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

Shearing and tumbling of a rigid polymer

This part should be written on a separate paper. It will be graded over 10 points.
It is possible to start the problem at question 6 (the first 5 questions will not be generously graded).
La rédaction pourra se faire en français pour ceux qui le souhaitent.

We are interested in the behaviour of a rod-like colloid in a uniform shear flow. The rod-like object undergoes Brownian motion, and has a tendency to align with the local flow, under the action of viscous drag forces. We will focus on the orientational degrees of freedom of the rod, discarding its center-of-mass coordinates. We will thus introduce two spherical angles θ and φ to monitor the rod's orientation, given by unit vector $\widehat{n}$ (see Fig. 1). In addition, inertial effects will be neglected (over-damped limit), and noise is responsible for a diffusive behaviour of orientation $\widehat{n}$, with rotational diffusion constant D. We will therefore study rotational Brownian motion in an external force field. To completely set the stage, it remains to specify that for the uniform shear flow, the fluid velocity at point $\vec{r}$ with Cartesian coordinates (x, y, z) reads

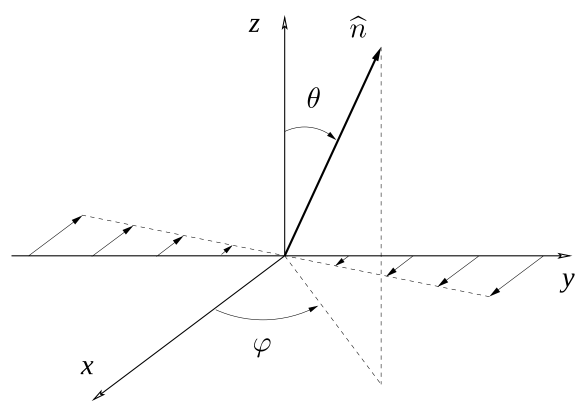

FIGURE 1 – *Sketch of the shear flow and definition of angular variables (usual spherical coordinates where the angle φ is defined in the xy plane). The rod has orientation $\widehat{n}$ and the flow is along x, depending solely on y.*

$$\vec{v} = \dot{\gamma}\, y\, \widehat{x},$$

where $\dot{\gamma}$ is the shear rate and $\widehat{x}$ is the unit vector along the x-direction.

1) What is the physical dimension of the shear rate $\dot{\gamma}$? To which other relevant scale should this quantity be compared to in the present case ?

2) What is the physical origin of the noise term ?

3) (subsidiary) In the over-damped limit to which we restrict the description, the torque on the rod should vanish at all times, but for the effect of the noise. We start by the noiseless limit (no noise), in order to derive the differential equation obeyed by θ and φ. Show that

$$\dot{\theta} = \dot{\gamma}\, F(\theta)\, F(\varphi) \tag{1}$$
$$\dot{\varphi} = -\dot{\gamma}\, \sin^2 \varphi. \tag{2}$$

Determine the function F.

4) Provide the solution of Eq. (2), given that $\varphi = \varphi_0$ at $t = 0$. Is the motion periodic, or not ?
Hint : Compute $\dfrac{d}{d\varphi}\left(\dfrac{\cos\varphi}{\sin\varphi}\right)$

5) Still in the noiseless case, transform (1) into an equation for $d\theta/d\varphi$, introduce $t = \tan\theta$ and then give the solution $\theta(t)$. How does θ behave in the long time limit ?

From now on, we study the effect of noise on the dynamics of the rod-like colloid, whereby Eqs. (1) and (2) become

$$\dot{\theta} \;=\; \dot{\gamma}\,\sin\theta\,\cos\theta\,\sin\varphi\,\cos\varphi \,+\, D\,\frac{\cos\theta}{\sin\theta} \,+ R_\Theta(t) \tag{3}$$

$$\dot{\varphi} \;=\; -\dot{\gamma}\,\sin^2\varphi \,+\, R_\Phi(t), \tag{4}$$

with $\langle R_\Theta(t)\rangle \;=\; \langle R_\Phi(t)\rangle \;=\; 0$ and

$$\big\langle R_\Theta(t)\,R_\Theta(t')\big\rangle \;=\; 2D\,\delta(t-t'), \tag{5}$$

$$\big\langle R_\Phi(t)\,R_\Phi(t')\big\rangle \;=\; 2\,\frac{D}{\sin^2\theta}\;\delta(t-t'). \tag{6}$$

We further introduce the Weissenberg number $W = \dot{\gamma}/D$.

6) For $\dot{\gamma} = 0$, why is there a drift term in Eq. (3) (contribution in $D\cos\theta/\sin\theta$) while there is none in Eq. (4) ?

We denote by $P(\widehat{n}, t)\,d\widehat{n}$ the probability for finding the rod's orientation at time t in a small solid angle $d\widehat{n}$ around $\widehat{n}$. P only depends on angles θ and φ (in addition to t) but differs from the joint probability density of the couple (θ, φ), that we define as $\widetilde{P}$. The latter is normalised as $\int \widetilde{P}\,d\theta d\varphi = 1$.

7) Show that

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

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

8) What is the Fokker-Planck equation obeyed by $\widetilde{P}$?

9) Show that the corresponding equation for P is

$$\frac{\partial P}{\partial t} \;+\; \frac{\dot{\gamma}}{\sin\theta}\,\frac{\partial}{\partial\theta}\left(\sin^2\theta\,\cos\theta\,\sin\varphi\,\cos\varphi\,P\right) \;-\; \frac{\dot{\gamma}}{\sin\theta}\frac{\partial}{\partial\varphi}\left(\sin^2\varphi\,\sin\theta\,P\right) \;=\; \begin{array}{c}\text{something...}\\ \text{what ?}\end{array} \tag{7}$$

10) Put the previous relation as a continuity (conservation) equation. What is the expression of the current $\overrightarrow{J}$? Explain why its form was to be expected.

11) Is it possible or not to find solutions with $W \neq 0$ and $\overrightarrow{J} = \overrightarrow{0}$?

In the remainder and unless otherwise stated, we focus on the steady state behaviour for small W.

12) What form does P take when $W = 0$?

13) We now look for a solution in a perturbative fashion

$$P(\theta, \varphi) \;=\; \text{cst} \,+\, \alpha\,W\,(\sin\theta)^2\,\sin(2\varphi) \,+\, \mathcal{O}(W^2) \tag{8}$$

What are the expressions of the constants cst and α ?
Hint : note that $(\sin\theta)^2\,\sin(2\varphi)$ is an eigenfunction of ∇^2 (with integer eigenvalue).

14) We define a fictitious particle having angles Θ and Φ such that its velocity $\overrightarrow{\mathcal{V}}$ matches the current $\overrightarrow{J}$: $\overrightarrow{J} \;=\; P\overrightarrow{\mathcal{V}}$. Show that to leading order in W, Φ only changes and has furthermore a constant time derivative.

15) From what precedes, conclude that the fictitious particle undergoes periodic motion. What is the period ? Compare to the noiseless case $W \to \infty$. Speculate freely on the effect of increasing W.

16) What is the qualitative form of the steady state solution P for large W ?

In this final part, the goal is to retrieve the form (8) by going back to the Langevin description of Eqs. (3) and (4)

17) In the strong noise regime, P is to leading order isotropic. Averaging out the Langevin equations over this distribution, explain why the variable φ only does matter. A schematic argument only is expected.

18) We therefore assume that θ is given, and concentrate on Eq. (4). What is the Fokker-Planck equation obeyed by the probability density $p(\varphi, t)$ of variable φ ?

19) Look for a stationary solution of this equation in the form

$$p(\varphi) = \frac{1}{2\pi} + W\, g(\varphi) + \mathcal{O}(W^2)$$

where g is a simple trigonometric function of φ to be specified, depending also on θ as a parameter. Explain the connection with Eq. (8).

Reminder / glossary :

- a rod-like molecule : *une molécule en forme de bâtonnet.*
- drag force : *force de traînée*
- $\cos(2\theta) = 2\cos^2\theta - 1\,; \quad \sin(2\theta) = 2\cos\theta\,\sin\theta.$
- in spherical coordinates, discarding radial dependence (with radial distance $r = 1$), and introducing the unit vectors $\vec{u}_\theta$ and $\vec{u}_\varphi$ as in Fig. 2, the velocity of a point with coordinates (θ, φ) is $\dot\theta\,\vec{u}_\theta + \sin\theta\,\dot\varphi\,\vec{u}_\varphi$, the dot denoting time derivative. In addition, one has : $\vec{\nabla} = \vec{u}_\theta\,\partial_\theta + (\vec{u}_\varphi/\sin\theta)\,\partial_\varphi$

For a vector field $\vec{A} = A_\theta\,\vec{u}_\theta + A_\varphi\,\vec{u}_\varphi$:

$$\operatorname{div}\vec{A} = \nabla\cdot\vec{A} = \frac{1}{\sin\theta}\frac{\partial(\sin\theta\,A_\theta)}{\partial\theta} + \frac{1}{\sin\theta}\frac{\partial A_\varphi}{\partial\varphi}$$

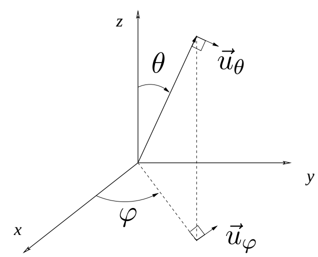

FIGURE 2 – *Unit vectors in spherical coordinates*

Finally : $$\nabla^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} = \frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial\theta^2} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}.$$

References :

→ *On the motion of small particles of elongated form suspended in a viscous liquid*, J.M. Burgers, in Second Report on Viscosity and Plasticity, Chapter 3, 16 (4), 113, Kon. Ned. Akad. Wet., North-Holland Publ., Amsterdam, 1938.

→ *Tumbling polymers in a sheared fluid*, G.T. Barkema, D. Panja and J.M.J. van Leeuwen, Dec 2012, seminar in LPT Orsay, unpublished.