Master 2 iCFP - Soft Matter & Physics for biology

Advanced Statistical Physics – Exam

Monday 3 january 2022

Duration : 3h30min.

Lecture notes are NOT allowed.

⚠ Write Exercices 1 & 2 and Exercice 3 on separate sheets (with your name on both!) ⚠

1 Subdiffusion of a monomer embedded in a long polymer

A. Preliminary : Ornstein-Ulhenbeck process.— We consider a particle submitted to a force $F(y) = -V'(y)$ for potential $V(y) = \frac{\lambda}{2}y^2$ and a Langevin force :

$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} = -V'(y(t)) + \sqrt{2D}\,\eta(t) \tag{1}$$

where $\eta(t)$ is a normalized Gaussian white noise, $\langle\eta(t)\rangle = 0$ and $\langle\eta(t)\eta(t')\rangle = \delta(t-t')$.

1/ Express the solution $y(t)$ as an integral of the noise, for $y(0) = y_0$ fixed.

2/ Deduce $\langle y(t)\rangle$ and $\mathrm{Var}(y(t))$.

3/ Give the conditional probability $P_t(y|y_0)$ (no further calculation needed).

B. Motion of a polymer.— We consider an elongated polymer modelled as an elastic line : the y coordinates of the monomers fluctuate, while the x coordinates are fixed on a lattice, $x \in \mathbb{Z}$ (figure). Monomers are linked by elastic forces, i.e. the potential energy of the line is

$$V(\{y_x\}) = \sum_x \frac{\lambda}{2}(y_{x+1} - y_x)^2 \tag{2}$$

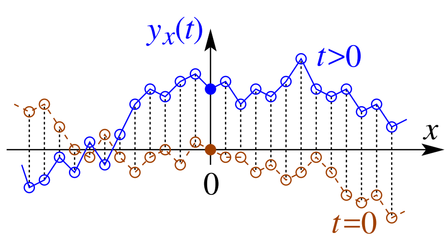


Figure 1: *Directed polymer model.*

1/ Write explicitly the Langevin equation describing the motion of the monomer x

$$\frac{\partial y_x(t)}{\partial t} = -\frac{\partial V}{\partial y_x} + \sqrt{2D}\,\eta_x(t) \tag{3}$$

where the noises are independent Gaussian white noises

$$\left\langle \eta_x(t)\eta_{x'}(t')\right\rangle = \delta_{x,x'}\,\delta(t-t') \tag{4}$$

The continuum limit of this model is known as the *Edwards-Wilkinson model.*

2/ In order to solve the set of coupled equations, we use the discrete Fourier transform :

$$\tilde{y}_k(t) = \sum_x y_x(t)\,\mathrm{e}^{-\mathrm{i}kx} \qquad \text{and} \qquad y_x(t) = \frac{1}{N}\sum_k \tilde{y}_k(t)\,\mathrm{e}^{\mathrm{i}kx} \tag{5}$$

Here we assume a finite number N of monomers. In this case, the summation $\sum_k$ runs over quantized wave vectors $k = 2\pi m/N \in [-\pi, +\pi]$ (with $m \in \mathbb{Z}$). Thus $\frac{1}{N}\sum_k \to \int_{-\pi}^{\pi}\frac{\mathrm{d}k}{2\pi}$ in the large N limit. Note also the useful identities $\sum_x \mathrm{e}^{\mathrm{i}kx} = N\,\delta_{k,0}$ and $\sum_k \mathrm{e}^{\mathrm{i}kx} = N\,\delta_{x,0}$.

Compute the correlator $\langle\tilde{\eta}_k(t)\tilde{\eta}_{k'}(t')\rangle$ for the Fourier components of the noise.

Give the Langevin equation for the Fourier component $\tilde{y}_k(t)$.

3/ Express $\tilde{y}_k(t)$ as an integral of the noise $\tilde{\eta}_k(t)$ [introduce the notation $\Lambda_k = 4\lambda\,\sin^2(k/2)$].

4/ For a non random initial condition $y_x(0) = y_x^0$, show that the fluctuations of the position of the monomer at x are characterized (in the limit $N\to\infty$) by

$$\mathrm{Var}(y_x(t)) = D\int_0^{\pi}\frac{\mathrm{d}k}{\pi}\,\frac{1-\mathrm{e}^{-2\Lambda_k t}}{\Lambda_k} \tag{6}$$

5/ Plot Λ_k as a function of k. For short times, $\lambda t \ll 1$, what is behaviour of $\mathrm{Var}(y_x(t))$? Explain physically.

6/ We now study the long time limit, $\lambda t \gg 1$. Argue that one can approximate the integral over k as $\int_{k_c(t)}^{\pi}\frac{\mathrm{d}k}{\pi}\frac{1}{\Lambda_k}$, where $k_c(t)$ is a time dependent cutoff. Give the expression of $k_c(t)$. Deduce an estimate for the variance and show that $\mathrm{Var}(y_x(t)) \sim t^{2\theta}$ for large time. Give the exponent θ. Comment the result.

2 Scaling of the correlation length

We consider a magnetic system. The correlation length depends on the temperature $t = (T - T_c)/T_c$ and the conjugated field : $\xi(t,h)$. The scaling hypothesis leads to the relation

$$\xi(t,h) = \ell\,\xi(\ell^{y_t}\,t, \ell^{y_h}\,h) \tag{7}$$

where ℓ is the scaling factor. y_t and y_h are the thermal and magnetic exponents.

1/ The critical exponent for the correlation length at zero field is denoted ν and defined by $\xi \propto |T - T_c|^{-\nu}$. Express ν in terms of y_t and y_h.

2/ Similarly, characterize the divergence of ξ as $h \to 0$ when $T = T_c$ in terms of y_t and y_h.

3/ The Onsager-Yang solution for the 2D Ising model shows that the specific heat critical exponent and the order parameter exponent are : $\alpha = 0$ and $\beta = 1/8$. Deduce explicitly the behaviours $\xi(t,0)$ for $t\to 0$ and $\xi(0,h)$ for $h \to 0$ in this case.

Appendix

We recall the two relations $\alpha = 2 - d/y_t$ and $\beta = (d - y_h)/y_t$, where d is the dimension.

3 Liquid crystal

Introduction.— the liquid crystal state is a mesophase with properties intermediate between liquid and crystalline phases. We are here interested in the *nematic* phase which is translationally invariant, like a liquid, but with rotational symmetry partially broken, like in a solid.

Long molecules are in suspension in a liquid, with fluctuating orientations. In the disordered phase the distribution of the orientation of the molecules is *isotropic*, while in the ordered phase (*nematic*) the molecules are on average oriented along a fixed direction given by the unit vector $\vec{n}$.

The three parts **A**, **B** and **C** are independent.

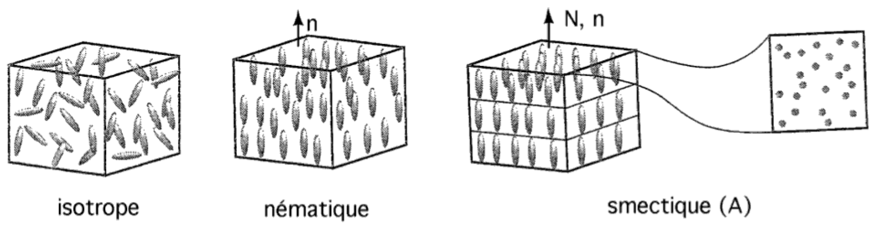


Figure 2: *Three phases of a liquid crystal : isotropic, nematic and smectic.*

A. Order parameter.— In this first part, we clarify the nature of the order parameter. The molecules have an orientation but no direction (i.e. if the axis of the molecule number i is carried by the unit vector $\vec{u}^{(i)}$, the two directions $\vec{u}^{(i)}$ and $-\vec{u}^{(i)}$ correspond to the same state).

1/ Deduce the symmetry of $p(\theta)$, the distribution of the angles $\theta_i \in [0, \pi]$ between the vectors $\vec{u}^{(i)}$ (fluctuating) and $\vec{n}$ (fixed). Give $p(\theta)$ corresponding to the isotropic phase and sketch $p(\theta)$ corresponding to the nematic phase (choose the normalisation $\int_0^\pi \mathrm{d}\theta\, p(\theta) = 1$).

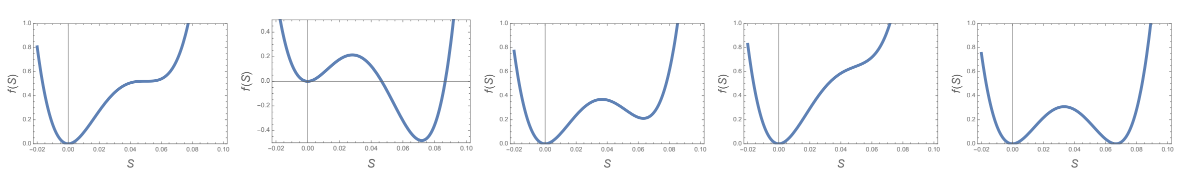
2/ Deduce $\langle \vec{u}^{(i)} \rangle$ in general ($\langle \cdots \rangle$ denotes thermal averaging). Can the order parameter be a vector ?

3/ For each molecule i, we introduce the tensor $Q^{(i)}_{\alpha\beta} = u^{(i)}_\alpha u^{(i)}_\beta - \frac{1}{3}\delta_{\alpha\beta}$ (the greek indices label the three directions x, y and z). Show that the averaged tensor $Q = \langle Q^{(i)} \rangle$ is diagonal for $\vec{n} = \vec{e}_z$ (unit vector along axis Oz). Express the components of Q in term of $S = \langle P_2(\cos\theta_i) \rangle = \int_0^\pi \mathrm{d}\theta\, p(\theta)\, P_2(\cos(\theta))$, where $P_2(x) = (3x^2 - 1)/2$. Give its value corresponding to the isotropic phase, and when the molecules are perfectly aligned (nematic state far from the transition).

4/ Maier and Saupe have proposed a model where the molecules i and j interact through a term of the form $E_{ij} = -\varepsilon \,\mathrm{Tr}\left\{ Q^{(i)} Q^{(j)} \right\} = -\varepsilon \sum_{\alpha,\beta} Q^{(i)}_{\alpha\beta} Q^{(j)}_{\beta\alpha}$ with $\varepsilon > 0$. Argue that this favors the nematic phase.

B. Isotropic-nematic transition.— The nematic state is characterised by the parameter S and the director $\vec{n}$. For symmetry reasons, the Landau free energy only depends on S. Within the Maier-Saupe model, one can show that it presents the $S \to 0$ expansion

$$f(S) = \frac{1}{2} a(T)\, S^2 - \frac{b}{3} S^3 + \frac{c}{4} S^4 \qquad \text{with } a(T) = \tilde{a}\,(T - T_*) \text{ and } \tilde{a},\ b,\ c \text{ positive}\,. \tag{8}$$



(a) $T = T_0$ (b) (c) (d) (e) $T = T_1$

1/ What is the correct ordering for the five plots of $f(S)$ (for decreasing temperature T) ?

2/ Express T_0 and T_1 as a function of T_*, $\tilde{a}$, b and c.
Hint : in order to determine T_1, solve $f(S) = f(0)$ and $f'(S) = 0$.

3/ Does this describe the isotropic-nematic transition ? Is the transition first or second order ? What is the transition temperature ? Plot $S_\star(T)$, the minimum of $f(S)$, as a function of T.

C. Nematic phase.— In this last section, we consider a fixed temperature (below the transition temperature). The Ginzburg-Landau theory involves an elastic energy depending on the local orientation $\vec{n}(\vec{r})$. From symmetry considerations, Frank (1958) has proposed the form

$$F_{\mathrm{el}}[\vec{n}] = \frac{1}{2}\int \mathrm{d}^3\vec{r}\,\left\{K_1\left(\vec{\nabla}\cdot\vec{n}\right)^2 + K_2\left[\vec{n}\cdot\left(\vec{\nabla}\times\vec{n}\right)\right]^2 + K_3\left[\vec{n}\times\left(\vec{\nabla}\times\vec{n}\right)\right]^2\right\} \tag{9}$$

where K_1 (splay), K_2 (twist) and K_3 (bend) are three positive parameters. We study below the case where the director is in the xOy plane, $\vec{n}(\vec{r}) = (\cos\psi(z)\,,\,\sin\psi(z)\,,\,0)$, with the angle depending only on the coordinate z. In the presence of a homogeneous magnetic field $\vec{H} = (0, H, 0)$, the free energy has a magnetic contribution $F_{\mathrm{magn}}[\vec{n}] = -\frac{1}{2}\chi_a\int \mathrm{d}^3\vec{r}\,\left(\vec{H}\cdot\vec{n}\right)^2$, where χ_a is the anistropic contribution to the magnetic susceptibility.

1/ Show that the free energy per unit surface is

$$F[\psi(z)] = \frac{F_{\mathrm{el}} + F_{\mathrm{magn}}}{\text{Surface}} = g\int \mathrm{d}z\,\left\{\frac{1}{2}\left[\psi'(z)\right]^2 - \frac{1}{\xi^2}\,\sin^2\psi(z)\right\} \tag{10}$$

Give the expressions of g and ξ in terms of K_i, $\chi_a > 0$ and H.

2/ Field equation.— What is the equation for the field $\psi(z)$ which minimizes $F[\psi]$?

3/ If $\psi(z)$ satisfies the field equation, show that $\mathscr{E} = \frac{1}{2}\left[\psi'(z)\right]^2 + \xi^{-2}\sin^2\psi(z)$ is independent of z.

4/ In this last question, we are interested in a field configuration with $\psi(z) \to \pm\pi/2$ for $z \to \pm\infty$. What is the value of $\mathscr{E}$ in this case ? Deduce the solution $\psi(z)$ such that $\psi(0) = 0$. Plot neatly $\psi(z)$.
Compare the free energy for this solution with the free energy for the uniform solution $\psi(z) = \text{cste}$ (no detailed calculation ; an order of magnitude is sufficient).
Hint : $\frac{\mathrm{d}}{\mathrm{d}t}\ln|\tan(t/2)| = 1/\sin t$.

Solutions will be avalaible at `http://lptms.u-psud.fr/christophe_texier/`