Master Icfp - M2

Advanced Statistical Physics

Tutorials

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Practical information

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Contents

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

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

where γ is a damping coefficient and ξ, a Langevin force. The latter is assumed to be a white noise with zero mean and peaked correlations

$$\langle \xi(t) \rangle = 0\,, \quad \left\langle \xi(t)\xi(t') \right\rangle = q\,\delta(t-t')\,, \tag{1.2}$$

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

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

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

3. In the stationary limit, when t and $t' \to \infty$, we define the temperature $\left\langle \frac{1}{2} m v^2 \right\rangle = \frac{1}{2} k_B T$. Deduce the relation between q, τ and T.

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

4. Show that in this regime

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

We recall that for a gaussian white noise (1.2)

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

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

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

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

1.2 Time and statistical averages

One considers the random "function" given by the sum of impulses

$$\xi(t) = \sum_{n=1}^{N} \kappa_n\,\delta(t - t_n) \tag{1.7}$$

defined over the interval $[0, T]$, where

- the t_n's are independent and identically distributed (i.i.d) random times *uniformly* distributed (i.e. one t_n has distribution $p(t_n) = 1/T$). We denote by $\lambda = N/T$ (for $N \to \infty$ and $T \to \infty$) the rate of occurence of the random times.
- the κ_n's are i.i.d random variables with common distribution $w(\kappa)$ with finite $\left\langle \kappa_n^2\right\rangle$.

1. Compute the time average of $\overline{\xi(t)}$, over the time interval $[0, T]$. Compare with the statistical average (over t_n's and κ_n's).
2. Compute the time averaged correlator $\widetilde{C}(t, t') = \overline{\xi(t)\xi(t')}^c = \overline{\xi(t)\xi(t')} - \overline{\xi(t)}\ \overline{\xi(t')}$. Is it invariant with respect to time ? Compare to $C(t, t') = \langle\xi(t)\xi(t')\rangle_c = \langle\xi(t)\xi(t')\rangle - \langle\xi(t)\rangle\langle\xi(t')\rangle$.

1.3 *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

$$\frac{\mathrm{d}v(t)}{\mathrm{d}t} + \frac{1}{\tau}v(t) = \frac{1}{m}\xi(t) \tag{1.8}$$

where ξ a a Gaussian white noise of zero mean and local time correlations

$$\left\langle\xi(t)\xi(t')\right\rangle = C\,\delta(t - t') \tag{1.9}$$

Our aim is to compute the mean square displacement $\left\langle x(t)^2\right\rangle$ 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

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} x(t)^2 + \frac{1}{\tau}\frac{\mathrm{d}}{\mathrm{d}t} x(t)^2 = 2v(t)^2 + \frac{2}{m} x(t)\,\xi(t) \tag{1.10}$$

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

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

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

$$\left\langle x(t)^2 \right\rangle = \frac{2k_{\mathrm{B}}T\tau}{m}\left[t - \tau\left(1 - \mathrm{e}^{-t/\tau}\right)\right] \tag{1.11}$$

Analyze carefully the limiting behaviours and plot the function.

Tutorial 2

Master equation

2.1 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 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 $N+1$.

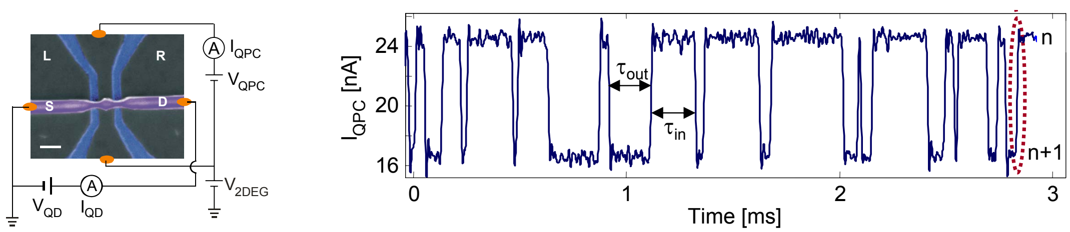

Figure 2.1: *The charge inside the conductor is measured as a function of the time : I_{QPC} is proportional to the number of electron inside the central island, which fluctuates by one unit (one electron).*

Consider the Markov process $X(t)$ taking two values X_1 or X_2. The transition rates are λ_1 (from X_1 to X_2) and λ_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, deno ted by P_i^* (hint : consider $P_1(t) + P_2(t)$ and $y(t) = P_1(t) - P_2(t)$).
An interesting exercice is to write the system of equations in a matricial form $\frac{\mathrm{d}}{\mathrm{d}t}\vec{P}(t) = M\vec{P}(t)$ and diagonalize the non-symmetric stochastic matrix M. Show that

$$\exp\left[t\begin{pmatrix}-\lambda_1 & \lambda_2\\ \lambda_1 & -\lambda_2\end{pmatrix}\right] = \begin{pmatrix}P_1^* & P_1^*\\ P_2^* & P_2^*\end{pmatrix} + \begin{pmatrix}P_2^* & -P_1^*\\ -P_2^* & P_1^*\end{pmatrix}\mathrm{e}^{-(\lambda_1+\lambda_2)t} \tag{2.1}$$

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

$$P_t(1|2)\, P_2^* = P_t(2|1)\, P_1^* \tag{2.2}$$

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.

In the experiments, the fluctuations of the charge in the QD can be characterized by measuring the power spectrum $S(\omega)$. Compute $S(\omega)$ for the random telegraph process. The measurment is reported in another article, Fig. 2.2. Compare your result with the data.

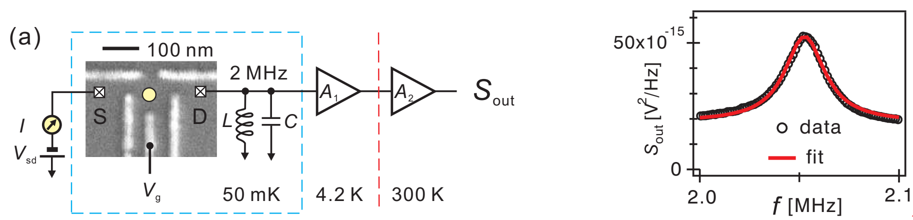

Figure 2.2: Left : *The microstructure studied.* Right : *Power spectrum.* From : Y. Okazaki, S. Sasaki and K. Muraki, *Shot noise spectroscopy on a semiconductor quantum dot in the elastic and inelastic cotunneling regimes*, Phys. Rev. B **87**, 041302(R) (2013).

2.2 Poisson jump process

In this exercise, we study the "Compound Poisson process" (or "Poisson jump process"). The process starts at $X(0) = 0$ and makes jumps at random times t_n occuring with rate λ :

$$X(t_n^+) = X(t_n^-) + \eta_n\,. \tag{2.3}$$

The jump amplitudes η_n's are i.i.d. random variables, distributed according to a distribution $w(\eta)$, assumed *symmetric* for simplicity. We denote by $P(x,t)$ the distribution of the process $X(t)$.

1/ Show that $P(x,t)$ obeys the integro-differential equation

$$\frac{\partial P(x,t)}{\partial t} = \lambda \int \mathrm{d}\eta\, w(\eta)\ [P(x-\eta,t) - P(x,t)] \tag{2.4}$$

Check conservation of normalisation.

2/ Using that the problem is translation invariant (both in time and space), solve the master equation by using Fourier transformation : show that $\widehat{P}(k,t) = \int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx}\, P(x;t)$ obeys a simple differential equation. Deduce a general integral representation of $P(x,t)$ involving the Fourier transform $\hat{w}(k)$ of the jump distribution.

3/ We have $\hat{w}(k) \simeq 1 - a_2 k^2 + a_4 k^4 + o(k^4)$ for $k \to 0$. Give the interpretation of the two positive coefficients a_2 and a_4.

Argue that the large time limit of $P(x,t)$ involves the $k \to 0$ behaviour of $\hat{w}(k)$. Deduce that the distribution is Gaussian at large time. Give $\langle X(t)^2 \rangle$ and interpret.

4/ We now consider the case where the jump distribution exhibits a power law tail $w(\eta) \sim |\eta|^{-\mu-1}$ for $\eta \to \infty$, with $0 < \mu < 2$. One can show that $\hat{w}(k) \simeq 1 - c\,|k|^{\mu} + o(k^{\mu})$ for $k \to 0$, where $c > 0$. Show that, at large time, the distribution can ne written as $P(x,t) \simeq F(x/t^{\theta})/t^{\theta}$. Give the exponent θ in terms of μ and express $F(x)$ as an integral.

Compute explicitly $F(x)$ for $\mu = 1$.

What is the expected asymptotic behaviour of $F(x)$ $\forall \mu \in]0,2[$?

2.3 *To go further : 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

$$\partial_t P_n(t) = W_{n,n-1} P_{n-1}(t) + W_{n,n+1} P_{n+1}(t) - \left(W_{n-1,n} + W_{n+1,n}\right) P_n(t) \tag{2.5}$$

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

$$\partial_t P_n = -J_n + J_{n-1} \tag{2.6}$$

and express the "current density" J_n related to the distribution of the P_n's.

2/ We now choose the matrix such that

$$W_{n,m} = \mathrm{e}^{[V(m)-V(n)]/2} \quad \text{for } m \neq n\,, \tag{2.7}$$

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

Equilibrium state.— Show that

$$P_n^* = C\,\mathrm{e}^{-V(n)} \tag{2.8}$$

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

$$P_n^* = J\,\mathrm{e}^{-V(n)} \sum_{m=n}^{\infty} \mathrm{e}^{[V(m+1)+V(m)]/2} \tag{2.9}$$

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

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

2.4 *To go further : Gaussian-versus-non Gaussian white noise – Shottky noise*

We consider the noise

$$F(t) = \sum_{n=1}^{N} \kappa_n \, \delta(t - t_n) \qquad \text{for } t \in [0, T] \tag{2.10}$$

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

$$P_T(N) = \frac{(\lambda T)^N}{N!} \mathrm{e}^{-\lambda T} \tag{2.11}$$

The t_n are uniformly distributed over the interval $[0, T]$, i.e. the joint distribution of the N times simply $P_N(t_1, \cdots, t_N) = 1/T^N$. The weights κ_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

$$G[\phi(t)] \stackrel{\text{def}}{=} \left\langle \mathrm{e}^{\int \mathrm{d}t \, \phi(t) \, F(t)} \right\rangle \tag{2.12}$$

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

$$\frac{\delta \phi(t')}{\delta \phi(t)} = \delta(t - t') \tag{2.13}$$

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

2/ Using that averaging over the random variables is

$$\langle (\cdots) \rangle_{N, \{t_n\}} = \sum_{N=0}^{\infty} \frac{(\lambda T)^N}{N!} \mathrm{e}^{-\lambda T} \int_0^T \frac{\mathrm{d}t_1}{T} \cdots \frac{\mathrm{d}t_N}{T} (\cdots) \tag{2.14}$$

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

3/ Functional derivations of $G[\phi]$ generate the correlation functions $\langle F(t_1) \cdots F(t_n) \rangle$ 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

[1] i.i.d. = independent and identically distributed.

be written under the form of independent implulses $i(t) = q\sum_n \delta(t-t_n)$. The average rate is λ. Express the two first cumulants of current, $\langle i(t)\rangle$ and $\langle i(t)\, i(t')\rangle_c$. Deduce the power spectrum

$$S(\omega) \stackrel{\text{def}}{=} \int \mathrm{d}(t-t')\, \mathrm{e}^{\mathrm{i}\omega(t-t')} \langle i(t)\, i(t')\rangle_c \tag{2.15}$$

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/ Transfered charge (Poisson process).– We consider the stochastic differential equation

$$\frac{\mathrm{d}Q(t)}{\mathrm{d}t} = i(t) \tag{2.16}$$

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

$$\frac{\mathrm{d}Q(t)}{\mathrm{d}t} = \mathcal{I}(Q(t)) + i(t)\,. \tag{2.17}$$

Consider separatly the effect of the drift and the jumps to relate $P(Q;t+\mathrm{d}t)$ to $P(Q;t)$. Show that the distribution obeys

$$\partial_t P(Q;t) = -\partial_Q \left[\mathcal{I}(Q)\, P(Q;t)\right] + \lambda \left[P(Q-q;t) - P(Q;t)\right]\,. \tag{2.18}$$

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

a) Find the new expression of the generating functional $G[\phi]$.

b) Show that it is possible to define a limit (changing λ and $w(\kappa)$) where the noise becomes a Gaussian white noise.

c) Show that the generalisation of (2.18) is

$$\boxed{\partial_t P(Q;t) = -\partial_Q \left[\mathcal{I}(Q)\, P(Q;t)\right] + \lambda \int \mathrm{d}q\, w(q)\, \left[P(Q-q;t) - P(Q;t)\right]} \tag{2.19}$$

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 $q \to 0$, i.e. when $w(q)$ is concentrated at the origin. Assuming $\langle q\rangle = 0$, show that (2.19) 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

$$m\frac{\mathrm{d}}{\mathrm{d}t}v(t) = -\int \mathrm{d}t'\,\gamma(t-t')\,v(t') + F(t) \tag{3.1}$$

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

1/ Show that the correlation function of the velocity is

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

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 σ in terms of the diffusion constant $D \stackrel{\text{def}}{=} \lim_{t\to\infty} \frac{1}{2t}\left\langle x(t)^2 \right\rangle$.

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

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

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 $\gamma(\tau) = \theta_{\mathrm{H}}(\tau)\,(\lambda/\tau_m)\,\mathrm{e}^{-\tau/\tau_m}$.
Discuss the hypothesis $\gamma(t) = \lambda\,\delta(t)$ in this case.
For a finite τ_m, give a physical argument to express the correct hierarchy of times $1/\lambda$, τ_m and τ_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 $f_{\rm ext}(t)$. The position of the particle is described by the Langevin equation

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = -\lambda\, x(t) + f_{\rm ext}(t) + F(t) \tag{3.4}$$

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

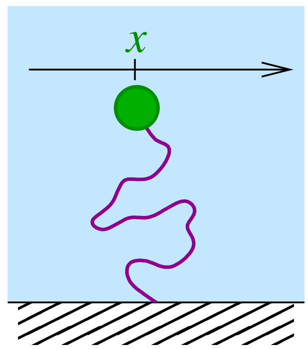

Figure 3.1: *A small particle is bound to a surface thanks to a polymer which acts like a spring.*

1/ Correlations at equilibrium.– We consider the case $f_{\rm ext}(t) = 0$. Compute de correlation function $C(t-t') \stackrel{\rm def}{=} \langle x(t)x(t')\rangle_{\rm eq}$. Deduce what is the stationary distribution $P_{\rm eq}(x)$ 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 χ for this linear problem. We recall that it is defined by

$$\langle x(t)\rangle_{\rm out\ of\ eq.} = \langle x\rangle_{\rm eq} + \int \mathrm{d}t'\,\chi(t-t')\,f_{\rm ext}(t') + \mathcal{O}(f_{\rm ext}^2) \tag{3.5}$$

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

$$\boxed{\chi(t) = -\beta\;\theta_{\rm H}(t)\,\frac{\mathrm{d}}{\mathrm{d}t}C(t)} \tag{3.6}$$

where $\beta = 1/(k_BT)$.

Tutorial 4

Fokker-Planck approach

4.1 The moments for a linear drift

We study a diffusion on $\mathbb{R}$ for a linear drift, described by the Fokker-Planck equation

$$\partial_t P_t(x) = -\partial_x\big[(a+b\,x)P_t(x)\big] + \partial_x^2\big[D(x)P_t(x)\big]\,. \tag{4.1}$$

1/ Express $\frac{\mathrm{d}}{\mathrm{d}t}\langle x(t)\rangle$ in terms of $P_t(x)$. Deduce that $\langle x(t)\rangle$ obeys a simple differential equation. Solve this differential equation for initial condition $x(0)=0$. Discuss the solution briefly : assuming $a>0$, plot *neatly* $\langle x(t)\rangle$ for $b>0$ and $b<0$.

2/ Consider now $\frac{\mathrm{d}}{\mathrm{d}t}\langle x(t)^n\rangle$. Under what condition on $D(x)$ *would it be possible in principle* to solve a differential equation for $\langle x(t)^n\rangle$? (do *not* solve it yet).

3/ We choose $D(x)=D_0+D_1\,x+D_2\,x^2$ ($>0\ \forall\,x$). Show that the variance $\langle x(t)^2\rangle_c=\langle x(t)^2\rangle-\langle x(t)\rangle^2$ obeys a linear differential equation with a source term $D(\langle x(t)\rangle)$. Solve the equation for $x(0)=0$. *Estimate* the main behaviour for large t (for $b>0$ and $D_2>0$). Prefactor *not* asked. Discuss $\sqrt{\langle x(t)^2\rangle_c}/\langle x(t)\rangle$ in this limit.

4.2 Ornstein-Uhlenbeck process and the Fokker-Planck equation

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

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = -\lambda\,x(t) + F(t) \tag{4.2}$$

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 stationnary distribution $P_{\mathrm{eq}}(x)$ and the conditional probability $P_\tau(x|x_0)$.

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

2. **Method 2.–** Write the corresponding Fokker-Planck equation.

In order to solve this partial differential equation, we can use its equivalence with the Schrödinger equation. Indeed, the Fokker-Planck equation

$$\partial_t P(x,t) = \partial_x \big[D\partial_x - F(x) \big] P(x,t) \tag{4.3}$$

can be mapped onto the imaginary time Schrödinger equation

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

thanks to the transformation $P(x,t) = \psi_0(x)\,\psi(x,t)$ with $\psi_0(x) = \sqrt{P_{\mathrm{eq}}(x)} \propto \exp[-U(x)/2D]$ where $U(x) = -\int^x \mathrm{d}\xi\, F(\xi)$ is the potential.

3. Demonstrate the formula (4.4) and give the corresponding supersymmetric Schrödinger operator H_+ associated with the Fokker-Planck equation of the over-damped regime. Give the spectrum of its eigenvalues.

4. We recall the expression of the quantum mechanical propagator for the harmonic oscillator

$$\langle\, x\,|\mathrm{e}^{-tH_\omega}|\, x_0\,\rangle = \sqrt{\frac{m\omega}{2\pi\,\mathrm{sh}(\omega t)}}\,\exp -\frac{m\omega}{2\,\mathrm{sh}(\omega t)}\left[\mathrm{ch}(\omega t)\,(x^2+x_0^2) - 2\,x\,x_0\right] \tag{4.5}$$

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

4.3 *To go further : Diffusion on a ring*

4.3.1 Free diffusion

We consider the free diffusion in a ring

$$\partial_t P(x,t) = D\partial_x^2 P(x,t) \qquad \text{for } x \in [0,L] \tag{4.6}$$

with periodic boundary conditions

$$P(0) = P(L) \tag{4.7}$$
$$P'(0) = P'(L) \tag{4.8}$$

(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 characterisitic time τ_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.

4.3.2 Effect of a drift

Same question when a constant drift is introduced :

$$\partial_t P(x,t) = \left(D\partial_x^2 - v\,\partial_x\right) P(x,t) \qquad \text{for } x \in [0,L] \tag{4.9}$$

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

4.3.3 Boundary conditions induced current

We now come back to the analysis of the free diffusion (4.6), however we now study the problem for a new set of boundary conditions :

$$P(L) = 0 \tag{4.10}$$

$$P'(0) = P'(L) \tag{4.11}$$

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 in 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 2×2 matrix.

Appendix : a Poisson formula

$$\sum_{n\in\mathbb{Z}} \mathrm{e}^{2\mathrm{i}\pi n\eta}\,\mathrm{e}^{-\pi^2(n+\alpha)^2 y} = \frac{1}{\sqrt{\pi y}} \sum_{n\in\mathbb{Z}} \mathrm{e}^{2\mathrm{i}\pi(n-\eta)\alpha}\,\mathrm{e}^{-\frac{(n-\eta)^2}{y}} \,. \tag{4.12}$$

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

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.

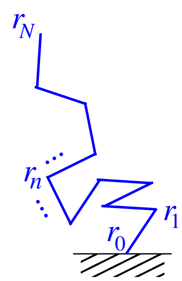

Figure 5.1: *The "Gaussian polymer" : N independent monomers.*

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

$$P_N(\vec{r}\,|\,\vec{r}_0) = \int \frac{\mathrm{d}^d\vec{u}}{S_d a^{d-1}}\,\delta(||\vec{u}|| - a)\,P_{N-1}(\vec{r}-\vec{u}\,|\,\vec{r}_0)\,. \tag{5.1}$$

   where 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 in the $d = 3$ case.

3. We define the "giration radius" as $R_G^2 = \int \mathrm{d}^d\vec{r}\,P_N(\vec{r}\,|\,0)\,\vec{r}^{\,2}$. By studying the small wavevector expansion of the Fourier transform, deduce R_G.
   Compare R_G (in unit of a) with the length of the polymer $\mathscr{L}_N = Na$.

4. Study the continuum limit $a \to 0$ and $N \to \infty$ with $t = Na^2$ fixed.

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. We write $P_0(x)$ the initial condition $P_0(x) = P(x, t = 0)$. Construct the solution of the diffusion equation

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

   (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 :

$$S_{x_0}(t) = \int_0^\infty \mathrm{d}x\, \mathcal{P}_t^+(x|x_0) \tag{5.3}$$

   Remark : what would have been the result if $\mathcal{P}_t^+(x|x_0)$ would have satisfied a Neunmann 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 :

$$S_{x_0}(t) = \int_t^\infty \mathrm{d}T\, P_{x_0}(T) \tag{5.4}$$

   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 $m \geqslant 0$ its maximum and $Q_t(m)$ the corresponding distribution. Justify the following identity

$$\int_0^m \mathrm{d}m'\, Q_t(m') = S_m(t) \tag{5.5}$$

   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 θ for the Brownian motion.

Appendix : the error function

$$\mathrm{erf}(z) \stackrel{\text{def}}{=} \frac{2}{\sqrt{\pi}} \int_0^z \mathrm{d}t\, \mathrm{e}^{-t^2} \tag{5.6}$$

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

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

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

6.1 Connection between stochastic and Fokker-Planck equations

We consider the stochastic differential equation (SDE)

$$\mathrm{d}x(t) = a[x(t)]\,\mathrm{d}t + b[x(t)]\,\mathrm{d}W(t) \qquad \text{(Itô)}. \tag{6.1}$$

A simple manner to make the connection between stochastic equations and Fokker-Planck equation (FPE) is to use the independence of $x(t)$ and $\mathrm{d}W(t)$ at coinciding times and $\langle \mathrm{d}W(t)^2\rangle_{\text{noise}} = \mathrm{d}t$ (physicist's notation). Thus, the drift and the "diffusion" terms in the related FPE

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

are given by

$$a(x) = \frac{\langle \mathrm{d}x\rangle_{\text{noise}}}{\mathrm{d}t} \qquad \text{and} \qquad b(x)^2 = \frac{\langle \mathrm{d}x^2\rangle_{\text{noise}}}{\mathrm{d}t} \tag{6.3}$$

1. We consider the multidimensional case

   $$\mathrm{d}x_i(t) = a_i(\vec{x})\,\mathrm{d}t + b_{ij}(\vec{x})\,\mathrm{d}W_j(t) \qquad \text{(Itô)}. \tag{6.4}$$

   with $\langle \mathrm{d}W_i(t)\rangle_{\text{noise}} = 0$ and $\langle \mathrm{d}W_i(t)\mathrm{d}W_j(t)\rangle_{\text{noise}} = \delta_{ij}\mathrm{d}t$. Show that the related FPE is

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

   (with implicit summation over repeated indices).

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

   $$\begin{cases} \mathrm{d}x = v\,\mathrm{d}t \\ \mathrm{d}v = \left(-\frac{v}{\tau} + \frac{F(x)}{m}\right)\mathrm{d}t + \frac{1}{m}\sqrt{2k_\mathrm{B}T\gamma}\,\mathrm{d}W(t) \end{cases} \tag{6.6}$$

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

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

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 $P_t(x) = \int \mathrm{d}v\, P_t(x, v)$ in the limit of strong friction is

$$\partial_t P_t(x) \simeq \frac{1}{\gamma}\left[-\partial_x F(x) + k_\mathrm{B}T\partial_x^2\right] P_t(x) \tag{6.8}$$

6.2 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 $a < x_0$:

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

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

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

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

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

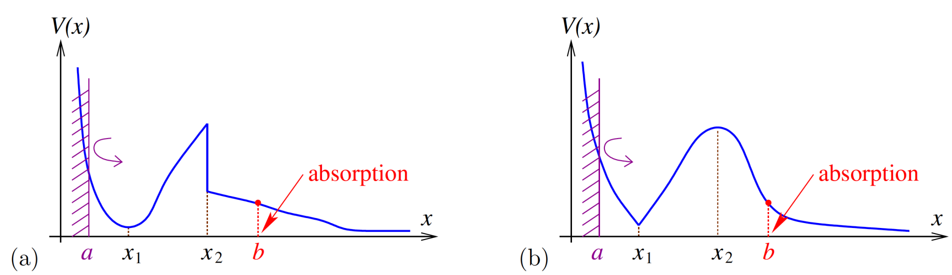

Figure 6.1: *Two other types of trapping potentials.*

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

$$\left(p + \frac{N^2}{V^2}a\right)(V - Nb) = Nk_\mathrm{B}T \tag{7.1}$$

1/ Using dimensionless analysis, relate the three coordinates (T_c, V_c, p_c) of the critical point to a and b.

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 $p_c V_c/(Nk_\mathrm{B}T_c)$. Compare with the experimental data of the table

	T_c (K)	V_c (cm^3)	p_c (atm)	$\frac{p_c V_c}{N k_\mathrm{B} T_c}$
He	5.2	57.8	2.26	0.30
H_2	33.1	65.0	12.8	0.31
N_2	126.1	90.1	33.5	0.29
O_2	154.4	74.4	49.7	0.29
CO_2	304.2	94.0	72.9	0.27
H_2O	647.4	56.3	218.3	0.23

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

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

(justifiy 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 β_{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.

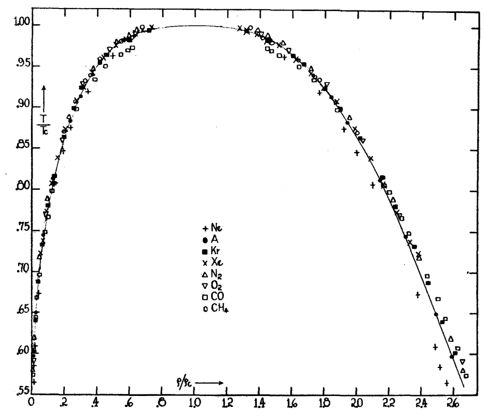

FIG. 2.

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 δ_{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 χ_T in the vicinity of the critical point ? Deduce the critical exponent γ_{VdW}.

8/ 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.

Tutorial 8

Mean field - Demixing transition

8.1 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).

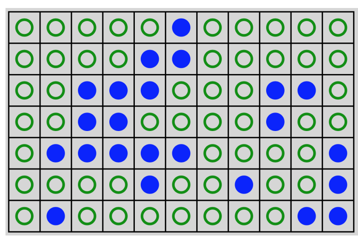

Figure 8.1: *Two types of molecules on a lattice : solute particles (•) and solvent molecules (∘).*

We introduce the concentration of solute

$$\phi = \frac{N_p}{N} . \tag{8.1}$$

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

$$\begin{cases} \bullet\bullet : & \varepsilon_{pp} \\ \circ\bullet : & \varepsilon_{ps} \\ \circ\circ : & \varepsilon_{ss} \end{cases} \tag{8.2}$$

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

$$E(\mathcal{C}) = N_{pp}(\mathcal{C})\, \varepsilon_{pp} + N_{ps}(\mathcal{C})\, \varepsilon_{ps} + N_{ss}(\mathcal{C})\, \varepsilon_{ss} \tag{8.3}$$

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

$$Z = \sum_{\mathcal{C}} \mathrm{e}^{-\beta E(\mathcal{C})} \tag{8.4}$$

with a mean field approximation.

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

$$\begin{cases} \overline{N}_{pp} = \frac{1}{2} N z \phi^2 \\ \overline{N}_{ps} = N z \phi (1-\phi) \\ \overline{N}_{ss} = \frac{1}{2} N z (1-\phi)^2 \end{cases} \tag{8.5}$$

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

$$\frac{1}{N}\overline{E} = \varepsilon_0 + c_1\,\phi + \frac{z}{2}\,\Delta\varepsilon\,\phi^2 \tag{8.6}$$

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 ε_{ps}.

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

3/ **Partition function :** The mean field approximation corresponds to $Z = \sum_{\mathcal{C}} \mathrm{e}^{-\beta E(\mathcal{C})} \equiv \Omega \left\langle \mathrm{e}^{-\beta E} \right\rangle \approx \Omega\, \mathrm{e}^{-\beta \overline{E}}$. Show that

$$Z \sim \mathrm{e}^{-N\beta f_L(\phi)} \tag{8.7}$$

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 $\overline{E}$ 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 $\eta = -z\Delta\varepsilon/(2k_{\mathrm{B}}T)$: what is the critical value η_c corresponding to T_c ?

5/ We consider $T < T_c$. We denote by ϕ_1 and ϕ_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 $T \to T_c^-$, 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 8.2).

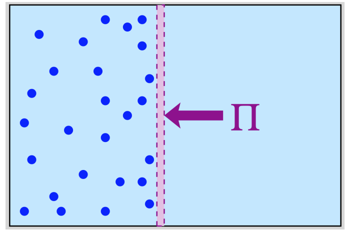

Figure 8.2: *The left volume contains solute+solvent and the right volume only solvent. The two volumes are separated by a semi-permeable wall allowing only sovent to pass through.*

The volume of the solution is N (in appropriate units) and the total volume N_{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

$$\Pi(\phi) = -\frac{\partial F_{\text{tot}}(N)}{\partial N} \tag{8.8}$$

as a function of ϕ (be careful that ϕ depends on the volume N).

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

Tutorial 9

Charged fluids

9.1 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 $\overline{n}_+$, and one with negative charge q_- and density $\overline{n}_-$. One may show that equilibrium may occur only when the global electroneutrality is satisfied, $q_+\overline{n}_+ + q_-\overline{n}_- = 0$. In presence of an external potential $\phi^{ext}(\mathbf{r})$, the Hamiltonian of the system is

$$\mathcal{H}^{int} = \frac{1}{2} \sum_{(i,\sigma)\neq(j,\tau)} q_\sigma q_\tau v_C(\mathbf{r}_i^\sigma - \mathbf{r}_j^\tau) + \sum_{i,\sigma} q_\sigma \phi^{ext}(\mathbf{r}_i^\sigma)\,, \tag{9.1}$$

where the Coulomb potential satisfies $\mathbf{\Delta_r} v_C(\mathbf{r},\mathbf{r}') = -4\pi\delta(\mathbf{r}-\mathbf{r}')$. 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 $f = k_B T n \left[\ln(n\lambda^3) - 1\right]$ 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

$$\mathcal{F} = \frac{1}{2}\int d\mathbf{r}\, d\mathbf{r}'\, \langle\rho_q(\mathbf{r})\rangle v_C(\mathbf{r}-\mathbf{r}')\langle\rho_q(\mathbf{r}')\rangle + \int d\mathbf{r}\, \langle\rho_q(\mathbf{r})\rangle\, \phi^{ext}(\mathbf{r})$$
$$+ k_B T \int d\mathbf{r}\langle n_+(\mathbf{r})\rangle \ln[\langle n_+(\mathbf{r})\rangle\lambda^3] + k_B T \int d\mathbf{r}\langle n_-(\mathbf{r})\rangle \ln[\langle n_-(\mathbf{r})\rangle\lambda^3] \tag{9.2}$$

   in 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, the local densities at equilibrium are given by

$$\frac{\delta}{\delta\langle n_+(\mathbf{r})\rangle}\left[\mathcal{F} - \mu_+ \int d\mathbf{r}\, \langle n_+(\mathbf{r})\rangle - \mu_- \int d\mathbf{r}\, \langle n_-(\mathbf{r})\rangle\right] = 0 \tag{9.3}$$

Show that the solution is

$$\langle n_\sigma(\mathbf{r})\rangle = A_\sigma \exp\left[-\beta q_\sigma \phi(\mathbf{r})\right] , \tag{9.4}$$

with some constants A_σ and the total electric potential

$$\phi(\mathbf{r}) = \phi^{ext}(\mathbf{r}) + \int d\mathbf{r}'\, v_C(\mathbf{r}-\mathbf{r}')\,\langle \rho_q(\mathbf{r}')\rangle , \tag{9.5}$$

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_σ ? In the special case where $\phi^{ext} = 0$, what are the values of the different densities ?

We consider the charge-density response function $\chi_{\rho\,\rho}(\mathbf{r},\mathbf{r}') = -\frac{\delta\langle \rho_q(\mathbf{r})\rangle}{\delta\phi^{ext}(\mathbf{r}')}\Big|_{\phi^{ext}=0}$.

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

$$\widetilde{\chi}_{\rho\,\rho}(\mathbf{k}) = \frac{\kappa^2}{4\pi}\frac{\widetilde{\delta\phi}}{\delta\phi^{ext}}(\mathbf{k}) , \tag{9.6}$$

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

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

$$\widetilde{\chi}_{\rho\,\rho}(\mathbf{k}) = \frac{\kappa^2}{4\pi}\frac{\mathbf{k}^2}{\mathbf{k}^2+\kappa^2} . \tag{9.7}$$

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_BT, $\overline{n}$ and q^2 ?

7. Argue that the mean-field approximation is valid when $\langle \delta\rho_q(\mathbf{r})\delta\rho_q(\mathbf{r}')\rangle \ll q^2\overline{n}^2$, where $\delta\rho_q(\mathbf{r}) = \rho_q(\mathbf{r}) - \langle \rho_q(\mathbf{r})\rangle$. What is the link between $\langle \delta\rho_q(\mathbf{r})\delta\rho_q(\mathbf{r}')\rangle$ 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 (9.2) in terms of the fluctuations in the densities. Hence we decompose the local densities as $\langle n_\pm(\mathbf{r})\rangle = \overline{n}_\pm + \delta n_\pm(\mathbf{r})$.

8. Expand the free energy (9.2) up to and including the second order δn. We introduce the auxiliary fields $\langle \rho_q(\mathbf{r})\rangle = q_+\delta n_+(\mathbf{r}) + q_-\delta n_-(\mathbf{r})$ and

$$\psi(\mathbf{r}) = -q_-\sqrt{\frac{\overline{n}_-}{\overline{n}_+}}\delta n_+(\mathbf{r}) + q_+\sqrt{\frac{\overline{n}_+}{\overline{n}_-}}\delta n_-(\mathbf{r}) \tag{9.8}$$

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

$$F = \frac{1}{2}\int d\mathbf{r}\, d\mathbf{r}'\, \langle\rho_q(\mathbf{r})\rangle U(\mathbf{r}-\mathbf{r}')\langle\rho_q(\mathbf{r}')\rangle + \int d\mathbf{r}\langle\rho_q(\mathbf{r})\rangle\, \phi^{ext}(\mathbf{r}) + \frac{2\pi}{\kappa^2}\int d\mathbf{r}\psi(\mathbf{r})^2\,, \tag{9.9}$$

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

9. Deduce that $\dfrac{1}{V}\langle\widetilde{\rho_q}(\mathbf{k})\widetilde{\rho_q}^*(\mathbf{k})\rangle = k_B T/\tilde{U}(\mathbf{k})$
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 10

Ginzburg-Landau mean field approach

10.1 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

$$F_L[\phi] = \int \mathrm{d}^d\vec{r}\, \left\{ g\left(\vec{\nabla}\phi(\vec{r})\right)^2 + f_L\left(\phi(\vec{r})\right) \right\} \quad \text{with } f_L(\phi) \simeq f_0(T) + \frac{a(T)}{2}\,\phi^2 + \frac{b}{4}\,\phi^4 \qquad (10.1)$$

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

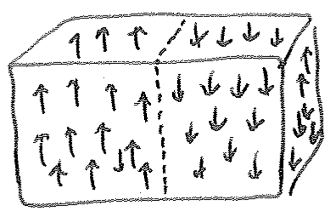

Figure 10.1: *Interface between two regions of opposite magnetization.*

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 $V(x) = \frac{1}{2}m\omega^2x^2$.

c) If the potential grows faster than the harmonic potential, for example $V(x) = \frac{1}{2}m\omega^2x^2 + \lambda\,x^4$, plot a sketch of $T(E)$.

d) *Optional:* 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 : $\phi(\vec{r}) \to \phi(x)$.

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 ϕ_0. Find the solution of the field equation which statisfy $\phi(x \to \pm\infty) = \pm\phi_0$. 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 :

$$\sigma = \frac{F[\phi(x)] - F[\phi_0]}{\text{Surf}} \tag{10.2}$$

Show that

$$\sigma = 2g \int_{-\infty}^{+\infty} \mathrm{d}x \, \left[\phi'(x)\right]^2 \tag{10.3}$$

Compute explicitly the integral. Comment on the temperature dependence.

Tutorial 11

Real space renormalization of an Ising model

11.1 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 Scientic, 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 $K = J/k_BT$.

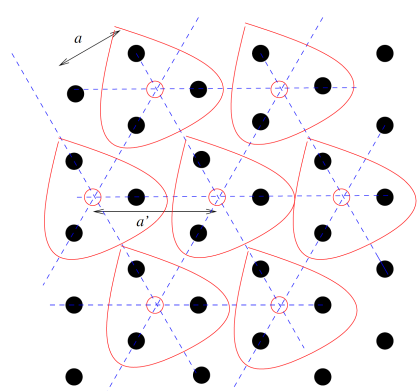

Figure 11.1: *The original spins σ_i lie at the black bullets while the plaquette lie at the empty circles. They form a triangular lattice.*

1. The lattice is divided into triangular plaquettes as shown in Figure 11.1. 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 $H = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j$ involves interactions of all the nearest neighbors. We gather on one hand interactions between spins σ_i that belong to the same plaquette I, and on the other hand, interactions between spins σ_i and σ_j that belong to different nearest neighbor plaquettes I and J. We thus split the Hamiltonian into two parts, $H = H_1 + H_2$, where $H_1 = \sum_I h_1(I)$ encompass all the nearest-neighbor interactions of spins that belong to same plaquettes, and $H_2 = \sum_{\langle I,J\rangle} h_2(I,J)$, that describes interactions of spins of different plaquettes. 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

$$Z(K,N,a) = \sum_{\{S_I\}}\sum_{\{\sigma_i\}}{}' e^{-\beta H(\sigma_i)} \quad , \tag{11.1}$$

where Σ' denotes a summation over all the $\{\sigma_i\}$ configurations at fixed plaquette configurations $S_I = \text{sign}\left(\sum_{i\in I}\sigma_i\right)$. 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

$$Z(K,N,a) = \sum_{\{S_I\}} Z_1 \left\langle e^{-\beta H_2}\right\rangle_1 \tag{11.2}$$

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

5. Let σ_i be a spin belonging to a plaquette I. Show that

$$\langle\sigma_i\rangle_1 = S_I\frac{e^{3K}+e^{-K}}{e^{3K}+3e^{-K}} \quad . \tag{11.3}$$

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 $\langle\ldots\rangle_1$.

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

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

$$Z(K,N,a) = \left(e^{3K}+3e^{-K}\right)^{N'} Z(K',N',a') \quad , \tag{11.4}$$

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 ν 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 Leewen 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.