Universités Paris 6, Paris 7 & Paris-Sud, École Normale Supérieure, École Polytechnique.
M2 – Parcours de Physique Quantique ; M2– Parcours de Physique Macroscopique

Statistical approaches to condensed matter - exam

Walking on the sphere

This part should be written on a separate paper. It will be graded over 10 points.
Question 12 is quite independent from the others.
La rédaction pourra se faire en français pour ceux qui le souhaitent

Introduction. The goal is here to retrieve the expression of the angular dependence of Laplace operator (∇^2) in spherical coordinates, from a Fokker-Plack treatment of a well chosen stochastic process on the unit sphere. To this end, we consider a random walker on the surface of the sphere, the position of which is measured by a unit vector $\widehat{n}$. The walker follows a path made up of a succession of random steps such that its probability density $P(\widehat{n}, t)$ at time t follows the diffusion equation

$$\frac{\partial P}{\partial t} = D_r \, \nabla^2 P, \tag{1}$$

where D_r is the rotational diffusion coefficient.

1/ Provide a physical example where such a process could be realized.

2/ What is the dimension of D_r ? Try to estimate a typical value of D_r for the above physical process.

3/ What is the value of $P^*(\widehat{n})$, the stationary long-time solution to (1) ? No heavy calculation required here.

We define by (θ, ϕ) the standard spherical coordinates of $\widehat{n}$, such that the walker's position reads, in Cartesian coordinates

$$\left\{ \begin{array}{l} x = \sin\theta \, \cos\phi \\ y = \sin\theta \, \sin\phi \\ z = \cos\theta \end{array} \right. \qquad \text{with} \qquad \left| \begin{array}{l} 0 \leqslant \theta \leqslant \pi \\ 0 \leqslant \phi \leqslant 2\pi \end{array} \right.$$

We denote by $\widetilde{P}(\theta, \phi)$ the joint probability distribution function of θ and ϕ, which fulfills

$$\int \widetilde{P}(\theta, \phi) \, d\theta d\phi = 1.$$

Attention must be paid to the fact that $\widetilde{P}(\theta, \phi)$ and P, which is itself a function of θ and ϕ only, do differ.

4/ Show that

$$\widetilde{P}(\theta, \phi) = f(\theta) \, P(\theta, \phi)$$

where f if a simple function (which one ?).

5/ What are the stationary distributions of θ (referred to as $p^*(\theta)$) and ϕ (referred to as $q^*(\phi)$) ?

We now enter into the specification of the stochastic process, for each of the variables θ and ϕ. Due to the random displacements, the angle ϕ obeys a Langevin equation of the form

$$\frac{d\phi}{dt} = R_\Phi(t)$$

where the noise term is such that

$$\langle R_\Phi(t)\rangle = 0 , \qquad \big\langle R_\Phi(t)\, R_\Phi(t')\big\rangle = 2D_\Phi\, \delta(t-t')$$

with D_Φ to be specified below. Likewise, we have for θ

$$\frac{d\theta}{dt} = -\frac{\partial V}{\partial \theta} + R_\Theta(t) \qquad \text{with} \qquad \langle R_\Theta(t)\rangle = 0 , \qquad \big\langle R_\Theta(t)\, R_\Theta(t')\big\rangle = 2D_\Theta\, \delta(t-t').$$

6/ Why do we have to enforce an external potential $V(\theta)$ acting on θ, while there is none for ϕ ? (no calculation required).

7/ Write the Fokker-Planck equation obeyed by the distribution of θ, $p(\theta,t)$. Knowing the desired long time solution $p^*(\theta)$, show that $V(\theta) = -D_\Theta \log f(\theta)$, where $f(\theta)$ is the same simple function as in question 4.

8/ We wish to determine the noise amplitude D_Φ. What is the displacement on the sphere associated to an incremental change $\theta \to \theta + d\theta$? Same question when $\phi \to \phi + d\phi$. Invoking an isotropy argument of the random walk, show that $g(\theta)\, D_\Phi = D_\Theta$, where g is another simple function to be precized.

9/ Gathering results, write the Fokker-Planck equation for the joint probability distribution $\widetilde{P}(\theta,\phi)$.

10/ Remembering the connection between $\widetilde{P}$ and P, rewrite the previous Fokker-Planck relation into a partial differential equation for $P(\theta,\phi)$. What is the resulting expression of ∇^2 in spherical coordinates ? How is D_Θ related to D_r ?

11/ What form does the diffusion equation for P take when D_Φ is chosen independent from θ ?

12/ Assuming that the initial conditions are such that P is a function of the sole coordinate θ, reproduce the key arguments for an arbitrary space dimension d, and give the relevant expression of ∇^2. Check that the result makes sense for $d = 2$ (cylindrical/circular geometry). More difficult : write ∇^2 in dimension 4 (again excluding the radial dependence, i.e. on the 3-sphere), but now in full glory, accounting for all angles (denoted θ, ϕ, ψ). Hint : it is useful to find a recursive expression connecting ∇^2 in dimension d to its counterpart in dimension $d-1$.

13/ Back to three dimensions ($d = 3$, i.e. the 2-sphere). The walker starts from a given arbitrary point on the sphere. Write the general form of the solution to the diffusion equation. It is useful here to remember that as far as angular dependence is concerned, one has $\nabla^2 = -\widehat{L}^2$, $\widehat{L}$ being the angular momentum operator (setting $\hbar = 1$). In addition, the spherical harmonics Y_ℓ^m provide a convenient complete orthonormal family of eigenfunctions verifying

$$\widehat{L}^2\, Y_\ell^m = \ell(\ell+1) Y_\ell^m \qquad \text{with closure relation} \qquad \delta(\widehat{n} - \widehat{n}_0) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y_\ell^m(\widehat{n}) \overline{Y_\ell^m}(\widehat{n}_0),$$

where the over-bar denotes the complex conjugate. What is the spectrum of relaxation times for the diffusion process ? Can you put forward a way to have the system relax according to a particular given mode ?

14/ When (roughly) did Adriaan Fokker and Max Planck complete their work on stochastic processes ?