a linear combination of up to 50 exponentials (1.1.34a), with the a - and b -coefficients calculated by fitting the corresponding dataset, which has been loaded from a file in the folder “V/Kohn-Sham”. These coefficients are stored in the files “V/Kohn-Sham/FitData.txt” and “V/Kohn-Sham/FitData_lo.txt” (see also the description of parameters No. 1.1.22–23 in Section 4.1). The only non-default option used in generating those files was “R_atom_max=1e4” (see the description of parameter No. 5.1.10 in Section 8.1). The folder “V/Kohn-Sham_appr/” contains the files obtained by transforming the same interaction potential into tabular format. The data in these files are identical to the point-nucleus interaction potential used in the case “IV=2 appr=4” and with the other control parameters equal to their default values (see also the description of parameter No. 1.1.8 “appr” in Section 4.1). This means that the results obtained using “IV=3 dirV=V/Kohn-Sham_appr/” should be identical to the results obtained using “IV=2 appr=4”, if the other control parameters are equal to their default values in both cases.

In the case of an ion, the screening function is defined according to Eq. (1.2.5). Everything that was said above about the screening function pertains only to the “normalized” variable part of the point-nucleus screening function, i.e., to the term $\tilde{V}_p(r)$ in Eq. (1.2.4a–c). The input screening function data (either loaded from a file or defined on the command line) are used to construct only the mentioned term, and the final screening function is subsequently calculated by applying the linear transform defined by Eq. (1.2.5). However, the input data files may contain the true (unnormalized) point-nucleus screening function of an ion (i.e., it may approach a non-zero value as r approaches ∞). In such a case, the term $\tilde{V}_p(r)$ in Eq. (1.2.4c) is calculated by applying the opposite transform to the input data:

$$\tilde{V}_p(r) = \frac{\tilde{V}_{in}(r) - i_{in}}{1 - i_{in}}, \quad (12.1)$$

where $\tilde{V}_{in}(r)$ is the input screening function, which is assumed to be equal to 1 at $r=0$ and to i_{in} at $r \rightarrow \infty$. Thus, the ion charge used for the calculations (Zi) may be different from the ion charge corresponding to the input data (Zi_{in}).

13. The test run

13.1. The description of the test run and the output files

In the subfolder “Test_runs” of the BREMS installation folder, there is the Windows batch file “Brems_79_100keV_KS.bat”, which performs the entire set of calculations described in Section 2 for the case when the target is gold ($Z=79$), incident electron energy is 100 keV, the photon energy is 10 keV or zero, and the Kohn-Sham (KS) interaction potential is used. The corresponding two command lines are

```
..\Brems.exe Z=79 T1=0.1 Ep=0.01 suffix=_KS del_S_int=0
```

and

```
..\Brems.exe Z=79 T1=0.1 Ep=0 suffix=_KS KS del_S_int=1
```

All files created by running the mentioned batch file are in the same subfolder. The file “Screen_output_Z=79_T1=0.1_Ep=0.01.txt” contains the complete text that is displayed on the screen during the first mentioned call to Brems.exe. These files were created by executing the mentioned batch file on a notebook computer with an Intel Core i5-8300H processor and 64-bit

Windows 10 (no other processor-intensive tasks were being run at the same time). Explanations of various parts of the screen output contained in the file “Screen_output_Z=79_T1=0.1_Ep=0.01.txt” are provided in Section 13.2. The batch file “Read_S_integrals_79_100keV_10keV_KS.bat” can be used to display all the phase shifts, the normalization factors, and the values of the S integrals corresponding to $\kappa_1 = 14$ and $\kappa_2 = 15$, which are stored in the binary file with the S integral data created by the first mentioned call to Brems.exe.

Since some of the stages of the calculation are relatively long, the program displays some intermediate data every few seconds in order to inform the user about the progress of the calculation. When $k \neq 0$, BREMS calculates two sets of numerical integrals (in stage 1): the one corresponding to the specified parameters, and the “test” set, which is calculated with all computational tolerances and step sizes greater by a factor of 2 (this is done in order to estimate the uncertainties of the S integrals). When $k = 0$, the numerical integration is much shorter (because in this case the S integrals are not calculated numerically; only the system of ODEs (1.1.16a,b) is solved at the stage of the numerical integration). At the end of the calculation, the values of the scaled single differential cross section and the extrapolated cross section are displayed. If the user does not request to keep the files with the intermediate data (such as the values of the S integrals and the values of the CS and the DCS for each value of κ_{\max}) and does not request to create the additional files (such as the file with the comparison of the fitted values of the CS obtained at several values of the endpoint of the fitting interval of κ_{\max}), then the output data of Brems.exe are written to four ASCII files (file name extension “.txt”). This number does not include up to four files with the data of the reference DCS and shape function (SF) No. 1 (which are calculated using the Born approximation with or without screening by default) and reference DCS and SF No. 2 (which are calculated using the Sommerfeld-Maue approximation with the next-to-leading order correction and with or without the screening correction by default), as well as the file “CS_Born_SM.txt” with the corresponding values of the approximate CS. Those files are created if the mentioned reference data are needed and the corresponding data files are initially absent (conversely, if those files already exist at the start of the calculation, then the reference data will be loaded from them). A line of text with the values of the physical parameters, the main control parameters and the scaled CS calculated in stage 2 (before extrapolation of its dependence on κ_{\max}) is appended to the file “CS.txt”, and a line of text with the κ_{\max} -fitted (i.e., extrapolated to $\kappa_{\max} \rightarrow \infty$) value of the scaled CS is appended to the file “CS_fitted.txt” (in this file, the values of the original and κ_{\max} -fitted CS are in the columns with headers “CS_MA[kmax]” and “CS_fitted[k->Inf]” respectively). The values of the scaled DCS and SF are written to the two files whose names start with “DCS_fitted_” and “ShapeFn_fitted_”, respectively. The remaining part of the latter two filenames indicates the values of Z , T_1 and k , using the format “Z_T.TE±XX_k.kkkE±YY_KS.txt”, where “Z” is the atomic number, “T.TE±XX” is the kinetic energy of the incident electron (MeV) rounded to 2 significant digits in scientific notation, and “k.kkkE±YY” is the energy of the bremsstrahlung photon (MeV) rounded to 4 significant digits in scientific notation (“E±XX” and “E±YY” are the respective decimal exponents). The first four columns in the latter two files contain values of the angle θ in degrees, values of the original (unfitted) scaled partial-wave (PW) DCS or SF, values of the spline-fitted PW DCS or SF, and values of the κ_{\max} -fitted (i.e., extrapolated to $\kappa_{\max} \rightarrow \infty$) scaled DCS or SF. In all output files, the values of the scaled CS and DCS are given with 15- or 18-digit precision using scientific notation. The units of the scaled CS and DCS are mb and mb/sr, respectively. When $T_1 < 1$ MeV (where T_1 denotes the initial kinetic energy of the electron), the values of the DCS and the SF are calculated for 181 equidistant values of θ from 0° to 180° by default (when $1 \text{ MeV} \leq T_1 \leq 3 \text{ MeV}$, the default density of points in the angular range $0^\circ \leq \theta \leq 10^\circ$ is increased by a factor of 5, and when $T_1 > 3 \text{ MeV}$, the density in the entire angular range $0^\circ \leq \theta \leq 180^\circ$ is additionally doubled by default). If the mentioned batch file is executed repeatedly, then additional lines will be appended to the files “CS.txt” and “CS_fitted.txt”, and the other two mentioned files will be overwritten.

Notes: 1. The values of the scaled CS and DCS in the output data (including the data displayed on the screen) are defined as the left-hand sides of Eq. (1.1.5) and Eq. (1.1.4), respectively, i.e., they are equal to the true cross sections multiplied by k/Z^2 (the units are indicated after Eq. (1.1.5) and Eq. (1.1.4)).

2. The values of the shape function are defined as the ratio of the DCS and the angular integral of the same DCS (the latter integral is calculated numerically).

3. During the calculation, in order to avoid text wrapping (which would reduce readability of the output data on the screen), the screen buffer width must be at least 235. On Windows, this can be achieved, e.g., by entering “mode 235” at the command prompt in the console window before starting the calculation (this command is included in the mentioned batch file).

13.2. The screen output of the test run

Below is the complete screen output displayed during the first call to Brems.exe in the Windows batch file “Test_runs\Brems_79_100keV_KS.bat” (the corresponding command line is “Brems.exe Z=79 T1=0.1 Ep=0.01”), with explanations of each part of the output text (the screen output and its explanations are printed in different typefaces). The only omitted part of the displayed text is the version number, which is displayed immediately after starting BREMS. This output was produced using a notebook computer with an Intel Core i5-8300H processor and 64-bit Windows 10, without any other processor-intensive tasks running in the background at the same time. The complete text that is displayed on the screen during the mentioned call to Brems.exe is in the file “Test_runs\Screen_output_Z=79_T1=0.1_Ep=0.01.txt”. The nine ASCII files created during this run are also included in the BREMS distribution package.

1) At first, the values of several control parameters that were not explicitly specified by the user are displayed:

```

IV = 3
accuracy_level = 1
ndp = -300
k12ratio = 1
Kmax1 = 80
Kmax2 = 80
isAbs_K1 = 1
isAbs_K2 = 1
k2_breakpoint1 = 30
k2_step = 5
lmax = 80
lmax_MP = 32
tol_A = 0.000000E+00
tol_delta = 0.000000E+00
Q_last = -1.000000E-08
R_atom = -2.000000E+01
pr_transition2 = -8.000000E+02
r_incr_max = -1.000000E-02
delta_V_max = 1.000000E-02
maxRelErr = 5.000000E-02
maxRelErr2 = 1.000000E-03
nErrMax = 6
vary_h_CS = 10
vary_h_DCS = 0
fitRange_CS = 3
fitRange_DCS = 2
avg_period_min_CS = 5
avg_period_min_DCS = 5

```

2) The next eight lines display the sequence number of the current stage, the relative deviation of the tabular point-nucleus screening function at the first radial breakpoint of the data table $\tilde{V}(r_1)$ from its “reference” value $\tilde{V}_{\text{ref}}(r_1)$ (see also the description of parameter No. 1.1.26 “file_Taylor”), the total number of S integrals (1.1.15a,b), the total number of S_{ij} integrals ($i, j = 1, 2$) defined by Eq. (1.2.7), and the total number of terms of the form (1.2.13) that have to be added up during

calculation of the coefficients of the linear combinations of the integrals (1.2.14a,b). It is denoted “`nterms_tot`”. The time of the analytical integration is proportional to the latter number (another factor that affects the time of the analytical integration is the precision level used). The alternative values of the same numbers to be used in QP or MP mode are shown with the suffix “MP”. These numbers are less than the ones to be used in DP mode because of the smaller maximum value of l in the sum (1.1.10). In this example, the maximum value of l_{\max} in DP mode is 80 (it is denoted “`lmax`” in the previous excerpt), but in QP or MP mode it is less by a factor of 2.5, i.e., 32 (denoted “`lmax_MP`” in the previous excerpt):

STAGE 1:

Relative deviation of the screening function at the first radial breakpoint from the reference value specified in the file “`..\V/Kohn-Sham/TaylorCoefs.txt`”: -1.7755881E-04

Number of S integrals = 415000
 Number of S integrals using MP = 127724

Number of integrals of $r^2*(j \text{ or } y)_{n1}*(j \text{ or } y)_{n2}*j_{n3}$ = 294404
 Number of integrals of $r^2*(j \text{ or } y)_{n1}*(j \text{ or } y)_{n2}*j_{n3}$ using MP = 84828

`nterms_tot` = 7138212801
`nterms_tot_MP` = 789216035

3) After the preliminary information described above, the numerical integration begins. During the numerical integration, a line with the current values of several variables is printed on the screen every 5 seconds. This line contains the following information: (a) the current time of the numerical integration (in seconds), (b) the sequence number of the last step of the numerical quadrature (“`i`”), (c) the current value of the radial coordinate r (“`r`”), (d) the percentage done, i.e., the ratio of the current value of r and the limiting radius (this entry is present only if the limiting radius has been defined, i.e., when the interaction potential is “truncated”, i.e., when $R_{\text{atom}} \neq 0$, or during the “test” numerical integration, or when $pr_{\text{transition}2} \neq 0$ and $r < pr_{\text{transition}2} / p_2$), (e) the current values of $p_1 r$ and $p_2 r$ (“`p(1)*r`” and “`p(2)*r`”, respectively), (f) the number of wave functions that have not attained the asymptotic form yet (“`Nasymp`”), (g) the current values of the S integrals (“`S1`” and “`S2`”) corresponding to the largest κ_1 , κ_2 and l , with an additional condition that $\kappa_2 \neq \kappa_1$ (the indices of the displayed S integrals are indicated in parentheses after “`S1`” or “`S2`” in this order: κ_1 , κ_2 , l), (h) the maximum ranges of variation of A_κ and $\tilde{\delta}_\kappa$ over the last 10 “test” points (“`A_range`” and “`delta_range`”). If `A_range` and `delta_range` have not been calculated yet, then they are not shown. If all wave functions have attained the asymptotic form (1.1.18), i.e., if “`Nasymp`” is zero, but the other conditions for terminating the numerical integration are not satisfied yet, then the last two entries of the output line change: “`A_range`” and “`delta_range`” are replaced by the values of the two phase correction integrals (“`Q(1)`” and “`Q(2)`”). Since these lines are rather long (234 characters), some of the mentioned entries are omitted in the sample output, which is presented below. The omitted text is marked by an ellipsis (however, if the ellipsis is at the end of a line and is not preceded by a comma, then it is actually present in the text displayed by BREMS):

Inverse minimum momentum transfer = 59.3602411010909
 Cutoff radius of the potential function = 1187.20482202182

Calculating the continuum wave functions and the numerical integrals...

The integration step became too large. Restarting the numerical integration...

5.3 s: `i` = 100, `r` = 3.813853E+00 (0.3%), ...

10.3 s: `i` = 2360, `r` = 3.142615E+02 (26.4%), ...

15.3 s: `i` = 6040, `r` = 8.756607E+02 (73.7%), ... `A_range`= 1.061334E-03, `delta_range`= 9.438250E-03.

Wave functions corresponding to energy No.1 attained asymptotic form at $r \leq 1.187205E+03$, ...

The power-series solution algorithm terminated at $r = 1.187205E+03$, ...

Time of the initial numerical integration = 18.3 s

`r0` = 1.18720482202181779E+03, ... `Max|S1,2|` = 1.056759E+01, `Min|S1,2|` = 2.962741E-39.

Recalculating ... with the computational tolerances and step sizes greater by a factor of 2...

The integration step became too large. Restarting the numerical integration...

5.0 s: `i` = 1480, `r` = 4.065568E+02 (34.2%), ...

Wave functions corresponding to energy No.1 attained asymptotic form at $r \leq 1.187205E+03$, ...

The power-series solution algorithm terminated at $r = 1.187205E+03$, ...

Time of the test numerical integration = 8.5 s

Total time = 30.2 s

r0 = 1.18720482202181756E+03, ... Max|S1,2| = 1.056758E+01, Min|S1,2| = 2.962736E-39.

4) The information that is displayed after terminating the numerical integration is mostly self-explanatory. It consists of the following items: (a) the maximum change of the numerical S_1 and S_2 integrals after increasing the computational tolerances and step sizes by a factor of 2 (the maximum absolute change is denoted “S1_num_maxDiff_abs” and “S2_num_maxDiff_abs”, respectively, and the maximum relative change is denoted “S1_num_maxDiff_rel” and “S2_num_maxDiff_rel”, respectively), (b) the values of the numerical S integrals and their uncertainties corresponding to the largest absolute values of κ_1 , κ_2 , and l (with the additional condition that $\kappa_2 \neq \kappa_1$), (c) the values of the factors A_{κ_1} and A_{κ_2} in Eqs. (1.1.18) and the corresponding values of $\tilde{\delta}_{\kappa_1}$ and $\tilde{\delta}_{\kappa_2}$ for the same values of κ_1 and κ_2 (the values of $\tilde{\delta}_{\kappa_1}$ and $\tilde{\delta}_{\kappa_2}$ are adjusted by adding $2\pi n$, where n is an integer number, so that the final values of the phase shifts are between $-\pi$ and π), (d) the final values of the phase correction integrals corresponding to the two energies of the electron (those values are displayed only when at least one of them is non-zero, and hence they are not shown in the case of a truncated interaction potential, as in the current example):

The maximum change of the S1 integrals after increasing the ... tolerances and step sizes by a factor of 2:
S1_num_maxDiff_abs = 5.9501128722772023E-05, S1_num_maxDiff_rel = 1.7087470659973444E-01

The maximum change of the S2 integrals after increasing the ... tolerances and step sizes by a factor of 2:
S2_num_maxDiff_abs = 5.6337146108198510E-05, S2_num_maxDiff_rel = 2.2629534673137808E-01

S1(80, 75, 80):
Numerical integral = -1.092983979632039E-035
Test integral = -1.092983979602472E-035
Difference = -2.956719232892391E-046
Relative difference = 2.705180760186248E-011

S2(80, 75, 80):
Numerical integral = 9.921851823579637E-036
Test integral = 9.921851823898483E-036
Difference = -3.188461297080934E-046
Relative difference = -3.213574798107186E-011

Energy No. 1: A(80) = 3.57019724897103E+00, delta(80) = 1.00813975687311E-01
Energy No. 2: A(75) = 3.75291441758888E+00, delta(75) = 1.06236411934692E-01

5) Before calculating the analytical part of the S integrals, the program attempts by default to determine the maximum value of l_{\max} such that double precision is sufficient for the analytical integration and l_{\max} belongs to the interval with the endpoints equal to the values of the two parameters “lmax” and “lmax_MP” mentioned above (thus, not only the precision level is optimized as described in Section 1.3.1, but also the value of l_{\max} is optimized). If no such value of l_{\max} is found, then the analytical integration will be performed using QP or MP, with $l_{\max} = \text{lmax_MP}$. The precision level is optimized for each tested value of l_{\max} . In this example, the final precision level corresponds to QP, and $l_{\max} = 32$. During the subsequent analytical integration, feedback is provided to the user every 10 seconds in the form of messages indicating the percentage of the terms of the type (1.2.13) calculated:

Performing analytical integration to infinity:

Calculating the trigonometric integrals...

p' = p(1) + p(2) + p(3)
p' = p(1) + p(2) - p(3)
p' = p(1) - p(2) + p(3)
p' = p(1) - p(2) - p(3)

Optimizing the precision level...

... 86 digits required with lmax = 80 (maximum relative error = -7.35778E-10). Calculating with lmax = 72...
... 72 digits required with lmax = 72 (maximum relative error = 1.03298E-07). Calculating with lmax = 65...
... 65 digits required with lmax = 65 (maximum relative error = -2.05377E-11). Calculating with lmax = 59...
... 57 digits required with lmax = 59 (maximum relative error = 1.14413E-12). Calculating with lmax = 53...
... 43 digits required with lmax = 53 (maximum relative error = 3.10056E-07). Calculating with lmax = 48...

```

... 43 digits required with lmax = 48 (maximum relative error = -1.22886E-13). Calculating with lmax = 43...
... 28 digits required with lmax = 43 (maximum relative error = 2.87862E-07). Calculating with lmax = 38...
... 28 digits required with lmax = 38 (maximum relative error = 8.07816E-13). Calculating with lmax = 33...
... 28 digits required with lmax = 33 (maximum relative error = -1.50527E-17). Calculating with lmax = 32...
Quadruple precision will be used (~30 significant digits, maximum relative error = 2.72727E-18).

```

```

kmax(1) = 80
kmax(2) = 80
kmax(3) = 32
kmax_tot = 192

```

```

nterms = 789216035

```

```

Number of S integrals = 127724

```

```

Number of integrals of r^2*(j or y)_n1*(j or y)_n2*j_n3 = 84828

```

```

10.0 s: 9.7% of terms calculated.
20.0 s: 18.7% of terms calculated.
30.1 s: 29.7% of terms calculated.
40.1 s: 40.7% of terms calculated.
50.2 s: 50.0% of terms calculated.
60.3 s: 61.7% of terms calculated.
70.3 s: 72.2% of terms calculated.
80.4 s: 83.8% of terms calculated.
90.4 s: 95.9% of terms calculated.

```

6) After terminating the analytical integration, the maximum change of the total S_1 and S_2 integrals, when the phase shift is changed by the value of the corresponding range of δ_{κ} , is displayed (the maximum absolute change is denoted “S1_maxDiff_abs” and “S2_maxDiff_abs”, respectively, and the maximum relative change is denoted “S1_maxDiff_rel” and “S2_maxDiff_rel”, respectively). The last piece of information displayed after terminating the analytical integration and before exiting subroutine “S_integrals” (i.e., before ending stage 1) consists of the final values of the total S integrals (from 0 to ∞) corresponding to the largest absolute values of κ_1 , κ_2 , and l (with the additional condition that $\kappa_2 \neq \kappa_1$), their uncertainties due to the uncertainty of the phase shift, and the total uncertainties. The total uncertainties are calculated by combining the errors of the numerical integration with the errors caused by the uncertainty of the phase shift (the latter two errors are assumed to be independent, hence they are combined in quadrature):

```

The maximum change of S1 integrals after changing the phase shift:
S1_maxDiff_abs = 3.8566088571618806E-06, S1_maxDiff_rel = 1.2017207829324203E+04

```

```

The maximum change of S2 integrals after changing the phase shift:
S2_maxDiff_abs = 4.0098973306709303E-06, S2_maxDiff_rel = 1.1427442645666975E+04

```

```

Analytical integrals calculated in 286.8 s

```

```

S1( 80, 75, 32):
Total integral: -1.055493927801026E-009
Change after modifying delta: 1.025242033836508E-016
Relative change: 9.713386376105979E-008
Total absolute uncertainty: 6.179382195330957E-014
Total relative uncertainty: 5.854493363315537E-005

```

```

S2( 80, 75, 32):
Total integral: 1.207714643976189E-009
Change after modifying delta: 1.126363075090059E-016
Relative change: 9.326400741334938E-008
Total absolute uncertainty: 6.452456101530252E-014
Total relative uncertainty: 5.342699232565957E-005

```

```

Subroutine S_INTEGRALS: elapsed time = 329.6 s

```

7) At the beginning of stage 2, subroutine “Bremsstrahlung” loads the S integral data from the binary files created in stage 1 by subroutine “S_integrals”. If the values of $|\kappa_1|_{\max}$, $|\kappa_2|_{\max}$ or l_{\max} in the available data are less than the values indicated by the input parameters, the latter parameters will be reduced and a corresponding message will be displayed (this is the case in the current example: the original value of l_{\max} is 80, but its value after the mentioned optimization in stage 1 is 32). After that, the “ R factors” (defined by Eq. (1.1.10)) and the spherical harmonics are calculated, and the messages indicating the duration of each of those two stages are displayed. Those two times

are usually a small fraction of the total duration of stage 2, but only if the pre-computed values of the Wigner 3j coefficients in Eq. (1.1.14) are available, or if the maximum values of l_1 and l_2 do not exceed 160. The Wigner 3j coefficients corresponding to $l_{1,2} > 80$ are loaded from the files located in the subfolder “3j”, and if those files are not available, then the mentioned 3j coefficients will be calculated and those files will be created. If the maximum value of l_1 or l_2 is greater than 160 and both l_1 and l_2 are less than 431, then some of the 3j coefficients will be calculated using multiple precision at the precision level of 100 digits, and if $l_1 > 430$ or $l_2 > 430$, then 200-digit precision will be used, which may cause a significant increase of the total processing time:

STAGE 2:

Values of 287276 S integrals are missing.

lmax reduced to 32

Number of R factors = 665600
R factors calculated in 13.1 s

Calculating spherical harmonics...
Spherical harmonics calculated in 1.3 s

8) After calculating the R factors and the spherical harmonics, the calculation of the truncated series (1.1.4) and (1.1.5) begins. The terms of these two series are grouped into sets of terms having the same value of $|\kappa_1|$, $|\bar{\kappa}_1|$ or $|\kappa_2|$. This makes it possible to calculate the values of the mentioned series corresponding to a sequence of increasing values of $\kappa_{\max} = \max(|\kappa_2|)$ and $\max(|\kappa_1|)$ (which is a multiple of κ_{\max} , according to Eq. (1.5.2)). The values of the scaled CS (1.1.5) and DCS (1.1.4) at each angle θ , corresponding to the last (maximum) value of κ_{\max} , are displayed every 5 seconds or at longer intervals (depending on the time needed to process one value of the angle θ). If the “test” values of the CS and DCS have been requested (see the description of parameter No. 2.2.19 in Section 5.2 and the description of the output files of stage 2 in Section 5.8), then the three corresponding sets of cross sections are calculated sequentially, and the current set is indicated by the text “test = 0”, “test = 1” or “test = 2” in the messages that are displayed on the screen:

Calculating cross sections...
0.0 s: test = 0, kmax = 80, CS = 2.78481756580462800E+01
3.0 s: test = 1, kmax = 80, CS = 2.78481988575084891E+01
6.3 s: test = 2, kmax = 80, CS = 2.78481756580447843E+01

Cross sections calculated in 9.7 s

CS = 2.78481756580462800E+01, DCS integral = 2.78482199368491159E+01, rel. diff. = 1.5900073E-06

Subroutine BREMSSTRAHLUNG: elapsed time = 24.2 s (total time = 353.8 s)

9) If reference functions have to be used in stage 3 (see Section 6.5), then the program attempts to load the reference function data from the corresponding files at the start of stage 3. If those files do not exist, then BREMS will recreate them. In order to do that, BREMS enters temporarily into the “special” operation mode described in Section 7. During the calculation of the reference DCS, its values are displayed on the screen every 5 seconds or at longer intervals (depending on the time needed to process one value of the angle θ):

STAGE 3:

Reference DCS No. 1 will be used for cubic spline fitting of the angular dependence of the DCS, or for comparison with it. If this is not required, use T1_thr1>T1, or T2_thr1>T2, or Ep_thr1>Ep.

The reference data file "DCS_Born_screened_79_1.0E-01_1.000E-02.txt" does not exist or is empty. The corresponding data will be recalculated and the file will be recreated.

The screened Born approximation with the Elwert factor will be applied. The analytical expression of the DDCS will be used.

5.0 s: theta = 74.00, DDCS = 2.07072644290354146E+00

10.0 s: theta = 140.00, DDCS = 9.19525399018059408E-01

The SDCS will be calculated by adaptive numerical angular integration of the DDCS.

15.9 s: SDCS = 2.70554545144368639E+01, relErr = 4.4410919E-07, nEval = 45

DDCS integral (10th order Newton-Cotes formula) = 2.70554545144311831E+01 (relative deviation from the value obtained by adaptive numerical integration = -2.0994317E-13)

Subroutine BORN_SM_APPR: elapsed time = 15.9 s (total time = 369.7 s)

Reference DCS No. 2 will be used for cubic spline fitting of the angular dependence of the DCS, or for comparison with it. If this is not required, use T1_thr2>T1, or T2_thr2>T2, or Ep_thr2>Ep.

The reference data file "DCS_SM_NLO_screened_79_1.0E-01_1.000E-02.txt" does not exist or is empty. The corresponding data will be recalculated and the file will be recreated.

The Sommerfeld-Maue approximation with the next-to-leading-order correction, and the screening correction with the Elwert factor will be applied.

5.2 s:	theta = 33.00,	DDCS = 3.70017266048993054E+00,	relErr = 9.7244853E-06,	nEval = 6475
10.2 s:	theta = 61.00,	DDCS = 2.06859722194008633E+00,	relErr = 9.7819157E-06,	nEval = 6623
15.4 s:	theta = 92.00,	DDCS = 1.16899628876405415E+00,	relErr = 9.3067240E-06,	nEval = 4773
20.5 s:	theta = 129.00,	DDCS = 7.65673564868925460E-01,	relErr = 9.9628927E-06,	nEval = 3885

DDCS integral (10th order Newton-Cotes formula) = 2.07587050490960792E+01

Subroutine BORN_SM_APPR: elapsed time = 25.4 s (total time = 395.0 s)

10) The text that is displayed afterwards starts with a reminder about the cubic spline fitting (if it has been requested). The next line repeats the value of $\max(\kappa_{\max})$ and CS from stage 2. Afterwards, the program may display the messages informing the user about the progress of the angular spline fitting of the original partial-wave DCS, if such fitting has been requested (these messages are absent in the example below due to short time of the angular spline fitting in this example). During the subsequent κ_{\max} -fitting of the (D)CS (whose angular dependence may have been spline-fitted previously), the messages informing about the current stage of the calculation are displayed at 5-second or longer intervals. Those messages use the following terms and notations:

- “shift” is the sequence number of the current fitting interval (also called “shift” in this document), which starts from $-\text{shift_k_max}$ (see the description of parameters No. 3.2.7–8) and ends at 0,
- “k_start” and “k_end” are the first and last values of κ_{\max} in the current fitting interval,
- “Nfit” is the number of values of κ_{\max} in the current fitting interval ($\text{Nfit}=\text{k_end}-\text{k_start}+1$),
- “cycle” is the number 1 or 2 indicating which of the two intervals with the same endpoint is currently used (the corresponding number of values of κ_{\max} in the interval is calculated using Eq. (1.5.11b) or Eq. (1.5.11a), respectively, or is equal to the value of parameter $\text{Nfit}_{\text{(D)CS}}$ or to $0.5*\text{Nfit}_{\text{(D)CS}}$, respectively),
- “n” is the sequence number of the current value of the angle θ (if the DCS is currently being fitted), or the number 0 if the CS is currently being fitted (in the latter case, there is also the text “(CS)” after the current elapsed time of stage 3, which is shown at the start of the line),
- “theta” is the current value of the angle θ (in degrees).

The first entry in the first line displayed after the κ_{\max} -fitting (“tol_range”) is the tolerance for the relative range of variation of the DCS in the fitting interval of κ_{\max} . If the range of variation of the DCS as a function of κ_{\max} for a particular value of θ is less than this tolerance, then BREMS will assume that there is no significant change, and the nonlinear fitting will not be performed for that angle. The second and third entries in the same line are the two limiting values of the angle θ (“theta_limits”) where the dependence of the DCS on κ_{\max} changes its direction. The first limit is the last value of θ where the mentioned dependence is a monotonous increase, and the second limit is the first value of θ where the mentioned dependence is a monotonous decrease (the range of variation of the DCS in the fitting interval is greater than tol_range in both cases). If the value of a limit is equal to -1 , this means that the DCS does not belong to the corresponding category at any value of θ .

Afterwards, the program may display the messages informing the user about the progress of the angular spline fitting of the κ_{\max} -fitted DCS, if such fitting has been requested (these messages are absent in the example below due to short time of the angular spline fitting in this example).

Since the κ_{\max} -fitting is by default performed three times (using the original partial-wave DCS and the two “test” sets of the partial-wave DCS, as explained in Section 6.16), there are three sets of messages. Each one of them is preceded by a message informing about the data that are currently being fitted (the “test” datasets are fitted first). The last four lines contain the value of the fitted CS, its relative deviation (in percent) from the original (unfitted) value of the CS, the angular integral of the fitted DCS and its relative deviation from the fitted CS, the duration of stage 3, and the total duration of the current run of BREMS:

```
Cubic spline fitting of the angular dependence of the original partial-wave DCS and kmax-fitted DCS will be
performed. If this is not required, use splineRef=0 and splineRef_fitted=0.
```

```
kmax =          80 ,   CS =   27.8481756580463
```

```
Processing the data in files "_CS_..._test2" and "DCS_..._test2":
```

```
Performing the angular spline fitting of the partial-wave DCS...
```

```
[shift = -8] The relative correction of the DCS due to kmax-fitting is equal to 0.0E+00 at theta = 180.00.
The endpoint of the angular spline-fitting interval will be changed to 180.00 degrees.
```

```
5.3 s: shift = -7, k_start = 45, k_end = 73, Nfit = 29, n = 1, theta = 0.00
10.8 s: shift = -3, k_start = 48, k_end = 77, Nfit = 30, n = 1, theta = 0.00
tol_range = 1.0E-03, theta_limits = 61.00 and -1.00
```

```
Processing the data in files "_CS_..._test" and "DCS_..._test":
```

```
Performing the angular spline fitting of the partial-wave DCS...
```

```
[shift = -8] The relative correction of the DCS due to kmax-fitting is equal to 0.0E+00 at theta = 180.00.
The endpoint of the angular spline-fitting interval will be changed to 180.00 degrees.
```

```
5.6 s: shift = -6, k_start = 46, k_end = 74, Nfit = 29, n = 1, theta = 0.00
11.7 s: shift = -1, k_start = 50, k_end = 79, Nfit = 30, n = 1, theta = 0.00
tol_range = 1.0E-03, theta_limits = 61.00 and -1.00
```

```
Processing the data in the main "_CS_..." and "DCS_..." files:
```

```
Performing the angular spline fitting of the partial-wave DCS...
```

```
[shift = -8] The relative correction of the DCS due to kmax-fitting is equal to 0.0E+00 at theta = 180.00.
The endpoint of the angular spline-fitting interval will be changed to 180.00 degrees.
```

```
5.3 s: shift = -7, k_start = 45, k_end = 73, Nfit = 29, n = 1, theta = 0.00
11.2 s: shift = -2, k_start = 49, k_end = 78, Nfit = 30, n = 1, theta = 0.00
tol_range = 1.0E-03, theta_limits = 61.00 and -1.00
```

```
Fitted CS =                2.78510972630472438E+01
Correction due to fitting = 1.2565E-02 %
Fitted DCS integral =      2.78532654882837143E+01 (deviation from the fitted CS = 7.7851E-03 %)
```

```
Subroutine BREMS_FIT: elapsed time =      89.7 s (total time =      443.5 s)
```

It should be noted that some variation in the format and quantity of the information that is displayed and written to files is possible, depending on the values of some input parameters. For example, if the photon energy is zero, then the format of the information that is displayed in stage 1 is different from the above example due to significant differences of the calculation procedure.

References

- [1] H. K. Tseng and R. H. Pratt, *Exact Screened Calculations of Atomic-Field Bremsstrahlung* // Physical Review A, Vol. 3, No. 1 (1971) pp. 100–115.
- [2] R. D. Schmickley and R. H. Pratt, *K-, L-, and M-Shell Atomic Photoeffect for Screened-Potential Models* // Physical Review, Vol. 164, No. 1 (1967) pp. 104–116.

- [3] P. Csavinszky, *Approximate Variational Solution of the Thomas-Fermi Equation for Atoms* // Physical Review, Vol. 166, No. 1 (1968) pp. 53–56.
- [4] W. Kohn and L. J. Sham, *Self-Consistent Equations Including Exchange and Correlation Effects* // Physical Review, Vol. 140, No. 4A (1965) pp. A1133–A1138.
- [5] D. A. Liberman, D. T. Cromer, J. T. Waber, *Relativistic self-consistent field program for atoms and ions* // Computer Physics Communications, Vol. 2 (1971) pp. 107–113; D. A. Liberman, D. T. Cromer, J. T. Waber, *Erratum notice* // Computer Physics Communications, Vol. 9 (1975) p. 129.
- [6] M. E. Rose, *Relativistic Electron Theory*, New York: John Wiley & Sons, 1961, 302 p.
- [7] H. K. Tseng, *Energy-angle distributions of bremsstrahlung from intermediate-energy electrons on atoms* // Physical Review A, Vol. 56 (1997) pp. 2868–2871.
- [8] A. Poškus, *BREMS: A program for calculating spectra and angular distributions of bremsstrahlung at electron energies less than 3 MeV* // Computer Physics Communications, Vol. 232 (2018) pp. 237–255.
- [9] A. Poškus, *Shape functions and singly differential cross sections of bremsstrahlung at electron energies from 10 eV to 3 MeV for $Z=1-100$* // Atomic Data and Nuclear Data Tables, Vol. 129–130 (2019) art. No.101277, pp. 1–39.
- [10] H. K. Tseng and R. H. Pratt, *Electron Bremsstrahlung from Neutral Atoms* // Physical Review Letters, Vol. 33 (1974), pp. 516–518.
- [11] H. K. Tseng, R. H. Pratt, C. M. Lee, *Electron bremsstrahlung angular distributions in the 1–500 keV energy range* // Physical Review A, Vol. 19 (1979), pp. 187–195.
- [12] W. Greiner, *Quantum Electrodynamics. Fourth Edition*, Berlin: Springer Verlag, 2009, 448 p.
- [13] L. C. Maximon, A. de Miniac, T. Aniel, E. Ganz, *Tagged photons: An analysis of the Bremsstrahlung cross section* // Physics Reports, Vol. 147, Issue 4 (1987) pp. 189–252.
- [14] A. Mangiarotti and M. N. Martins, *A review of electron-nucleus bremsstrahlung cross sections between 1 and 10 MeV* // Radiation Physics and Chemistry, Vol. 141 (2017) pp. 312–338.
- [15] H. A. Bethe and W. Heitler, *On the stopping of fast particles and on the creation of positive electrons* // Proceedings of the Royal Society of London, Ser. A, Vol. 146 (1934) pp. 83–112.
- [16] F. Sauter, *Über die Bremsstrahlung schneller Elektronen* // Annalen der Physik, Vol. 412 (1934) pp. 404–412.
- [17] H. W. Koch and J. W. Motz, *Bremsstrahlung Cross-Section Formulas and Related Data* // Reviews of Modern Physics, Vol. 31 (1959) pp. 920–955.
- [18] C. Fronsdal and H. Überall, *Polarization of bremsstrahlung from polarized electrons* // Physical Review, Vol. 111 (1958) pp. 580–586.
- [19] A. Sommerfeld and A. W. Maue, *Verfahren zur näherungsweise Anpassung einer Lösung der Schrödinger- an die Diracgleichung* // Annalen der Physik (Leipzig), Vol. 414 (1935) pp. 629–642.
- [20] H. A. Bethe and L. C. Maximon, *Theory of Bremsstrahlung and Pair Production. I. Differential Cross Section* // Physical Review, Vol. 93 (1954) pp. 768–784.
- [21] G. Elwert and E. Haug, *Calculation of Bremsstrahlung Cross Sections with Sommerfeld-Maue Eigenfunctions* // Physical Review, Vol. 183 (1969) pp. 90–105.
- [22] E. Haug, *Bremsstrahlung cross-section with screening and Coulomb corrections at high energies* // Radiation Physics and Chemistry, Vol. 77 (2008) pp. 207–214.
- [23] G. Roche, C. Ducos, J. Proriol, *Bremsstrahlung cross-section formula including a high-order Coulomb correction* // Physical Review A, Vol. 5 (1972) pp. 2403–2408.

- [24] I. S. Gradshteyn and I. M. Ryzhik, *Table Of Integrals, Series, and Products. Seventh Edition*, Elsevier Academic Press, 2007, 1220 p.
- [25] A. Mangiarotti, D. H. Jakubassa-Amundsen, M. N. Martins, *On higher-order corrections to nuclear bremsstrahlung cross sections* // Radiation Physics and Chemistry, Vol. 167 (2020) art. No. 108292, pp. 1–5
- [26] H. Olsen, L. C. Maximon, H. Wergeland, *Theory of High-Energy Bremsstrahlung and Pair Production in a Screened Field* // Physical Review, Vol. 106 (1957) pp. 27–46.
- [27] G. Elwert, *Verschärfte Berechnung von Intensität und Polarisation im kontinuierlichen Röntgenspektrum* // Annalen der Physik, Vol. 426 (1939) pp. 178–208.
- [28] R. H. Pratt and H. K. Tseng, *Tip region of the bremsstrahlung spectrum from incident electrons of kinetic energy 50 keV – 1.84 MeV* // Physical Review A, Vol. 11 (1975) pp. 1797–1803.
- [29] J. C. Slater, *A Simplification of the Hartree-Fock Method* // Physical Review, Vol. 81 (1951) pp. 385–390.
- [30] L. H. Thomas, *The calculation of atomic fields* // Mathematical Proceedings of the Cambridge Philosophical Society, Vol. 23 (1927), pp. 542–548.
- [31] E. Fermi, *Eine statistische Methode zur Bestimmung einiger Eigenschaften des Atoms und ihre Anwendung auf die Theorie des periodischen Systems der Elemente* // Zeitschrift für Physik, Vol. 48 (1928), pp. 73–79.
- [32] P. A. M. Dirac, *Note on exchange phenomena in the Thomas atom* // Mathematical Proceedings of the Cambridge Philosophical Society, Vol. 26 (1930), pp. 376–385.
- [33] R. Latter, *Atomic Energy Levels for the Thomas-Fermi and Thomas-Fermi-Dirac Potential* // Physical Review, Vol. 99 (1955), pp. 510–519.
- [34] D. A. Liberman, *New Potential Function for Atomic and Solid-State Calculations* // Physical Review B, Vol. 2 (1970), pp. 244–248.
- [35] B. Hahn, D. G. Ravenhall, R. Hofstadter, *High-Energy Electron Scattering and the Charge Distributions of Selected Nuclei* // Physical Review, Vol. 101 (1956) pp. 1131–1142.
- [36] F. Salvat, A. Jablonski, C. J. Powell, *ELSEPA – Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules* // Computer Physics Communications, Vol. 165 (2005) pp. 157–190.
- [37] R. H. Helm, *Inelastic and Elastic Scattering of 187-Mev Electrons from Selected Even-Even Nuclei* // Physical Review, Vol. 104 (1956) pp. 1466–1475.
- [38] W. Bühring, *Computational improvements in phase shift calculations of elastic electron scattering* // Zeitschrift für Physik, Vol. 187 (1965), pp. 180–196.
- [39] F. Salvat and R. Mayol, *Accurate numerical solution of the Schrödinger and Dirac wave equations for central fields* // Computer Physics Communications, Vol. 62 (1991) pp. 65–79.
- [40] F. Salvat, J. M. Fernández-Varea, W. Williamson Jr., *Accurate numerical solution of the radial Schrödinger and Dirac wave equations* // Computer Physics Communications, Vol. 90 (1995) pp. 151–168.
- [41] F. J. Corbato and J. L. Uretsky, *Generation of Spherical Bessel Functions in Digital Computers* // Journal of the ACM, Vol. 6, No. 3 (1959) pp. 366–375.
- [42] T. A. Beu, *Introduction to Numerical Programming*, Boca Raton, FL: CRC Press, 2015, 654 p.
- [43] A. Ralston and H. S. Wilf, *Mathematical Methods for Digital Computers*, New York: John Wiley & Sons, 1960, 294 p.

- [44] A. Ralston, *Runge-Kutta Methods with Minimum Error Bounds* // Mathematics of Computation, Vol. 16 (1962) pp. 431–437.
- [45] R. May and J. Noye, *The Numerical Solution of Ordinary Differential Equations: Initial Value Problems* // Computational Techniques for Differential Equations, Elsevier Science Publishers, Amsterdam, 1984, pp. 1–94.
- [46] R. L. Malig, *Comparison of predictor-corrector methods*, Monterey, CA: Naval Postgraduate School, 1972, 204 p.
- [47] *NIST Digital Library of Mathematical Functions*. <http://dlmf.nist.gov/>, Release 1.0.15 of 2017-06-01. F. W. J. Olver, A. B. Olde Daalhuis, D. W. Lozier, B. I. Schneider, R. F. Boisvert, C. W. Clark, B. R. Miller, and B. V. Saunders, eds. [Online]
- [48] A. Messiah, *Quantum Mechanics*, New York: Dover Publications, Inc., 2014, 1152 p.
- [49] D. H. Bailey, *A Fortran-90 Based Multiprecision System* // RNR Technical Report RNR-94-013 (January 6, 1995), 10 p.
- [50] *High-Precision Software Directory, MPFUN90 (A Fortran-90 arbitrary precision package)*. <http://crd-legacy.lbl.gov/~dhbailey/mpdist/> [Online]
- [51] *Quadruple Precision Code*. <http://wp.csiro.au/alanmiller/F.html> [Online]
- [52] H. K. Tseng and R. H. Pratt, *Electron bremsstrahlung energy spectra above 2 MeV* // Physical Review A, Vol. 19, No. 4 (1979) pp. 1525–1528.
- [53] J. A. Nelder and R. Mead, *A Simplex Method for Function Minimization* // The Computer Journal, Vol. 7, Issue 4 (1965) pp. 308–313.
- [54] R. W. Hamming, *Numerical Methods for Scientists and Engineers. Second Edition*, New York: Dover Publications, Inc., 1986, 722 p.
- [55] A. Pořkus, *Calculation of double differential cross sections of electron–atom bremsstrahlung by the relativistic partial-wave method at electron energies greater than 3 MeV* // Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, Vol. 508 (2021) pp. 49–62.
- [56] W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, *Numerical Recipes in C: The Art of Scientific Computing. Second Edition*, Cambridge: Cambridge University Press, 1992, 994 p.
- [57] W. F. Perger, A. Atul Bhalla, M. Nardin, *A numerical evaluator for the generalized hypergeometric series* // Computer Physics Communications, Vol. 77, Issue 2 (1993) pp. 249–254.
- [58] R. S. Caswell and L. C. Maximon, *Fortran Programs for the Calculation Of Wigner 3j, 6j, and 9j Coefficients For Angular Momenta ≤ 80* . US Department Of Commerce, National Bureau of Standards, NBS Technical Note 409 (1966), 72 p.
- [59] F. Salvat, *PENELOPE-2014: A Code System for Monte Carlo Simulation of Electron and Photon Transport*, OECD Nuclear Energy Agency, Doc. No. NEA/NSC/DOC(2015)3.
- [60] *Computer Physics Communications Program Library*. <https://data.mendeley.com/journal/00104655> [Online]