Problems

5.8. Relaxation in rotational diffusion. Consider a spherical colloidal particle that has a labelled direction, which is immersed in a fluid. The director $\hat{n}$ experiences rotational diffusion described by the equation

$$\frac{\partial f}{\partial t} = D_r \vec{\nabla}^2_{\hat{n}} f \ . \tag{1}$$

Expanding the distribution function in Fourier modes in 2D or in spherical harmonics in 3D, show that the relaxation time of the slowest mode is proportional to $\tau_r = D_r^{-1}$. Compute the proportionality constant.

Reformulation: Solve eq. (1) in 2D or 3D.

2D:

- We can write the derivative operator $\vec{\nabla}$ from Cartesian into polar coordinates. Then we have simply to drop the radial dependence and we have our $\vec{\nabla}_{\hat{n}}$:

$$\vec{\nabla} = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} = \begin{pmatrix} \sin\phi \frac{\partial}{\partial r} + \frac{\cos\phi}{r}\frac{\partial}{\partial \phi} \\ \cos\phi \frac{\partial}{\partial r} - \frac{\sin\phi}{r}\frac{\partial}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \sin\phi & \frac{\cos\phi}{r} \\ \cos\phi & -\frac{\sin\phi}{r} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \phi} \end{pmatrix} = D_{2,\phi} \cdot \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \phi} \end{pmatrix} \ , \tag{2}$$

$$\vec{\nabla}_{\hat{n}} = D_{2,\phi} \cdot \begin{pmatrix} 0 \\ \frac{\partial}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \frac{\cos\phi}{r}\frac{\partial}{\partial \phi} \\ -\frac{\sin\phi}{r}\frac{\partial}{\partial \phi} \end{pmatrix} = \frac{1}{r}\begin{pmatrix} \cos\phi \\ -\sin\phi \end{pmatrix}\frac{\partial}{\partial \phi} \ , \tag{3}$$

and

$$\begin{aligned} \vec{\nabla}^2_{\hat{n}} =& \frac{1}{r}\begin{pmatrix} \cos\phi \\ -\sin\phi \end{pmatrix}^{\top} \cdot \frac{\partial}{\partial \phi}\left[\frac{1}{r}\begin{pmatrix} \cos\phi \\ -\sin\phi \end{pmatrix}\frac{\partial}{\partial \phi}\right] \\ =& \frac{1}{r^2}\begin{pmatrix} \cos\phi & -\sin\phi \end{pmatrix}\left[\begin{pmatrix} \cos\phi \\ -\sin\phi \end{pmatrix}\frac{\partial^2}{\partial \phi^2} + \begin{pmatrix} -\sin\phi \\ -\cos\phi \end{pmatrix}\frac{\partial}{\partial \phi}\right] \overset{r=1}{\equiv} \frac{\partial^2}{\partial \phi^2} \ . \end{aligned} \tag{4}$$

- Making the ansatz for f in terms of $\hat{n}$, which is just ϕ:

$$f(\hat{n};t) = f(\phi;t) = \sum_{k=-\infty}^{+\infty} f_k(t) e^{-ik\phi} \ , \tag{5}$$

we get eq. (1) as

$$\sum_{k=-\infty}^{+\infty} e^{-ik\phi}\frac{\partial f_k}{\partial t} = D_r \frac{\partial^2}{\partial \phi^2}\sum_{k=-\infty}^{+\infty} f_k e^{-ik\phi} = -D_r \sum_{k=-\infty}^{+\infty} k^2 f_k e^{-ik\phi} \tag{6}$$

- Integrating $\int_{-\pi}^{+\pi} d\phi\, e^{im\phi}$ gets rid of the sum and the exponent:

$$\frac{\partial f_m}{\partial t} = -D_r m^2 f_m \ , \tag{7}$$

giving immediately the solution

$$f_m(t) = f_m(0) e^{-D_r m^2 t} \ , \tag{8}$$

which gives for the smallest non-constant mode $m = 1$ the proportionality factor 1.

3D shortcut:

- Since we know that the Laplacian in 3D in spherical coordinates has the spherical harmonics $Y_\ell^m(\theta,\phi)$ as eigenfunctions

$$r^2\vec{\nabla}^2 Y_\ell^m(\theta,\phi) = -\,\ell(\ell+1)Y_\ell^m(\theta,\phi) \ , \tag{9}$$

and we simply drop the r dependence, we can write our function as

$$f(\theta,\phi;t) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} f_m^\ell(t) Y_\ell^m(\theta,\phi) \ . \tag{10}$$

Since the spherical harmonics fulfill the orthogonality relation

$$\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} Y_\ell^m(\theta,\phi) Y_{\ell'}^{m'\,*}(\theta,\phi) d^2\Omega = \delta_{\ell\ell'}\delta^{mm'} \ , \tag{11}$$

we can integrate over the angles and get from eq. (1)

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\frac{\partial f_m^\ell(t)}{\partial t} Y_\ell^m(\theta,\phi) = D_r\vec{\nabla}_{\hat{n}}^2\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} f_m^\ell(t) Y_\ell^m(\theta,\phi) = D_r\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} -\ell(\ell+1) f_m^\ell(t) Y_\ell^m(\theta,\phi) \tag{12}$$

the simple relation

$$\frac{\partial f_m^\ell(t)}{\partial t} = -D_r\ell(\ell+1) f_m^\ell(t) \ , \tag{13}$$

which has the immediate solution

$$f_m^\ell(t) = f_m^\ell(0) e^{-D_r\ell(\ell+1)t} \ , \tag{14}$$

which gives for the smallest non-constant mode $\ell = 1$ the proportionality factor 2.