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TUTORIALS



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## Informations pratiques

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# Contents

<b>1 Langevin model and random processes</b>	<b>5</b>
1.1 Brownian motion and stationary velocity distribution . . . . .	5
1.2 <i>To go further : Mean square displacement from the Langevin equation</i> . . . . .	6
1.3 <i>To go further : Random telegraph process</i> . . . . .	6
<b>2 Random processes and conservation</b>	<b>8</b>
2.1 Master equation for the diffusion on $\mathbb{Z}$ . . . . .	8
2.2 <i>To go further : Gaussian-versus-non Gaussian white noise – Shottky noise</i> . . . . .	9
<b>3 Correlations and fluctuations</b>	<b>11</b>
3.1 Generalised Langevin equation – Wiener-Khintchine theorem . . . . .	11
3.2 Response function for the Ornstein-Uhlenbeck process . . . . .	12
<b>4 Fokker-Planck approach</b>	<b>13</b>
4.1 Ornstein-Uhlenbeck process and the Fokker-Planck equation . . . . .	13
4.2 <i>To go further : Diffusion on a ring</i> . . . . .	14
4.2.1 Free diffusion . . . . .	14
4.2.2 Effect of a drift . . . . .	14
4.2.3 Boundary conditions induced current . . . . .	14
<b>5 Random walks</b>	<b>16</b>
5.1 The Gaussian model of polymer . . . . .	16
5.2 Few properties of the free diffusion on the line . . . . .	17
<b>6 Fokker-Planck and Stochastic Differential Equations</b>	<b>18</b>
6.1 Escape from a metastable state : Arrhenius law . . . . .	19
<b>7 Phase separation</b>	<b>20</b>
7.1 The critical point of the van der Waals model . . . . .	20
7.2 <i>To go further : Lattice gas model for the demixing transition</i> . . . . .	21
<b>8 Charged fluids</b>	<b>24</b>
8.1 The mean-field Debye-Hückel theory for charged fluids . . . . .	24

<b>9</b>	<b>Liquid crystals</b>	<b>27</b>
9.1	Cost of an interface . . . . .	27
<b>10</b>	<b>Real space renormalization of an Ising model</b>	<b>29</b>
10.1	The Niemeijer-Van Leeuwen decimation procedure . . . . .	29
<b>1</b>	<b>Home work : environment model</b>	<b>32</b>

# Tutorial 1

## Langevin model and random processes

### 1.1 Brownian motion and stationary velocity distribution

We consider a Langevin model for the diffusion of a Brownian particle in a thermal bath that obeys in one dimension the differential equation

$$\dot{v} + \frac{1}{\tau}v = \xi(t), \quad (1.1)$$

where  $\gamma$  is a damping coefficient and  $\xi$ , a Langevin force. The latter is assumed to be a white noise with zero mean and peaked correlations

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = q\delta(t-t'), \quad (1.2)$$

with some constant  $q$  related to the strength of the thermal fluctuations.

1. Solve the evolution equation (1.1) for a particle with a velocity  $v_0$  at  $t = 0$ .
2. Show that the velocity correlation is

$$\langle v(t)v(t') \rangle = v_0^2 e^{-(t+t')/\tau} + \frac{q\tau}{2} \left[ e^{-|t-t'|/\tau} - e^{-(t+t')/\tau} \right]. \quad (1.3)$$

3. In the stationary limit, when  $t$  and  $t' \rightarrow \infty$ , we define the temperature  $\langle \frac{1}{2}mv^2 \rangle = \frac{1}{2}k_B T$ . Deduce the relation between  $q$ ,  $\tau$  and  $T$ .

We look for the velocity distribution function in the stationary regime.

4. Show that in this regime

$$v(t) = \int_0^\infty e^{-t'/\tau} \xi(t-t') dt'. \quad (1.4)$$

We recall that for a gaussian white noise (1.2)

$$\langle \xi(t_1)\xi(t_2)\dots\xi(t_{2n+1}) \rangle = 0, \quad (1.5)$$

$$\langle \xi(t_1)\xi(t_2)\dots\xi(t_{2n}) \rangle = q^n \sum_{\pi} \delta(t_{\pi(1)} - t_{\pi(2)}) \delta(t_{\pi(3)} - t_{\pi(4)}) \dots \delta(t_{\pi(2n-1)} - t_{\pi(2n)}), \quad (1.6)$$

for an integer  $n$ , where we sum only those permutations  $\pi(i)$  that lead to different expressions for  $\delta(t_{\pi(1)} - t_{\pi(2)}) \delta(t_{\pi(3)} - t_{\pi(4)}) \dots \delta(t_{\pi(2n-1)} - t_{\pi(2n)})$ .

5. How many such permutations are involved in the sum (1.6) ?
6. Compute the average  $\langle v(t)^{2n+1} \rangle$  and  $\langle v(t)^{2n} \rangle$ .
7. Deduce the characteristic function  $C_v(u) = \langle e^{iuv} \rangle$ , and the resulting velocity distribution function  $P(v)$ . Comment.

## 1.2 To go further : Mean square displacement from the Langevin equation

We consider a particle in a fluid. We write the 1D equation of motion to simplify

$$\frac{dv(t)}{dt} + \frac{1}{\tau}v(t) = \frac{1}{m}\xi(t) \quad (1.7)$$

where  $\xi$  is a Gaussian white noise of zero mean and local time correlations

$$\langle \xi(t)\xi(t') \rangle = C \delta(t - t') \quad (1.8)$$

Our aim is to compute the mean square displacement  $\langle x(t)^2 \rangle$  assuming that  $x(0) = 0$ . We apply the method proposed by Langevin in his famous article, P. Langevin, *Sur la théorie du mouvement brownien*, C. R. Acad. Sc. (Paris) **146**, 530–533 (1908).

1/ Prove that

$$\frac{d^2}{dt^2}x(t)^2 + \frac{1}{\tau} \frac{d}{dt}x(t)^2 = 2v(t)^2 + \frac{2}{m}x(t)\xi(t) \quad (1.9)$$

2/ Give an argument to justify  $\langle x(t)\xi(t) \rangle = 0$ .

3/ What is  $\langle v(t)^2 \rangle$  in the stationary regime ?

4/ Argue that  $\left. \frac{d}{dt} \langle x(t)^2 \rangle \right|_{t=0} = 0$  and deduce

$$\langle x(t)^2 \rangle = \frac{2k_B T \tau}{m} \left[ t - \tau \left( 1 - e^{-t/\tau} \right) \right] \quad (1.10)$$

Analyze carefully the limiting behaviours and plot the function.

## 1.3 To go further : Random telegraph process

We consider a small electric conductor with two contacts which are pinned by gate voltages so that electrons enter one by one (this is the so called "Coulomb blockade regime"). The number of electrons inside the island can be controlled by the gate underneath, so that the number of electrons is either  $N$  or  $N + 1$ .

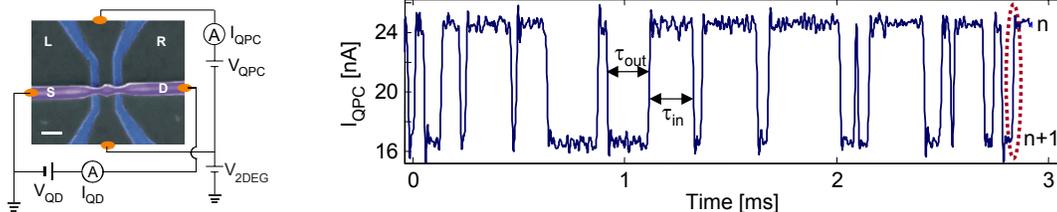


Figure 1.1: *The charge inside the conductor is measured as a function of the time :  $I_{\text{QPC}}$  is proportional to the number of electron inside the central island, which fluctuates by one unit (one electron).*

Consider the Markov process  $X(t)$  taking two values  $X_1$  or  $X_2$ . The transition rates are  $\lambda_1$  (from  $X_1$  to  $X_2$ ) and  $\lambda_2$  (from  $X_2$  to  $X_1$ ). The mean time spent in state  $X_{1,2}$  is  $1/\lambda_{1,2}$ . We denote by  $P_i(t) = \text{Proba}\{X(t) = X_i\}$  with  $i \in \{1, 2\}$ .

1/ Write the set of differential equations for  $P_1(t)$  and  $P_2(t)$ .

2/ Find the stationary solution, denoted by  $P_i^*$  (hint : consider  $P_1(t) + P_2(t)$  and  $y(t) = P_1(t) - P_2(t)$ ).

An interesting exercise is to write the system of equations in a matricial form  $\frac{d}{dt}\vec{P}(t) = M\vec{P}(t)$  and diagonalize the non-symmetric stochastic matrix  $M$ . Show that

$$\exp \left[ t \begin{pmatrix} -\lambda_1 & \lambda_2 \\ \lambda_1 & -\lambda_2 \end{pmatrix} \right] = \begin{pmatrix} P_1^* & P_1^* \\ P_2^* & P_2^* \end{pmatrix} + \begin{pmatrix} P_2^* & -P_1^* \\ -P_2^* & P_1^* \end{pmatrix} e^{-(\lambda_1 + \lambda_2)t} \quad (1.11)$$

3/ Find the conditional probability  $P_t(i|j)$  (i.e.  $P_t(i|j) = P_i(t)$  for  $P_j(0) = 1$ ). Check that the detailed balance condition

$$P_t(1|2) P_2^* = P_t(2|1) P_1^* \quad (1.12)$$

is fulfilled.

4/ We now want to characterize the correlation of the charge in the conductor. Express  $\langle X(t) \rangle$  and  $\langle X(t)X(t') \rangle$  in the stationary regime. For simplicity, we assume that  $X_1 = 0$  describes the conductor empty and  $X_2 = 1$  the conductor with one electron. Compute explicitly  $\langle X(t) \rangle$  and  $C(t - t') = \langle X(t)X(t') \rangle - \langle X(t) \rangle \langle X(t') \rangle$  in this case.

Deduce the power spectrum  $S(\omega)$ .

## Tutorial 2

# Random processes and conservation

### 2.1 Master equation for the diffusion on $\mathbb{Z}$

Let us consider the master equation describing the one dimensional diffusion on  $\mathbb{Z}$  with transitions between nearest neighbour sites

$$\partial_t P_n(t) = W_{n,n-1}P_{n-1}(t) + W_{n,n+1}P_{n+1}(t) - (W_{n-1,n} + W_{n+1,n})P_n(t) \quad (2.1)$$

i.e.  $W_{nm}$  is a tridiagonal (infinite) matrix with  $W_{n,n} = -W_{n-1,n} - W_{n+1,n}$ .

1/ *Current* : check that the master equation can be rewritten under the form

$$\partial_t P_n = -J_n + J_{n-1} \quad (2.2)$$

and express the "current density"  $J_n$  related to the distribution  $P_n$

2/ We now choose the matrix such that

$$W_{n,m} = e^{[V(m)-V(n)]/2} \quad \text{for } m \neq n, \quad (2.3)$$

where  $V(x)$  is a known function.

*Equilibrium state.*— Show that

$$P_n^* = C e^{-V(n)} \quad (2.4)$$

is a stationary solution corresponding to a vanishing current. Discuss the normalisability.

3/ *NESS* ( $J \neq 0$ ).— Find the stationary solution corresponding to  $J_n = J \forall n$ . Show that it is

$$P_n^* = J e^{-V(n)} \sum_{m=n}^{\infty} e^{[V(m+1)+V(m)]/2} \quad (2.5)$$

Discuss the normalisability (consider the continuum limit for simplicity).

4/ Provide an example where there is no stationary state.

## 2.2 To go further : Gaussian-versus-non Gaussian white noise – Shottky noise

We consider the noise

$$F(t) = \sum_{n=1}^N \kappa_n \delta(t - t_n) \quad \text{for } t \in [0, T] \quad (2.6)$$

where  $N$  is random.  $\{\kappa_n\}$  and  $\{t_n\}$  are two sets of i.i.d. random variables.<sup>1</sup> The probability to have  $N$  “impulses” in  $[0, T]$  is

$$P_T(N) = \frac{(\lambda T)^N}{N!} e^{-\lambda T} \quad (2.7)$$

The  $t_n$  are uniformly distributed over the interval  $[0, T]$ , i.e. the joint distribution of the  $N$  times simply  $P_N(t_1, \dots, t_N) = 1/T^N$ . The weights  $\kappa_n$ 's have a common law  $p(\kappa)$ .

We first consider the case where  $p(\kappa) = \delta(\kappa - q)$ .

1/ We introduce the generating functional

$$G[\phi(t)] \stackrel{\text{def}}{=} \left\langle e^{\int dt \phi(t) F(t)} \right\rangle \quad (2.8)$$

Show how one can deduce the correlation functions from the knowledge of  $G[\phi]$  (which will be calculated below).

Hint : Use the functional derivatives  $\frac{\delta G}{\delta \phi(t_1)}$ ,  $\frac{\delta^2 G}{\delta \phi(t_1) \delta \phi(t_2)}$ , etc. Functional derivatives are easily computed with the rule

$$\frac{\delta \phi(t')}{\delta \phi(t)} = \delta(t - t') \quad (2.9)$$

and usual rules for derivation. Example :  $\frac{\delta}{\delta \phi(t)} \int dt' \phi(t')^2 = 2 \phi(t)$ .

2/ Using that averaging over the random variables is

$$\langle (\dots) \rangle_{N, \{t_n\}} = \sum_{N=0}^{\infty} \frac{(\lambda T)^N}{N!} e^{-\lambda T} \int_0^T \frac{dt_1}{T} \dots \frac{dt_N}{T} (\dots) \quad (2.10)$$

compute explicitly  $G[\phi(t)]$ .

3/ Functional derivations of  $G[\phi]$  generate the correlation functions  $\langle F(t_1) \dots F(t_n) \rangle$  and the derivations of  $W[\phi] = \ln G[\phi]$  generate the connex correlation functions, i.e.  $\langle F(t) \rangle$ ,  $\langle F(t) F(t') \rangle_c \stackrel{\text{def}}{=} \langle F(t) F(t') \rangle - \langle F(t) \rangle \langle F(t') \rangle$ , etc. Deduce these latter.

4/ **Application : Classical theory of shot noise (Shottky noise).**– Some current  $i(t)$  flows through a conductor. Due to the discrete nature of the charge carriers, the current presents some fluctuations (noise) known as “shot noise”, which we aim to characterize here (not to be confused with the thermal fluctuations, i.e. the Johnson-Nyquist noise). We assume that the current can

<sup>1</sup> i.i.d. = independent and identically distributed.

be written under the form of independent impulses  $i(t) = q \sum_n \delta(t - t_n)$ . The average rate is  $\lambda$ . Express the two first cumulants of current. Deduce the power spectrum

$$S(\omega) \stackrel{\text{def}}{=} \int dt (t - t') e^{i\omega(t-t')} \langle i(t) i(t') \rangle_c \quad (2.11)$$

and express the relation between the shot noise and the averaged current  $\langle i \rangle$ .

**Remark :** This result has permitted to demonstrate the existence of charge carriers with *fractional charge* in the regime of the fractional quantum Hall effect (strong magnetic field, low temperature) :

- L. Saminadayar, D. C. Glattli, Y. Jin & B. Etienne, *Observation of the e/3 Fractionally Charged Laughlin Quasiparticle*, Phys. Rev. Lett. **79** (1997) 2526.
- M. Reznikov, R. de Picciotto, T. G. Griffiths, M. Heiblum & V. Umansky, *Observation of quasiparticles with 1/5 of an electron's charge*, Nature **399** (May 1999) 238.

**5/ Transferred charge (Poisson process).**– We consider the stochastic differential equation

$$\frac{dQ(t)}{dt} = i(t) \quad (2.12)$$

- a) Draw a typical realisation of the process  $Q(t)$ . Deduce the cumulants of the charge  $\langle Q(t)^n \rangle_c$ .
- b) Argue that on the large time scale  $\lambda t \gg 1$ , the cumulants with  $n > 2$  can be neglected. What is then the nature of the process  $Q(t)$  ?
- c) We introduce the distribution of the charge  $P(Q; t) = \langle \delta(Q - Q(t)) \rangle$  describing the evolution of the process with a drift

$$\frac{dQ(t)}{dt} = \mathcal{I}(Q(t)) + i(t) . \quad (2.13)$$

Consider separately the effect of the drift and the jumps to relate  $P(Q; t + dt)$  to  $P(Q; t)$ . Show that the distribution obeys

$$\partial_t P(Q; t) = -\partial_Q [\mathcal{I}(Q) P(Q; t)] + \lambda [P(Q - q; t) - P(Q; t)] . \quad (2.14)$$

**6/ Compound Poisson process.**– We now consider an arbitrary distribution  $w(\kappa)$  and introduce the generating function  $g(k) = \langle e^{k\kappa} \rangle$ .

- a) Find the new expression of the generating functional  $G[\phi]$ .
- b) Show that it is possible to define a limit (changing  $\lambda$  and  $w(\kappa)$ ) where the noise becomes a Gaussian white noise.
- c) Show that the generalisation of (2.14) is

$$\boxed{\partial_t P(Q; t) = -\partial_Q [\mathcal{I}(Q) P(Q; t)] + \lambda \int dq w(q) [P(Q - q; t) - P(Q; t)]} \quad (2.15)$$

Check the conservation of probability. Express the probability current  $\mathcal{J}(Q; t)$  related to the distribution by the conservation law  $\partial_t P(Q; t) = -\partial_Q \mathcal{J}(Q; t)$ .

Consider the limit of small jumps  $q \rightarrow 0$ , i.e. when  $w(q)$  is concentrated at the origin. Assuming  $\langle q \rangle = 0$ , show that (2.15) leads to a Fokker-Planck like equation of the form  $\partial_t P(Q; t) = -\partial_x [a_1(Q) P(Q; t) + \frac{1}{2} \partial_{xx} [a_2(Q) P(Q; t)]]$ , and express the diffusion constant  $D$  of the charge diffusion.

# Tutorial 3

## Correlations and fluctuations

### 3.1 Generalised Langevin equation – Wiener-Khintchine theorem

We consider a small particle in a fluid whose velocity can be analysed thanks to the generalised Langevin equation

$$m \frac{d}{dt} v(t) = - \int dt' \gamma(t-t') v(t') + F(t) \quad (3.1)$$

(set  $m = 1$ ). The Langevin force  $F(t)$  is correlated over a short “microscopic” time  $\tau_c$ . The integral term comes from damping.

1/ Show that the correlation function of the velocity is

$$C_{vv}(\tau) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\tilde{C}_{FF}(\omega)}{|\tilde{\gamma}(\omega) - i\omega|^2} e^{-i\omega\tau} \quad (3.2)$$

2/ We first consider the limiting case where  $\gamma(t) = \lambda \delta(t)$  and  $C_{FF}(\tau) = \sigma \delta(\tau)$ . Compute the correlator  $C_{vv}(\tau)$  and express  $\sigma$  in terms of the diffusion constant  $D \stackrel{\text{def}}{=} \lim_{t \rightarrow \infty} \frac{1}{2t} \langle x(t)^2 \rangle$ .

3/ We now consider  $C_{FF}(t) = 2D\lambda^2 \frac{1}{2\tau_c} e^{-|t|/\tau_c}$  with  $\tau_c \ll 1/\lambda$ . Show that

$$\int_{\mathbb{R}} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{(\omega^2 + a^2)(\omega^2 + b^2)} = \frac{1}{2(b^2 - a^2)} \left( \frac{1}{a} e^{-a|t|} - \frac{1}{b} e^{-b|t|} \right) \quad (3.3)$$

and deduce  $C_{vv}(t)$ . Analyze its limiting behaviors.

4/ We can assume that damping occurs over a finite memory time  $\tau_m \gg \tau_c$ , so that  $\gamma(\tau)$  is a causal function decaying fast over this time scale, like  $\gamma(\tau) = \theta_H(\tau) (\lambda/\tau_m) e^{-\tau/\tau_m}$ .

Discuss the hypothesis  $\gamma(t) = \lambda \delta(t)$  in this case.

For a finite  $\tau_m$ , give a physical argument to express the correct hierarchy of times  $1/\lambda$ ,  $\tau_m$  and  $\tau_c$ .

## 3.2 Response function for the Ornstein-Uhlenbeck process

We consider a small ball bound to a substrated by a polymer and submitted to a time dependent external force  $f_{\text{ext}}(t)$ . The position of the particle is described by the Langevin equation

$$\frac{d}{dt}x(t) = -\lambda x(t) + f_{\text{ext}}(t) + F(t) \quad (3.4)$$

where  $F(t)$  is the Langevin force. We choose to model the force as a Gaussian white noise,  $\langle F(t)F(t') \rangle = 2D \delta(t - t')$ .

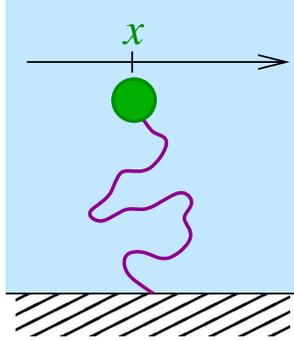


Figure 3.1: A small particle is bound to a surface thanks to a polymer which acts like a spring.

**1/ Correlations at equilibrium.**— We consider the case  $f_{\text{ext}}(t) = 0$ . Compute de correlation function  $C(t - t') \stackrel{\text{def}}{=} \langle x(t)x(t') \rangle_{\text{eq}}$ . Deduce what is the stationary distribution  $P_{\text{eq}}(x)$  of the process. Assuming equipartition theorem, relate  $D$  to the temperature.

**2/ Response (out of equilibrium).**— Show that we can easily determine the response function  $\chi$  for this linear problem. We recall that it is defined by

$$\langle x(t) \rangle_{\text{out of eq.}} = \langle x \rangle_{\text{eq}} + \int dt' \chi(t - t') f_{\text{ext}}(t') + \mathcal{O}(f_{\text{ext}}^2) \quad (3.5)$$

**3/ Fluctuation dissipation theorem.**— Check that the two functions satisfy the FDT

$$\boxed{\chi(t) = -\beta \theta_{\text{H}}(t) \frac{d}{dt} C(t)} \quad (3.6)$$

where  $\beta = 1/(k_B T)$ .

# Tutorial 4

## Fokker-Planck approach

### 4.1 Ornstein-Uhlenbeck process and the Fokker-Planck equation

We study the Ornstein-Uhlenbeck process, the only Markovian, stationary and Gaussian random process. It describes the motion of the particle submitted to a spring force in the **overdamped** regime. It obeys the Langevin equation

$$\frac{d}{dt}x(t) = -\lambda x(t) + F(t) \quad (4.1)$$

where  $F(t)$  is the Langevin force, a Gaussian white noise  $\langle F(t)F(t') \rangle = 2D\delta(t-t')$ . Our aim is here to determine the stationary distribution  $P_{\text{eq}}(x)$  and the conditional probability  $P_\tau(x|x_0)$ .

1/ Write the corresponding Fokker-Planck equation.

2/ **Method 1.**– Recall the expression of  $\langle x(t) \rangle$  and  $\text{Var}(x(t))$  obtained with the Langevin approach. Deduce the expression of the conditional probability  $P_\tau(x|x_0)$ . What is its  $\tau \rightarrow \infty$  limit ?

3/ **Method 2.**– We solve directly the Fokker-Planck equation. Express the corresponding supersymmetric Schrödinger operator  $H_+$ . Give its spectrum of eigenvalues and eigenfunctions. We recall the expression of the quantum mechanical propagator for the harmonic oscillator

$$\langle x | e^{-tH_\omega} | x_0 \rangle = \sqrt{\frac{m\omega}{2\pi \text{sh}(\omega t)}} \exp -\frac{m\omega}{2 \text{sh}(\omega t)} [\text{ch}(\omega t) (x^2 + x_0^2) - 2 x x_0] \quad (4.2)$$

where  $H_\omega = -\frac{1}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$ . Recover the expression of the propagator of the Ornstein-Uhlenbeck process.

APPENDIX : FPE *versus* Schrödinger Equation.– The Fokker-Planck equation

$$\partial_t P(x, t) = \partial_x [D\partial_x - F(x)] P(x, t) \quad (4.3)$$

can be mapped onto the imaginary time Schrödinger equation

$$-\partial_t \psi(x, t) = H_+ \psi(x, t) \quad \text{where } H_+ = -D \frac{d^2}{dx^2} + \frac{1}{4D} F(x)^2 + \frac{1}{2} F'(x) \quad (4.4)$$

thanks to the transformation  $P(x, t) = \psi_0(x) \psi(x, t)$  where  $\psi_0(x) = \sqrt{P_{\text{eq}}(x)} \propto \exp[-U(x)/D]$  where  $U(x) = -\int^x d\xi F(\xi)$  is the potential.

## 4.2 To go further : Diffusion on a ring

### 4.2.1 Free diffusion

We consider the free diffusion in a ring

$$\partial_t P(x, t) = D \partial_x^2 P(x, t) \quad \text{for } x \in [0, L] \quad (4.5)$$

with periodic boundary conditions

$$P(0) = P(L) \quad (4.6)$$

$$P'(0) = P'(L) \quad (4.7)$$

(time dependence is omitted).

1/ Analyze the spectrum of the diffusion operator  $D\partial_x^2$ . Deduce a first series representation of the propagator  $P(x, t|x_0, 0)$ . Is it convenient to analyze short or large time ? Identify the characteristic time  $\tau_D$  (Thouless time) separating the "short" and "long" time regimes.

2/ Using the Poisson formula (appendix), deduce another series representation for  $P(x, t|x_0, 0)$  convenient to analyze the other limit in time.

### 4.2.2 Effect of a drift

Same question when a constant drift is introduced :

$$\partial_t P(x, t) = (D\partial_x^2 - v\partial_x) P(x, t) \quad \text{for } x \in [0, L] \quad (4.8)$$

In particular, discuss the stationary limit  $t \rightarrow \infty$ . Compute the stationary current  $J_v$ .

### 4.2.3 Boundary conditions induced current

We now come back to the analysis of the free diffusion (4.5), however we now study the problem for a new set of boundary conditions :

$$P(L) = 0 \quad (4.9)$$

$$P'(0) = P'(L) \quad (4.10)$$

Interpret the two boundary conditions. Found the stationary state and deduce a formula for the current  $J_D$ . Discuss the  $L$  dependence (compare with  $J_v$ ).

**Remark :** the spectral analysis is more tricky in this case because the Fokker-Planck operator is not self adjoint (due to the choice of boundary conditions), which makes it non diagonalisable. The eigenvalues are doubly degenerated and in each subspace the operator must be written under the form of an upper triangular  $2 \times 2$  matrix.

### Appendix : a Poisson formula

$$\sum_{n \in \mathbb{Z}} e^{2i\pi n \eta} e^{-\pi^2 (n+\alpha)^2 y} = \frac{1}{\sqrt{\pi y}} \sum_{n \in \mathbb{Z}} e^{2i\pi (n-\eta)\alpha} e^{-\frac{(n-\eta)^2}{y}}. \quad (4.11)$$

Proof : apply  $\sum_{n \in \mathbb{Z}} f(n) = \sum_{n \in \mathbb{Z}} \hat{f}(2\pi n)$  where  $\hat{f}(k) = \int_{\mathbb{R}} dx f(x) e^{-ikx}$ .

# Tutorial 5

## Random walks

### 5.1 The Gaussian model of polymer

We discuss a simple model of polymer. We consider a sequence of  $N$  monomers attached at point  $\vec{r}_0$ . We denote by  $\vec{r}_n$  the end of the  $n$ -th monomer.

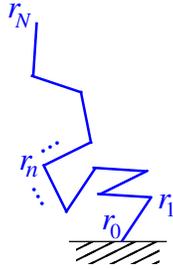


Figure 5.1: The “Gaussian polymer” :  $N$  independent monomers.

We assume that the  $n$ -th monomer  $\vec{u}_n = \vec{r}_n - \vec{r}_{n-1}$  has a fixed length  $a$  and its direction is uniformly distributed in space, independently of the other monomers.

We introduce the probability to find the end of the polymer at  $\vec{r}$  given that the other end is fixed at  $\vec{r}_0$ .

1/ Justify the recurrence

$$P_N(\vec{r} | \vec{r}_0) = \int_{\|\vec{u}\|=a} d^d \vec{u} P_{N-1}(\vec{r} - \vec{u} | \vec{r}_0). \quad (5.1)$$

where  $\int_{\|\vec{u}\|=a} d^d \vec{u} \dots \equiv \int \frac{d^d \vec{u}}{S_d a^{d-1}} \delta(\|\vec{u}\| - a) \dots$ ,  $S_d$  being the surface of the unit sphere in dimension  $d$  (e.g.  $S_3 = 4\pi$ )

2/ Solve the equation by using the Fourier transform (consider the  $d = 3$  case).

3/ Study the continuum limit  $a \rightarrow 0$  and  $N \rightarrow \infty$  with  $t = Na^2$  fixed.

4/ Deduce the “giration radius” defined as  $R_G^2 = \int d^d \vec{r} P_N(\vec{r} | 0) \vec{r}^2$

Compare  $R_G$  (in unit of  $a$ ) with the length of the polymer  $\mathcal{L}_N = Na$ .

## 5.2 Few properties of the free diffusion on the line

We illustrate how powerful is the Fokker-Planck approach by considering several properties of the Brownian motion.

**1/ Propagator on the half line.**— We consider the free diffusion on  $\mathbb{R}_+$  with a Dirichlet boundary condition at the origin. Construct the solution of the diffusion equation

$$\partial_t P(x, t) = D \partial_x^2 P(x, t) \quad \text{for } x > 0 \text{ with } P(0, t) = 0 \quad (5.2)$$

(use the image method). Apply the method to the propagator, denoted  $\mathcal{P}_t^+(x|x_0)$ .

**2/ Survival probability.**— Dirichlet boundary condition describes absorption at  $x = 0$ . Compute the survival probability for a particle starting from  $x_0$  :

$$S_{x_0}(t) = \int_0^\infty dx \mathcal{P}_\tau^+(x|x_0) \quad (5.3)$$

Remark : what would have been the result if  $\mathcal{P}_\tau^+(x|x_0)$  would have satisfied a Neumann boundary condition ?

**3/ First passage time.**— We denote by  $T$  the first time at which the process starting from  $x_0 > 0$  reaches  $x = 0$  (it is a random quantity depending on the process), and  $P_{x_0}(T)$  is distribution. The survival probability is the probability that the process did not reach  $x = 0$  up to time  $t$  :

$$S_{x_0}(t) = \int_t^\infty dT P_{x_0}(T) \quad (5.4)$$

Deduce  $P_{x_0}(T)$  and plot it.

**4/ Maximum.**— We now consider another property of the Brownian motion  $x(\tau)$  with  $\tau \in [0, t]$  starting from  $x_0 = 0$  : we denote by  $m \geq 0$  its maximum and  $Q_t(m)$  the corresponding distribution. Justify the following identity

$$\int_0^m dm' Q_t(m') = S_m(t) \quad (5.5)$$

Deduce the expression of  $Q_t(m)$ . What does  $Q_t(0)$  represent ? The exponent of the power law  $t^{-\theta}$  is called the persistence exponent. Give  $\theta$  for the Brownian motion.

### Appendix : the error function

$$\operatorname{erf}(z) \stackrel{\text{def}}{=} \frac{2}{\sqrt{\pi}} \int_0^z dt e^{-t^2} \quad (5.6)$$

and  $\operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$ . Asymptotics :

$$\operatorname{erfc}(z) \underset{z \rightarrow \infty}{\simeq} \frac{e^{-z^2}}{\sqrt{\pi}} \sum_{n=0}^N (-1)^n \left(\frac{1}{2}\right)_n \frac{1}{z^{2n+1}} + R_N(z) \quad (5.7)$$

where  $(a)_n \stackrel{\text{def}}{=} a(a+1) \cdots (a+n-1) = \Gamma(a+n)/\Gamma(a)$  is the Pochhammer symbol.

## Tutorial 6

# Fokker-Planck and Stochastic Differential Equations

We consider the stochastic differential equation (SDE)

$$dx(t) = a(x(t)) dt + b(x(t)) dW(t) \quad (\text{It}\hat{o}). \quad (6.1)$$

A simple manner to make the connection between SDE and FPE is to use the independence of  $x(t)$  and  $dW(t)$  at coinciding times and  $\langle dW(t)^2 \rangle_{\text{noise}} = dt$  (physicist's notation). Thus, the drift and the "diffusion" in the related FPE

$$\partial_t P_t(x) = \left[ -\partial_x a(x) + \frac{1}{2} \partial_x^2 b(x)^2 \right] P_t(x) \quad (6.2)$$

are given by

$$a(x) = \frac{\langle dx \rangle_{\text{noise}}}{dt} \quad \text{and} \quad b(x)^2 = \frac{\langle dx^2 \rangle_{\text{noise}}}{dt} \quad (6.3)$$

1/ As an application we consider the multidimensional case

$$dx_i(t) = a_i(\vec{x}) dt + b_{ij}(\vec{x}) dW_j(t) \quad (\text{It}\hat{o}). \quad (6.4)$$

with  $\langle dW_i(t) dW_j(t) \rangle_{\text{noise}} = \delta_{ij} dt$ . Show that the related FPE is

$$\partial_t P_t(\vec{x}) = \left[ -\partial_i a_i(\vec{x}) + \frac{1}{2} \partial_i \partial_j b_{ik}(\vec{x}) b_{jk}(\vec{x}) \right] P_t(\vec{x}) \quad (6.5)$$

(with implicit summation over repeated indices).

2/ **Application : Kramers equation.**— Consider the equations

$$\begin{cases} dx = v dt \\ dv = \left( -\frac{v}{\tau} + \frac{F(x)}{m} \right) dt + \frac{1}{m} \sqrt{2k_B T \gamma} dW(t) \end{cases} \quad (6.6)$$

Consider  $(x(t), v(t))$  as 2D random process. What are the drift  $a_i(x, v)$  (i.e.  $a_x$  and  $a_v$ ) and the diffusion matrix  $(b_{xx}, b_{xv}, b_{vx}, b_{vv})$  ? Deduce that the FPE equation is

$$\left( \partial_t + v \partial_x + \frac{F(x)}{m} \partial_v \right) P_t(x, v) = \frac{1}{\tau} \partial_v \left( v + \frac{k_B T}{m} \partial_v \right) P_t(x, v) \quad (6.7)$$

This equation is called the *Kramers equation*.

**3/ Smoluchowski equation.**— The Smoluchowski equation is the overdamped limit of the Kramers equation. The treatment at the level of FPE is complicated. It is more simple to start from SDE. Remembering that the overdamped limit corresponds to neglect the acceleration term in the Newton equation, show that the equation for the distribution  $P_t(x) = \int dv P_t(x, v)$  in the limit of strong friction is

$$\partial_t P_t(x) \simeq \frac{1}{\gamma} [-\partial_x F(x) + k_B T \partial_x^2] P_t(x) \quad (6.8)$$

## 6.1 Escape from a metastable state : Arrhenius law

We consider the first passage time problem : a particle starts at  $x(0) = x_0$  and reaches the point  $b$  for the first time at a (random) time  $T_{x_0}$  :  $x(T_{x_0}) = b$  with  $x(t) < b$  for  $t \in [0, T_{x_0}]$ . In the lectures, we have obtained a formula for the average time, assuming a reflecting boundary condition at  $a < x_0$  :

$$\langle T_{x_0} \rangle = \frac{1}{D} \int_{x_0}^b dx e^{V(x)/D} \int_a^x dx' e^{-V(x')/D} . \quad (6.9)$$

We have applied this formula to the case where the potential presents a well at  $x_1$  and a barrier at  $x_2$  (escape from a metastable state) and have obtained the formula

$$\langle T_{x_0} \rangle \simeq \frac{2\pi}{\sqrt{-V''(x_1)V''(x_2)}} \exp \left\{ \frac{V(x_2) - V(x_1)}{D} \right\} \quad (6.10)$$

in the  $D \rightarrow 0$  limit. This formula describes a smooth potential  $\in \mathcal{C}^2(\mathbb{R})$ .

Consider the potentials of the figure 6.1 and derive analogous formulae for the averaged escape time.

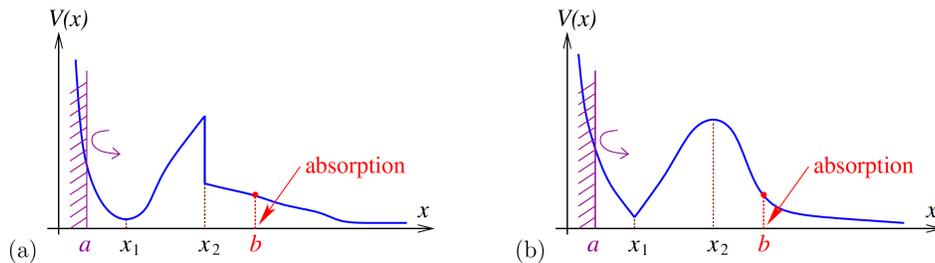


Figure 6.1: *Two other types of trapping potentials.*

# Tutorial 7

## Phase separation

### 7.1 The critical point of the van der Waals model

The Van der Waals model is a model for a real fluid, with a strong repulsion between atoms (or molecules) and a weak attraction. It is characterised by two parameters : the first one is related to the exclusion volume around each atom/molecule :  $b \sim r_0^3$ , where  $r_0$  is the interaction range. The second is the typical potential energy averaged in the volume  $a \sim u_0 r_0^3$ , where  $-u_0$  is the depth of the potential well. The van der Waals equation reads

$$\left(p + \frac{N^2}{V^2}a\right)(V - Nb) = Nk_B T \quad (7.1)$$

- 1/ Using dimensionless analysis, relate the three coordinates  $(T_c, V_c, p_c)$  of the critical point to  $a$  and  $b$ , up to dimensionless factors  $\sim 1$ .
- 2/ At the critical temperature  $T_c$ , the isotherm presents a vanishing slope and an inflexion point at point  $C$ . Write the three equations determining  $(T_c, V_c, p_c)$ . Solve them.
- 3/ Give the value of the dimensionless ratio  $p_c V_c / (N k_B T_c)$ . Compare with the experimental data of the table

	$T_c$ (K)	$V_c$ (cm <sup>3</sup> )	$p_c$ (atm)	$\frac{p_c V_c}{N k_B T_c}$
He	5.2	57.8	2.26	0.30
H <sub>2</sub>	33.1	65.0	12.8	0.31
N <sub>2</sub>	126.1	90.1	33.5	0.29
O <sub>2</sub>	154.4	74.4	49.7	0.29
CO <sub>2</sub>	304.2	94.0	72.9	0.27
H <sub>2</sub> O	647.4	56.3	218.3	0.23

- 4/ We now study the vicinity of the critical point  $C$ . We introduce the dimensionless variables  $v \stackrel{\text{def}}{=} \frac{V}{V_c} - 1$ ,  $\pi \stackrel{\text{def}}{=} \frac{p}{p_c} - 1$  and  $t \stackrel{\text{def}}{=} \frac{T}{T_c} - 1$ . Write the VdW equation with the new variables and show that its expansion in the vicinity of the critical point is

$$\pi \simeq 4t - 6vt - \frac{3}{2}v^3 \quad (7.2)$$

(justify that we can stop at order  $v^3$  and can neglect the term  $v^2 t$  and higher).

- 5/ For  $T < T_c$ , discuss explicitly the Maxwell construction with the simplified isotherm. What are the values of the volume of the liquid  $v_L$  and of gas  $v_G$ , defining the two ends of the liquefaction plateau ? What is the value of the saturation pressure  $\pi_s(t)$  ?

Deduce the critical exponent  $\beta_{\text{vdW}}$  (controlling the order parameter). In a famous set of experiments on various fluids, Guggenheim has plotted the ratio  $T/T_c$  as a function of the two densities (liquid and gas) : cf. Fig.7.1. Comment the figure.

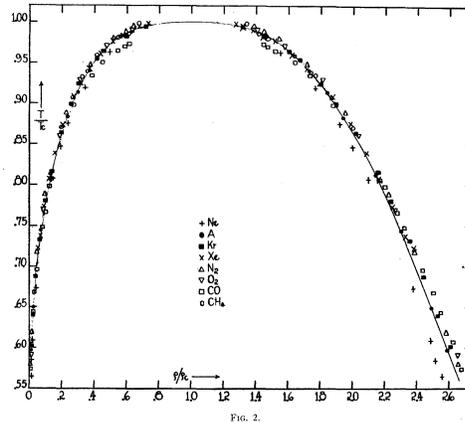


Figure 7.1: Figure from : E. A. Guggenheim, “*The principles of corresponding states*”, J. Chem. Phys. **13**(7), p. 253 (1945).

- 6/ Analyze the critical isotherm. Deduce the critical exponent  $\delta_{\text{vdW}}$ .
- 7/ The isothermal compressibility is defined as  $\chi_T \stackrel{\text{def}}{=} -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_T$ . What is the behaviour of  $\chi_T$  in the vicinity of the critical point ? Deduce the critical exponent  $\gamma_{\text{vdW}}$ .
- 8/ In the Clapeyron diagram  $(\pi, v)$ , the region where liquid and gas coexist is delimited by the "binodal" curve (i.e. the two values  $v_L$  and  $v_G$  as a function of  $\pi = \pi_s(t)$ ). Give the expression of the binodal curve.

The spinodal is the curve corresponding to the end of metastability (i.e. the set of points where  $\frac{\partial \pi}{\partial v} = 0$  in the Clapeyron diagram). Deduce the expression of the spinodal curve.

- 9/ Plot neatly the phase diagram in the Clapeyron representation and indicate the region of metastability.

## 7.2 To go further : Lattice gas model for the demixing transition

We study a lattice gas model for mixing of a solute (dissolved material) in a solvent (liquid). The lattice is made of  $N$  elementary cells, which each contains one molecule : the solute or the solvent. We denote by  $N_p$  the number of solute molecules (particles in the fluid) and  $N_s$  the number of solvent molecules. We denote by  $z$  the coordination number of the lattice ( $z = 2d$  for a square lattice in dimension  $d$ ).

We introduce the concentration of solute

$$\phi = \frac{N_p}{N}. \quad (7.3)$$

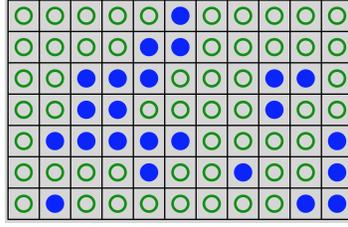


Figure 7.2: Two types of molecules on a lattice : solute particles ( $\bullet$ ) and solvent molecules ( $\circ$ ).

The molecules interact through the following rules (for neighbour molecules):

$$\begin{cases} \bullet\bullet : \varepsilon_{pp} \\ \circ\bullet : \varepsilon_{ps} \\ \circ\circ : \varepsilon_{ss} \end{cases} \quad (7.4)$$

We denote by  $E(\mathcal{C})$  the energy of a configuration  $\mathcal{C}$ , which can be written as

$$E(\mathcal{C}) = N_{pp}(\mathcal{C}) \varepsilon_{pp} + N_{ps}(\mathcal{C}) \varepsilon_{ps} + N_{ss}(\mathcal{C}) \varepsilon_{ss} \quad (7.5)$$

where  $N_{pp}(\mathcal{C})$ ,  $N_{ss}(\mathcal{C})$  and  $N_{ps}(\mathcal{C})$  are the numbers of bonds between two solute molecules, solvent molecules and solute/solvent molecules, respectively.  $N_{pp}(\mathcal{C}) + N_{ss}(\mathcal{C}) + N_{ps}(\mathcal{C}) = N_{\text{bonds}}$  with  $N_{\text{bonds}} = zN/2$ .

In a first time, we compute the partition function

$$Z = \sum_{\mathcal{C}} e^{-\beta E(\mathcal{C})} \quad (7.6)$$

with a mean field approximation.

1/ Justify the three following expression for the mean values :

$$\begin{cases} \overline{N}_{pp} = \frac{1}{2} N z \phi^2 \\ \overline{N}_{ps} = N z \phi (1 - \phi) \\ \overline{N}_{ss} = \frac{1}{2} N z (1 - \phi)^2 \end{cases} \quad (7.7)$$

Deduce the mean value of the energy  $\overline{E}$  as a function of  $\phi$ . Show that it is of the form

$$\frac{1}{N} \overline{E} = \varepsilon_0 + c_1 \phi + \frac{z}{2} \Delta \varepsilon \phi^2 \quad (7.8)$$

The energy  $\Delta \varepsilon$  is the *effective* interaction energy between solute molecules in the solvent (think at the energy of the Ising model). Discuss physically its dependence in  $\varepsilon_{ps}$ .

2/ What is the number of microstates of the fluid  $\Omega = \sum_{\mathcal{C}} 1$  ( $N_p$  and  $N_s$  are fixed) ? Compute the entropy per site  $s(\phi) \stackrel{\text{def}}{=} \lim_{N \rightarrow \infty} \frac{1}{N} \ln \Omega$ .

3/ **Partition function** : The mean field approximation corresponds to  $Z = \sum_C e^{-\beta E(C)} \equiv \Omega \langle e^{-\beta E} \rangle \approx \Omega e^{-\beta \bar{E}}$ . Show that

$$Z \sim e^{-N\beta f_L(\phi)} \quad (7.9)$$

and give the expression of  $f_L(\phi)$ , the Landau free energy per unit volume (remember that  $N$  is the volume in cell unit).

In the following, we simplify the analysis and adjust the coefficient  $c_1$  in  $\bar{E}$  so that the energy is symmetric with respect to  $\phi \leftrightarrow 1 - \phi$ . Give the expression of  $f_L(\phi)$  (disregard the constant).

- 4/ Analyze  $f_L(\phi)$  for different temperatures (plot the function). Interpret the behaviour. Show that there is a first order phase transition below a certain critical temperature  $T_c$ . Introduce the parameter  $\eta = -z\Delta\varepsilon/(2k_B T)$  : what is the critical value  $\eta_c$  corresponding to  $T_c$  ?
- 5/ We consider  $T < T_c$ . We denote by  $\phi_1$  and  $\phi_2$  the concentrations of the two phases. Give the equation for  $\phi_{1,2}$ . Plot  $T$  as a function of  $\phi_{1,2}$ . Analyzing the limit  $T \rightarrow T_c^-$ , give the critical exponent  $\delta\phi = \phi_2 - \phi_1 \sim (T_c - T)^\beta$ .
- 6/ **Osmotic pressure** : is the force per unit surface when a solution (solvent+solute) is in contact with pure solvent through a semi-permeable membrane (figure 7.3).

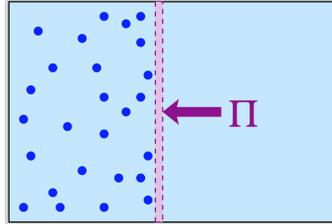


Figure 7.3: The left volume contains solute+solvent and the right volume only solvent. The two volumes are separated by a semi-permeable wall allowing only solvent to pass through.

The volume of the solution is  $N$  (in appropriate units) and the total volume  $N_{\text{tot}}$ . The total free energy is thus  $F_{\text{tot}}(N) = N f_L(\phi) + (N_{\text{tot}} - N) f_L(0)$ . Express the osmotic pressure

$$\Pi(\phi) = -\frac{\partial F_{\text{tot}}(N)}{\partial N} \quad (7.10)$$

as a function of  $\phi$  (be careful that  $\phi$  depends on the volume  $N$ ).

Plot  $\Pi(\phi)$ . Discuss the cases  $\eta < \eta_c$  and  $\eta > \eta_c$ .

# Tutorial 8

## Charged fluids

### 8.1 The mean-field Debye-Hückel theory for charged fluids

We will study the mean-field theory relevant at equilibrium for classical plasmas made of mobile charges of opposite signs, that is referred to as Debye-Hückel theory. This theory may be applied to dilute electrolytes where various charged ions are in solution or to the free carriers in semiconductors. It is also used to describe the disorder phase of two-dimensional  $xy$ -models where topological point defects called vortices interact via a Coulomb potential.

We will consider plasmas made of only two types of charge carriers, one with positive charge  $q_+$  with density  $\bar{n}_+$ , and one with negative charge  $q_-$  and density  $\bar{n}_-$ . One may show that equilibrium may occur only when the global electroneutrality is satisfied,  $q_+\bar{n}_+ + q_-\bar{n}_- = 0$ . In presence of an external potential  $\phi^{ext}(\mathbf{r})$ , the Hamiltonian of the system is

$$\mathcal{H}^{int} = \sum_{i,j,\sigma,\tau} q_\sigma q_\tau v_C(\mathbf{r}_i^\sigma - \mathbf{r}_j^\tau) + \sum_{i,\sigma} q_\sigma \phi^{ext}(\mathbf{r}), \quad (8.1)$$

where the Coulomb potential satisfies  $\Delta_{\mathbf{r}} v_C(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}')$ . We introduce the local densities  $\langle n_\sigma(\mathbf{r}) \rangle = \langle \sum_i \delta(\mathbf{r} - \mathbf{r}_i^\sigma) \rangle$  and the charge density  $\langle \rho_q(\mathbf{r}) \rangle = q_+ \langle n_+(\mathbf{r}) \rangle + q_- \langle n_-(\mathbf{r}) \rangle$ . We recall that the free energy density for a monoatomic ideal gas of density  $n$  at temperature  $T$  is  $f = k_B T n [\ln(n\lambda^3) - 1]$  with the de Broglie wavelength  $\lambda = h/\sqrt{2\pi m k_B T}$ . We consider the local densities  $\langle n_+(\mathbf{r}) \rangle$  and  $\langle n_-(\mathbf{r}) \rangle$  as variational functions and look for their solutions at equilibrium.

1. Argue that the mean-field free energy of the system is

$$\begin{aligned} \mathcal{F} = & \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \langle \rho_q(\mathbf{r}) \rangle v_C(\mathbf{r} - \mathbf{r}') \langle \rho_q(\mathbf{r}') \rangle + \int d\mathbf{r} \langle \rho_q(\mathbf{r}) \rangle \phi^{ext}(\mathbf{r}) \\ & + k_B T \int d\mathbf{r} \langle n_+(\mathbf{r}) \rangle \ln[\langle n_+(\mathbf{r}) \rangle \lambda^3] + k_B T \int d\mathbf{r} \langle n_-(\mathbf{r}) \rangle \ln[\langle n_-(\mathbf{r}) \rangle \lambda^3] \end{aligned} \quad (8.2)$$

n terms of  $\langle \rho_q(\mathbf{r}) \rangle$  together with  $\langle n_+(\mathbf{r}) \rangle$  and  $\langle n_-(\mathbf{r}) \rangle$  ?

2. What are the constraints on  $\langle n_-(\mathbf{r}) \rangle$  and  $\langle n_+(\mathbf{r}) \rangle$  ? By introducing Lagrange multipliers, what are the equilibrium conditions that determine the local densities ? Show that the

solution is

$$\langle n_\sigma(\mathbf{r}) \rangle = A_\sigma \exp[-\beta q_\sigma \phi(\mathbf{r})], \quad (8.3)$$

with some constants  $A_\sigma$  and the total electric potential

$$\phi(\mathbf{r}) = \phi^{ext}(\mathbf{r}) + \int d\mathbf{r}' v_C(\mathbf{r} - \mathbf{r}') \langle \rho_q(\mathbf{r}') \rangle, \quad (8.4)$$

that is the sum of the external potential and the induced part arising from the induced charge  $\langle \rho_q(\mathbf{r}) \rangle$ . What are the values of the constants  $A_\sigma$ ? In the special case where  $\phi^{ext} = 0$ , what are the values of the different densities?

We consider the charge-density response function  $\chi_{\rho\rho}(\mathbf{r}, \mathbf{r}') = -\frac{\delta \langle \rho_q(\mathbf{r}) \rangle}{\delta \phi^{ext}(\mathbf{r}')}$ .

3. Show that its Fourier transform is, for non-zero  $\mathbf{k}$ ,

$$\tilde{\chi}_{\rho\rho}(\mathbf{k}) = \frac{\kappa^2}{4\pi} \frac{\tilde{\delta\phi}}{\delta\phi^{ext}}(\mathbf{k}), \quad (8.5)$$

where we introduce the inverse Debye-Hückel length  $\kappa^2 = 4\pi\beta (q_+^2 \bar{n}_+ + q_-^2 \bar{n}_-)$ . What is its value for  $\mathbf{k} = \mathbf{0}$ ?

4. Considering the definition of  $\phi(\mathbf{r})$ , show that

$$\tilde{\chi}_{\rho\rho}(\mathbf{k}) = \frac{\kappa^2}{4\pi} \frac{\mathbf{k}^2}{\mathbf{k}^2 + \kappa^2}. \quad (8.6)$$

We consider a point charge of charge  $Q$  placed at the origin.

5. What is thence the electric potential induced by this charge in the whole system? What is the charge density? Comments?

We investigate the validity of the mean-field approximation.

6. What is the condition of its validity regarding the balance between the kinetic vs potential energy? What is the condition on  $k_B T$ ,  $\bar{n}$  and  $q^2$ ?

7. Argue that the mean-field approximation is valide when  $\langle \delta\rho_q(\mathbf{r})\delta_q(\mathbf{r}') \rangle \ll q^2 \bar{n}^2$ . What is the link between  $\langle \delta\rho_q(\mathbf{r})\delta_q(\mathbf{r}') \rangle$  and  $\chi_{\rho\rho}(\mathbf{r}, \mathbf{r}')$ ? What is then the condition of validity of the mean-field approximation?

We will expand the mean-field free energy (8.2) in terms of the fluctuations in the densities. Hence we decompose the local densities as  $\langle n_\pm(\mathbf{r}) \rangle = \bar{n}_\pm + \delta n_\pm(\mathbf{r})$ .

8. Expand the free energy (8.2) up to and including the second order  $\delta n$ . We introduce the auxiliary fields  $\langle \rho_q(\mathbf{r}) \rangle = q_+ \delta n_+(\mathbf{r}) + q_- \delta n_-(\mathbf{r})$  and

$$\psi(\mathbf{r}) = -q_- \sqrt{\frac{\bar{n}_-}{\bar{n}_+}} \delta n_+(\mathbf{r}) + q_+ \sqrt{\frac{\bar{n}_+}{\bar{n}_-}} \delta n_-(\mathbf{r}) \quad (8.7)$$

Give  $\delta n_{\pm}(\mathbf{r})$  as a function of  $\langle \rho_q(\mathbf{r}) \rangle$  and  $\psi(\mathbf{r})$ . Show that eventually

$$F = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \langle \rho_q(\mathbf{r}) \rangle U(\mathbf{r} - \mathbf{r}') \langle \rho_q(\mathbf{r}') \rangle + \int d\mathbf{r} \langle \rho_q(\mathbf{r}) \rangle \phi^{ext}(\mathbf{r}) + \frac{2\pi}{\kappa^2} \int d\mathbf{r} \psi(\mathbf{r})^2, \quad (8.8)$$

where  $U(\mathbf{r} - \mathbf{r}') = v_C(\mathbf{r} - \mathbf{r}') + \frac{4\pi}{\kappa^2} \delta(\mathbf{r} - \mathbf{r}')$ .

9. Deduce that  $\frac{1}{V} \langle \tilde{\rho}_q(\mathbf{k}) \tilde{\rho}_q^*(\mathbf{k}) \rangle = k_B T / \tilde{U}(\mathbf{k})$

10. Retrieve the previous results for  $\chi_{\rho\rho}$ .

*Bonus* Consider the case of a charged particle located at a distance  $d$  from a perfect conducting wall embedded in an electrolyte. What is the electric potential ? Comment ?

# Tutorial 9

## Liquid crystals

### 9.1 Cost of an interface

We study the interface between two domains where the order parameter takes opposite values (ex: between positive and negative magnetization, or between liquid and gas, etc). We consider the Ginzburg-Landau functional

$$F_L[\phi] = \int d^d \vec{r} \left\{ g \left( \vec{\nabla} \phi(\vec{r}) \right)^2 + f_L(\phi(\vec{r})) \right\} \quad \text{with } f_L(\phi) \simeq f_0(T) + \frac{a(T)}{2} \phi^2 + \frac{b}{4} \phi^4 \quad (9.1)$$

for  $a(T) = \tilde{a}(T - T_c)$  and  $b > 0$ .

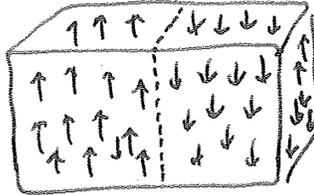


Figure 9.1: *Interface between two regions of opposite magnetization.*

- 1/ Preliminary : 1D Newton equation. Consider  $m\ddot{x} = F(x)$  with  $F(x) = -V'(x)$ .
  - a) Recall the expression of the conserved quantity.
  - b) We consider a confining potential  $V(x)$  Use the conservation law to find a representation of the period of oscillation  $T(E)$  as an integral, where  $E$  is the energy of the particle. Check your result for the harmonic potential  $V(x) = \frac{1}{2}m\omega^2 x^2$ .
  - c) If the potential grows faster than the harmonic potential, for example  $V(x) = \frac{1}{2}m\omega^2 x^2 + \lambda x^4$ , plot a sketch of  $T(E)$ .
  - d) Same question if the potential grows slower, for example  $V(x) = \frac{1}{2}m\omega^2 \sin^2 x$ .
- 2/ Derive the field equation (condition that  $F_L[\phi]$  is minimum). Simplify the equation by assuming translation invariance in two directions :  $\phi(\vec{r}) \rightarrow \phi(x)$ .

- 3/ The equation is solved by analogy with the 1D Newton equation : identify the conserved quantity.
- 4/ Remark : The resolution of the field equation is a boundary problem (for the interface problem the values at  $\pm\infty$  are fixed), while the resolution of the Newton equation is an initial value problem ( $x(0)$  and  $\dot{x}(0)$  are fixed). In this latter case, the energy is a parameter of the problem (related to the initial conditions), while in the first case, the "energy" is fixed by the requirement to satisfy the boundary conditions.
- We consider  $T < T_c$ . Recall the solution in bulk, denoted  $\phi_0$ . Find the solution of the field equation which satisfy  $\phi(x \rightarrow \pm\infty) = \pm\phi_0$ . Express the solution as a function of the correlation length  $\xi = \sqrt{g/(-a)}$ .
- 5/ The aim is here to find a formula for the cost of the interface :

$$\sigma = \frac{F[\phi(x)] - F[\phi_0]}{\text{Surf}} \quad (9.2)$$

Show that

$$\sigma = 2g \int_{-\infty}^{+\infty} dx [\phi'(x)]^2 \quad (9.3)$$

Compute explicitly the integral. Comment on the temperature dependence.

## Tutorial 10

# Real space renormalization of an Ising model

### 10.1 The Niemeijer-Van Leeuwen decimation procedure

The purpose of this problem is to learn how to implement the renormalization group ideas on simple physical systems, such as interacting spins, see Leo P. Kadanoff [Statistical Physics: Statics, Dynamics, and Renormalization, World Scientific, Singapore, (2000)]

In the early days of the renormalization, Niemeijer and Van Leeuwen [Phys. Rev. Lett. 31, 1411 (1973)] came up with an explicit, albeit approximate, procedure to integrate out a fraction of the degrees of freedom in a two-dimensional spin system. We consider a 2D Ising model with  $N$  spins living on a triangular lattice with spacing  $a$ . The normalized exchange energy is  $K = J/k_B T$ .

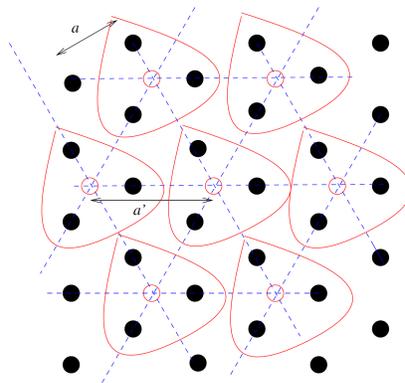


Figure 10.1: The original spins  $\sigma_i$  lie at the black bullets while the plaquette lie at the empty circles. They form a triangular lattice.

1. The lattice is divided into triangular plaquettes as shown in Figure 10.1. A spin variable  $S_I = \pm 1$  is associated to each plaquette  $I = \{i_1, i_2, i_3\}$  via a majority rule:  $S_I = \text{sign} \sigma_{i_1} +$

$\sigma_{i_2} + \sigma_{i_3}$ . What is the number  $N'$  of plaquettes and what is the spacing  $a'$  of the triangular lattice the plaquettes make up ?

2. The Hamiltonian  $H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$  features interactions between spins  $\sigma_i$  belonging to the same plaquette  $I$ , but it also features interactions between spins  $\sigma_i$  and  $\sigma_j$  belonging to different nearest neighbor plaquettes  $I$  and  $J$ . We thus split the Hamiltonian into  $H = H_1 + H_2$ , with  $H_1 = \sum_I h_1(I)$  and  $H_2 = \sum_{\langle I,J \rangle} h_2(I, J)$ . With these notations  $h_1(I)$  denotes a function of the spins belonging to plaquette  $I$ , and the same is true for  $h_2(I, J)$ . For a given triangular plaquette  $I = i_1, i_2, i_3$  and  $J = j_1, j_2, j_3$ , write  $h_2(I, J)$  as a function of  $\sigma_{i_1}, \sigma_{i_2}, \sigma_{i_3}$  and  $\sigma_{j_1}, \sigma_{j_2}, \sigma_{j_3}$ .

3. We would like to rewrite the original partition function  $Z$  in terms of a summation over the  $\{S_I\}$  configurations rather than over the  $\{\sigma_i\}$  configurations, be it at the expense of modifying the Hamiltonian. As a step in that direction, we note that

$$Z(K, N, a) = \sum_{\{S_I\}} \sum'_{\{\sigma_i\}} e^{-\beta H(\sigma_i)} \quad , \quad (10.1)$$

where  $\Sigma'$  denotes a summation over all the  $\{\sigma_i\}$  configurations at fixed plaquette configurations  $S_I = \text{sign}(\sum_{i \in I} \sigma_i)$ . Let  $Z(\{S_I\}) = \sum'_{\{\sigma_i\}} e^{\beta H(\sigma_i)}$ . Give the approximate expression of  $Z(\{S_I\})$ , denoted  $Z_1$  in the following, when the plaquette-plaquette interactions are discarded.

4. Show that

$$Z(K, N, a) = \sum_{\{S_I\}} Z_1 \langle e^{-\beta H_2} \rangle_1 \quad (10.2)$$

where  $\langle \mathcal{O} \rangle_1 = \frac{1}{Z_1} \sum'_{\{\sigma_i\}} e^{-\beta H_1} \mathcal{O}$

5. Let  $\sigma_i$  be a spin belonging to a plaquette  $I$ . Show that

$$\langle \sigma_i \rangle_1 = S_I \frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \quad . \quad (10.3)$$

6. In general, computing  $\langle e^{-\beta H_2} \rangle_1$  is a formidable task. Express the latter average in terms of the cumulants of  $H_2$  with respect to the measure  $\langle \dots \rangle_1$ .

We now implement the Niemeiher-Van Leeuwen approximation which consists in dropping all cumulants of order  $\geq 2$ .

7. What is the physical content, in terms of plaquette-plaquette interactions, of the second cumulant that is neglected ?
8. Within this approximation, show that

$$Z(K, N, a) = (e^{3K} + 3e^{-K})^{N'} Z(K', N', a') \quad , \quad (10.4)$$

where  $K' = f(K)$  is a function to be identified.

9. Find the fixed points of  $f(K)$ . Discuss their stability and their physical meaning. Find the critical temperature within this approximation scheme. Compare its value with the mean-field value and with the exact value that is close to  $3.6J/k_B$  as found by Onsager.
10. Let  $\nu$  be the exponent governing the divergence of the correlation length as criticality is approached. Find the value predicted by the Niemeijer-Van Leeuwen approximation and compare it with both its mean-field and exact values ( $\nu_{exact} = 1$ ).

A few years later, Van Leeuwen and collaborators [[Phys. Rev. Lett. 40, 1605 \(1978\)](#)] came up with a new decimation scheme that is exact in the limit of very large systems. While the specifics of the calculation itself are tedious, the idea was to begin with a system of  $N$  spins and to eliminate at each step of the decimation procedure, an infinitesimal fraction of spins.

# Home work 1

## Home work : environment model

In the lecture, we have introduced a microscopic model of a particle interacting with an environment of harmonic oscillators. Here we introduce the following model

$$H = \underbrace{\frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2}_{\text{system}} + \underbrace{\sum_k g_k \left( \sqrt{m\omega_0\Omega_k} x q_k + \frac{p \pi_k}{\sqrt{m\omega_0\Omega_k}} \right)}_{\text{coupling}} + \underbrace{\sum_k \left( \frac{\pi_k^2}{2} + \frac{\Omega_k^2}{2} q_k^2 \right)}_{\text{bath}} \quad (1.1)$$

$(x, p)$  are the canonical variables for the system and  $(q_k, \pi_k)$  for the bath.  $g_k$  are (real) coupling constants. Thus, we have chosen a more symmetric form of coupling between bath and environment. The most important property is the existence of a continuum of eigen-frequencies  $\Omega_k \in [0, \omega_D]$  (with non vanishing couplings) ensuring the possibility to transfer energy at any scale (below  $\omega_D$ , a "large" cutoff frequency).

1/ Derive the equations of motion. Introduce the set of complex variables

$$a \stackrel{\text{def}}{=} \sqrt{\frac{m\omega_0}{2}} x + i \frac{p}{\sqrt{2m\omega_0}} \quad \text{and} \quad b_k \stackrel{\text{def}}{=} \sqrt{\frac{\Omega_k}{2}} q_k + i \frac{\pi_k}{\sqrt{2\Omega_k}} \quad (1.2)$$

Show that the equations of motion can be recast under the form of two coupled first order differential equations

$$\dot{a}(t) = -i\omega_0 a(t) - i \sum_k g_k b_k(t) \quad (1.3)$$

$$\dot{b}_k(t) = -i\Omega_k b_k(t) - i g_k a(t) \quad (1.4)$$

2/ Integrate the equation of motion for the bath variable and inject the solution in the first differential equation. Show that the system is described by the effective equation

$$\dot{a}(t) = -i\omega_0 a(t) - \int_0^t d\tau \gamma(\tau) a(t - \tau) + \xi(t) \quad (1.5)$$

where  $\xi(t) \stackrel{\text{def}}{=} -i \sum_k g_k b_k(0) e^{-i\Omega_k t}$  is the "noise". Give the expression of the causal function  $\gamma(\tau)$ .

3/ Assume canonical equilibrium for the bath

$$P_{\text{eq}}(\{q_k, \pi_k\}) \propto e^{-\beta H_{\text{bath}}} \quad (1.6)$$

for  $q_k(0)$  and  $\pi_k(0)$ , i.e. the bath variables at time  $t = 0$ . Deduce the expression of the correlators  $\langle \xi(t)\xi(t') \rangle$  and  $\langle \xi(t)\xi(t')^* \rangle$ .

4/ The function  $\gamma(\tau)$  is expected to decay fast (at the scale of the evolution of the variables of the system). Justify the approximation

$$\int_0^t d\tau \gamma(\tau) a(t - \tau) \simeq \tilde{\gamma}(\omega_0) a(t) \quad (1.7)$$

where

$$\tilde{\gamma}(\omega_0) = \int_0^\infty d\tau e^{i\omega_0\tau} \gamma(\tau) = i\delta\omega_0 + \frac{\Gamma}{2}. \quad (1.8)$$

Express  $\delta\omega_0$  and  $\Gamma$  as sums of contributions of oscillators. We also introduce  $\omega_R \stackrel{\text{def}}{=} \omega_0 + \delta\omega_0$ . Injecting this form in the differential equation for  $a(t)$ , interpret these two parameters physically.

5/ Using the above approximation, deduce the simple integral representation of  $a(t)$

$$a(t) = a(0) e^{-(i\omega_R + \Gamma/2)t} + \int_0^t dt_1 \xi(t_1) e^{-(i\omega_R + \Gamma/2)(t-t_1)} \quad (1.9)$$

6/ We introduce the useful relation :

$$\sum_k g_k^2 \frac{e^{-i(\Omega_k - \omega_R)t}}{(\Omega_k - \omega_R)^2 + \Gamma^2/4} f(\Omega_k) \simeq f(\omega_R) e^{-\Gamma|t|/2} \quad (1.10)$$

for  $f(\omega)$  any smooth function (at the scale  $\Gamma$ ). You can prove it from the definition of  $\Gamma$ .

Use this relation to compute  $\langle |a(t)|^2 \rangle$ . What represents this quantity ? Show that

$$\langle |a(t)|^2 \rangle = \langle |a(0)|^2 \rangle e^{-\Gamma t} + \frac{k_B T}{\omega_R} (1 - e^{-\Gamma t}) \quad (1.11)$$

and interpret physically this equation.

**7/ Linear response.**

We now introduce an external force  $f(t)$ , i.e.

$$H_{\text{pert}}(t) = -x f(t) \quad (1.12)$$

Justify that the response function characterizing the response of  $x(t)$  to this perturbation is

$$\chi(t - t') = \frac{\theta_{\text{H}}(t - t')}{k_B T} \langle x(t)v(t') \rangle \quad (1.13)$$

With a calculation similar to the one of the previous question, shows that

$$\langle a(t)a(t')^* \rangle \simeq \frac{k_B T}{\omega_R} e^{-i\omega_R(t-t') - \frac{\Gamma}{2}|t-t'|} \quad (1.14)$$

and argue that  $\langle a(t)a(t') \rangle = 0$ . Deduce  $\chi(t)$ .

**8/ Dissipation.**

Analyze the dissipative power

$$\overline{\mathcal{P}}_{\text{diss}} = \frac{1}{2} \omega f_\omega^2 \text{Im}[\tilde{\chi}(\omega)] \quad (1.15)$$

for a harmonic external force  $f(t) = f_\omega \cos(\omega t)$