Physique statistique hors équilibre – Examen

Lundi 9 janvier 2017

Rédigez vos réponses à cette partie de l'examen sur une **copie SÉPARÉE**.

Vous pouvez rédiger en français si vous le souhaitez.

Subject : **Non-intersecting fluctuating lines and 1D fermions**

Introduction : We study a model of non-intersecting Brownian lines in dimension $1+1$, using the mapping on the 1D fermion gas. We consider lines going only forward in one of the two spatial directions (axis τ in Fig. 1), which can thus be considered as a fictitious "time". Each line is described by a displacement field $x_n(\tau) \in \mathbb{R}$ for $\tau \in [0, L]$. Such models appear in various contexts : directed polymers, fluctuating interface models (for atomic terraces, wetting problems,..), etc.

Single line : The basic ingredient of the model is the functional for the elastic energy

$$E[x(\tau)] = \frac{c}{2}\int\left(\sqrt{\mathrm{d}\tau^2+\mathrm{d}x^2}-\mathrm{d}\tau\right) \simeq \frac{c}{4}\int_0^L \mathrm{d}\tau\,(\partial_\tau x(\tau))^2\,,$$

where it is assumed that distorsions are small, $|\partial_\tau x| \ll 1$. The positive coefficient c is the elastic coefficient (the stress). The Gibbs measure $\exp\big\{-E[x(\tau)]/T\big\}$ is identified with the Wiener measure for the Brownian motion with diffusion constant $D = T/c$. Such a Brownian trajectory can be conveniently described by the Fokker-Planck equation

$$\partial_\tau P_\tau(x|y) = D\,\partial_x^2 P_\tau(x|y)\,, \tag{1}$$

where $P_\tau(x|y)$ is the conditional probability for the Wiener process (free Brownian motion).

Part C is almost independent of parts A and B.

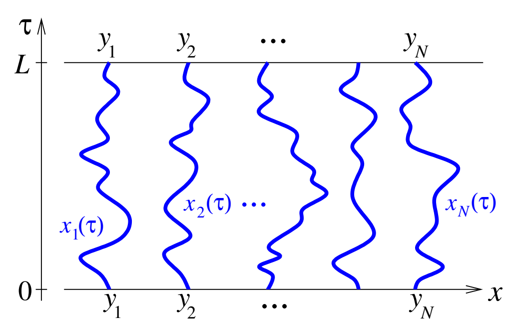

FIGURE 1 : *N non-intersecting elastic lines (directed polymers, fluctuating interfaces,...).*

A. Properties of a single line.– We first study the fluctuations of a single line.

1/ Eq. (1) describes the single line. Recall its solution on $\mathbb{R}$.

Hint : The initial condition is $\lim_{\tau\to0} P_\tau(x|y) = \delta(x-y)$.

2/ Fluctuations.– We consider the situation where the line issues and ends at the same point, say $x(0) = x(L) = 0$. Justify

$$\langle x(\tau)^2 \rangle = A_L \int_{\mathbb{R}} \mathrm{d}x\, P_{L-\tau}(0|x)\, x^2\, P_\tau(x|0) \tag{2}$$

What is the normalisation constant A_L ? Compute the variance $\langle x(\tau)^2 \rangle$ and plot it neatly as a function of $\tau \in [0, L]$. Where are the fluctuations maximum ?

B. *N* non-intersecting lines.– We now consider N lines $(x_1(\tau), \cdots, x_N(\tau)) \stackrel{\text{def}}{=} \vec{x}(\tau)$, still described by the free diffusion, with however some constraints for non-intersection

$$\partial_\tau P_\tau(\vec{x}|\vec{y}) = D\vec{\nabla}^2 P_\tau(\vec{x}|\vec{y}) \qquad \text{with } x_1 < x_2 < \cdots < x_N\ , \tag{3}$$

where $\vec{\nabla} \equiv (\cdots, \partial/\partial x_i, \cdots)$.

1/ Recall the general form for the decomposition of the propagator over the spectrum of the operator $H_N = -D\vec{\nabla}^2$, denoted $\{E_n,\ \Psi_n(\vec{x})\}_{n=0,1,\cdots,\infty}$ (with $\int \mathrm{d}^N\vec{x}\, \Psi_n^*(\vec{x})\Psi_m(\vec{x}) = \delta_{n,m}$).

Hint : Since the Fokker-Planck operator is Hermitian here, we can simply use the mapping of (3) onto the imaginary time Schrödinger equation with Hamiltonian H_N.

2/ We assume that the N lines start from $\vec{x}(0) = \vec{y}$ and reach the same set of values at final "time", $\vec{x}(L) = \vec{y}$ (like in Fig. 1). Express *formally* the average of an observable $\langle A(\vec{x}(\tau))\rangle$ at "time" τ in terms of the propagator $P_\tau(\vec{x}|\vec{y})$. Argue that for τ and $L - \tau \to \infty$, this average can simply be written in terms of the ground state $\Psi_0(\vec{x})$ of the operator H_N.

C. Compressibility and 1D fermionic gas.– We study the response of $N \gg 1$ lines to an external perturbation. In the limit $L \to \infty$, their statistical properties are controlled by the ground state $\Psi_0(\vec{x})$ of the operator H_N. Thus, we can use the mapping between (3) and the Schrödinger equation for a **gas of N free spinless fermions** of "mass" $m = 1/(2D) = c/(2T)$ (we set $\hbar = 1$), where T is the original temperature of the lines and c their elastic constant. We now consider the fermions, described by the Schrödinger equation $\mathrm{i}\partial_t\Psi(\vec{x},t) = H_N\Psi(\vec{x},t)$: fermions occupy 1D plane waves $\psi_k(x) = \frac{1}{\sqrt{\mathscr{L}}}\mathrm{e}^{\mathrm{i}kx}$ of energy $\varepsilon_k = \frac{k^2}{2m}$. In a box of finite size $\mathscr{L}$, the wave vector k is quantised (it is sufficient to remember that $\sum_k \to \mathscr{L}/(2\pi)\int \mathrm{d}k$).

1/ We consider a *single fermion* : the density operator is $\hat{n}(x) = \delta(x - \hat{x})$ and its Fourier component $\hat{n}_q = \mathrm{e}^{-\mathrm{i}q\hat{x}}$, where $\hat{x}$ is the position operator. Give the matrix element $\langle\, \psi_k \,|\hat{n}_q|\, \psi_{k'}\,\rangle$.

2/ We now consider the *fermion gas*. A perturbation is introduced under the form of a scalar external potential $V(x,t) = (1/\mathscr{L})\sum_q V_q(t)\,\mathrm{e}^{\mathrm{i}qx}$. The corresponding Hamiltonian is

$$\hat{H}_{\text{pert}}(t) = \sum_{i=1}^{N} V(\hat{x}_i, t) = \int \mathrm{d}x\, V(x,t)\,\hat{n}(x) = \frac{1}{\mathscr{L}}\sum_q V_q(t)\,\hat{n}_{-q}\ ; \tag{4}$$

from now on $\hat{n}_q = \sum_i \mathrm{e}^{-\mathrm{i}q\hat{x}_i}$ is the density operator of the *fermion gas*. Its response is

$$\langle \hat{n}(x,t)\rangle_V = \langle \hat{n}(x)\rangle + \int \mathrm{d}t'\mathrm{d}x'\, \chi(x - x', t - t')\, V(x', t') + \mathcal{O}(V^2) \tag{5}$$

i.e. $\langle \hat{n}_q(t)\rangle_V = n\,\mathscr{L}\,\delta_{q,0} + \int_{\mathbb{R}} \mathrm{d}t'\, \widetilde{\chi}_q(t - t')\, V_q(t') + \mathcal{O}(V^2)$, where $n = \langle \hat{n}(x)\rangle$ is the mean density.

a) Express $\widetilde{\chi}_q(t)$ as an equilibrium correlation function.

b) Write its Fourier transform $\widetilde{\chi}(q,\omega) = \int_{\mathbb{R}} \mathrm{d}t\, \widetilde{\chi}_q(t)\,\mathrm{e}^{\mathrm{i}\omega t}$ as a sum over contributions of plane waves. Analyse its analytical structure. Interpret the position of the poles of the integrand.

3/ Static compressibility.– The connection to the problem of fluctuating lines is made more transparent by considering the static response $\chi(q) \stackrel{\text{def}}{=} \widetilde{\chi}(q,0)$ at zero temperature.

a) We denote by $f(\varepsilon_k)$ the Fermi-Dirac distribution. Show that

$$\chi(q) = \fint \frac{\mathrm{d}k}{\pi} \frac{f(\varepsilon_k)}{\varepsilon_k - \varepsilon_{k+q}} \tag{6}$$

where the integral is a Cauchy principal part integral (see appendix).

b) The zero temperature fermion gas involves the Fermi energy $\varepsilon_F = \frac{1}{2m}k_F^2$ controlling the number of fermions N. Compute explicitely $\chi(q)$.

c) **Kohn anomaly.–** Show that $\lim_{q\to 0}\chi(q)$ is related to the density of states at Fermi level $\rho_0 = \frac{m}{\pi k_F}$. Analyse $\chi(q)$ for $q \to 2k_F$ and $q \to \infty$. Plot neatly $-\chi(q)/\rho_0$ as a function of $q/(2k_F)$. Express k_F and ρ_0 as a function of the parameters for the fluctuating lines (n, T and c).

d) Bonus.— Argue that the length of the lines L coincides with the inverse temperature of the fermions $\beta_{\text{ferm}} = 1/T_{\text{ferm}}$ (go back to question **B.2**). Discuss the validity of the $T_{\text{ferm}} = 0$ approximation, and then that of the small distorsion approximation made in the very begining (express the two conditions in terms of the parameters of the lines). For finite T_{ferm}, what is the value of $\chi(2k_F)$ (in terms of T, n and c) ?

Appendix :

• Convention for Fourier transform in dimension d :

$$\varphi_q = \int_{\text{Vol}} \mathrm{d}^d x\, \mathrm{e}^{-\mathrm{i}qx}\,\varphi(x) \quad \& \quad \varphi(x) = \frac{1}{\text{Vol}}\sum_q \varphi_q\,\mathrm{e}^{\mathrm{i}qx} \underset{\text{Vol}\to\infty}{\longrightarrow} \int \frac{\mathrm{d}^d q}{(2\pi)^d}\varphi_q\,\mathrm{e}^{\mathrm{i}qx} \tag{7}$$

• In pratice, Cauchy principal part integral $\fint \mathrm{d}x\,\frac{\varphi(x)}{x-x_0} = \mathrm{Re}\int \mathrm{d}x\,\frac{\varphi(x)}{x-x_0\pm \mathrm{i}0^+}$ can be calculated with

$$\fint_a^b \mathrm{d}x\,\frac{\varphi(x)}{x-x_0} = \lim_{\eta\to 0^+}\left(\int_a^{x_0-\eta} + \int_{x_0+\eta}^b\right)\mathrm{d}x\,\frac{\varphi(x)}{x-x_0}\,, \tag{8}$$

where $\varphi(x)$ is a regular function and $x_0 \in [a,b]$ (if $x_0 \notin [a,b]$, this is the usual integral).

• We recall that the grand canonical average of a commutator of many body operators, sums of one particle operators, of the form $\hat{A} = \sum_{i=1}^N \hat{a}^{(i)}$ and $\hat{B} = \sum_{i=1}^N \hat{b}^{(i)}$, is

$$\langle [\hat{A}\,,\hat{B}]\rangle = \sum_\alpha f_\alpha \,\langle\,\varphi_\alpha\,|\big[\hat{a},\hat{b}\big]|\,\varphi_\alpha\,\rangle = \sum_{\alpha,\beta}(f_\alpha - f_\beta)\,a_{\alpha\beta}\,b_{\beta\alpha}\,, \tag{9}$$

where the sum runs over one particle stationary states. $a_{\alpha\beta} = \langle\,\varphi_\alpha\,|\hat{a}|\,\varphi_\beta\,\rangle$ is a matrix element of the one particle operator and $f_\alpha = f(\varepsilon_\alpha)$ denotes the occupancy of the individual eigenstate.

The problem is inspired by the article :

P.-G. de Gennes, *Model for fibrous structures with steric constraints*, J. Chem. Phys. **48**(5), 2257–2259 (1968).

Solutions sur la page du cours : cf. http://lptms.u-psud.fr/christophe_texier/

NON-INTERSECTING FLUCTUATING LINES AND 1D FERMIONS – SOLUTIONS

A. Single line.

1/ Solution is $P_\tau(x|y) = \frac{1}{\sqrt{4\pi D\tau}} \exp\left\{-\frac{(x-y)^2}{4D\tau}\right\}$. Note that here, D has dimension $[D] = [x]^2/[\tau] =$ [length]

2/ Averaging takes the form

$$\langle x(\tau)^2 \rangle = \frac{\int_{\mathbb{R}} \mathrm{d}x\, P_{L-\tau}(0|x)\, x^2\, P_\tau(x|0)}{P_L(0|0)}$$

(if one removes the x^2 in the numerator, one gets obviously $\langle 1 \rangle = 1$, as required). The Gaussian integral gives the fluctuations of the *Brownian bridge*, $\langle x(\tau)^2 \rangle = 2D\,\tau\left(1 - \frac{\tau}{L}\right)$. Fluctuations are maximum at the middle $\tau = L/2$, where the line is less constrained $\langle x(L/2)^2 \rangle = DL/2 = TL/(2c)$. Discussion : fluctuations increase with temperature and decrease with the stress. Scaling with the length is $\delta x \sim \sqrt{L}$ as expected.
Dimensional analysis : $[T] =$ [energy] and $[c] =$ [force] $=$ [energy]/[length]. Ok.

B. N lines.

1/ The decomposition of the propagator over the spectrum of $H_N = -D\vec{\nabla}^2$ is

$$P_\tau(\vec{x}|\vec{y}) = \langle\, \vec{x}\, | \mathrm{e}^{-\tau H_N} |\, \vec{y}\, \rangle = \sum_{n=0}^{\infty} \Psi_n(\vec{x})\, \Psi_n^*(\vec{y})\, \mathrm{e}^{-\tau E_n} \,.$$

2/ Averaging of a function of coordinates at "time" τ has the same structure as for one line. Assuming a discrete spectrum, for long lines we write $P_\tau(\vec{x}|\vec{y}) \simeq \Psi_0(\vec{x})\, \Psi_0^*(\vec{y})\, \mathrm{e}^{-\tau E_0}$, hence

$$\langle A(\vec{x}(\tau)) \rangle = \frac{N! \int_{-\infty}^{\infty} \mathrm{d}x_1 \int_{x_1}^{\infty} \mathrm{d}x_2 \cdots \int_{x_{N-1}}^{\infty} \mathrm{d}x_N\, P_{L-\tau}(\vec{y}|\vec{x})\, A(\vec{x})\, P_\tau(\vec{x}|\vec{y})}{P_L(\vec{y}|\vec{y})} \tag{10}$$

$$\simeq \frac{N! \int_{-\infty}^{\infty} \mathrm{d}x_1 \int_{x_1}^{\infty} \mathrm{d}x_2 \cdots \int_{x_{N-1}}^{\infty} \mathrm{d}x_N\, \Psi_0(\vec{y})\, \Psi_0^*(\vec{x})\, \mathrm{e}^{-(L-\tau)E_0}\, A(\vec{x})\, \Psi_0(\vec{x})\, \Psi_0^*(\vec{y})\, \mathrm{e}^{-\tau E_0}}{\Psi_0(\vec{y})\, \Psi_0^*(\vec{y})\, \mathrm{e}^{-LE_0}} \,.$$

Finally

$$\langle A(\vec{x}(\tau)) \rangle \underset{\tau\,\&\,L-\tau\to\infty}{\simeq} N! \int_{-\infty}^{\infty} \mathrm{d}x_1 \int_{x_1}^{\infty} \mathrm{d}x_2 \cdots \int_{x_{N-1}}^{\infty} \mathrm{d}x_N\, |\Psi_0(\vec{x})|^2\, A(\vec{x}) \,. \tag{11}$$

which corresponds to average in the ground state of H_N. The factor $N!$ is required if we choose to normalise the eigenstates as $\int_{\mathbb{R}^N} \mathrm{d}\vec{x}\, |\Psi_n(\vec{x})|^2 = 1$.

From non-intersecting lines to 1D fermions : The constraints for non-intersection can be described by wave functions which vanish at coinciding points $\Psi(\cdots, x_i, x_{i+1} = x_i, \cdots) = 0$. Moreover, being restricted to the sector $x_1 < x_2 < \cdots < x_N$, we can construct a basis of wave functions antisymmetric under exchange of particles, i.e. *fermionic* eigenstates.

Remark : from the point of view of the diffusion, the Dirichlet boundary condition implies that normalisation is not conserved, i.e. $\int \mathrm{d}\vec{x}\, P_\tau(\vec{x}|\vec{y}) \sim \mathrm{e}^{-E_0\tau}$ decays as time grows. However, dividing by $P_L(\vec{y}|\vec{y})$ in (10) implies that averaging is taken only over non-intersecting trajectories which have survived.

C. Compressibility and 1D fermionic gas.– We now study the 1D fermion gas (the begining of the part **C** reproduces a result of the lectures).

1/ Matrix elements for the one-body density operator : $\langle\, \psi_k \,|\hat{n}_q|\, \psi_{k'}\,\rangle = \int \frac{\mathrm{d}x}{\mathscr{L}} \mathrm{e}^{-\mathrm{i}kx-\mathrm{i}qx+\mathrm{i}k'x} = \delta_{k',k+q}$.

2/ Compressibility.– We apply one of the main results of the lectures :

$$\widetilde{\chi}_q(t) = -\frac{\mathrm{i}}{\mathscr{L}}\,\theta_{\mathrm{H}}(t)\,\langle[\hat{n}_q(t), \hat{n}_{-q}]\rangle \tag{12}$$

in terms of many-body density operator. The correlator can be expressed in terms of one-body matrix elements (relation of the appendix) :

$$\widetilde{\chi}_q(t) = -\frac{\mathrm{i}}{\mathscr{L}}\,\theta_{\mathrm{H}}(t)\sum_{k,\,k'}(f_k - f_{k'})\,|\langle\, \psi_k \,|\hat{n}_q|\, \psi_{k'}\,\rangle|^2\,\mathrm{e}^{\mathrm{i}(\varepsilon_k-\varepsilon_{k'})t}$$

where $f_k \equiv f(\varepsilon_k) = 1/\big(\mathrm{e}^{\beta(\varepsilon_k-\mu)}+1\big)$. A Fourier transform over time finally gives the formula obtained in the exercice session (TD 8) :

$$\widetilde{\chi}(q,\omega) = \frac{1}{\mathscr{L}}\sum_k \frac{f_k - f_{k+q}}{\omega + \varepsilon_k - \varepsilon_{k+q} + \mathrm{i}0^+} \tag{13}$$

where the 0^+ in the denominator is a regulator. It ensures that singularities of the response function are in the lower complex plane of the frequency (causality). Besides we recognise the energy of a particle-hole excitation $\varepsilon_{k+q} - \varepsilon_k$.

3/ Static compressibility.– For zero frequency, we could drop the regulator which is not needed $\chi(q) = \frac{1}{\mathscr{L}}\sum_k \frac{f_k - f_{k+q}}{\varepsilon_k - \varepsilon_{k+q}}$. We prefer to use the symmetry of the spectrum $\varepsilon_k = \varepsilon_{-k}$ and split the sum (which requires to keep the regulator)

$$\begin{aligned}\chi(q) = \frac{1}{\mathscr{L}}\sum_k \frac{f_k - f_{k+q}}{\varepsilon_k - \varepsilon_{k+q} + \mathrm{i}0^+} &= \frac{1}{\mathscr{L}}\sum_k \frac{f_k}{\varepsilon_k - \varepsilon_{k+q} + \mathrm{i}0^+} - \frac{1}{\mathscr{L}}\sum_k \frac{f_k}{\varepsilon_{k-q} - \varepsilon_k + \mathrm{i}0^+} \\ &= \frac{1}{\mathscr{L}}\sum_k \frac{f_k}{\varepsilon_k - \varepsilon_{k+q} + \mathrm{i}0^+} + \frac{1}{\mathscr{L}}\sum_k \frac{f_k}{\varepsilon_k - \varepsilon_{k+q} - \mathrm{i}0^+}\end{aligned}$$

finally, using $\frac{1}{\Omega\pm\mathrm{i}0^+} = \mathcal{PP}\frac{1}{\Omega} \mp \mathrm{i}\pi\,\delta(\Omega)$,

$$\chi(q) = \frac{2}{\mathscr{L}}\sum_k \mathcal{PP}\frac{f_k}{\varepsilon_k - \varepsilon_{k+q}} = ⨍ \frac{\mathrm{d}k}{\pi}\,\frac{f_k}{\varepsilon_k - \varepsilon_{k+q}}$$

The Fermi-Dirac distribution at $T_{\mathrm{ferm}} = 0$ is $f_k = \theta_{\mathrm{H}}(k_F - |k|)$. Writing $\varepsilon_{k+q} - \varepsilon_k = \frac{q}{m}(k + q/2)$ we find

$$\chi(q) = -\frac{m}{q\,\pi}⨍_{-k_F}^{+k_F}\frac{\mathrm{d}k}{k+q/2} = \frac{m}{q\,\pi}\,\ln\left|\frac{q-2k_F}{q+2k_F}\right| \tag{14}$$

We obtain easily the limiting behaviours :

$$\chi(q) \simeq -\rho_0 \times \begin{cases} 1 & \text{for } q \ll k_F \\ \frac{1}{2}\ln\frac{4k_F}{|q-2k_F|} & \text{for } q \sim 2k_F \\ \left(\frac{2k_F}{q}\right)^2 & \text{for } q \gg k_F \end{cases} \tag{15}$$

where $\rho_0 = \frac{m}{\pi k_F}$ is the DoS per unit volume at Fermi level. The logarithmic singularity is called the **Kohn anomaly**. It is due to a particle-hole excitation where the particle and the hole are close to the two Fermi points.

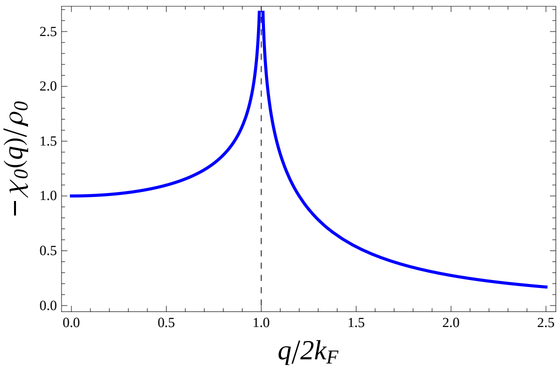

FIGURE 2 : *Zero temperature compressibility with logarithmic divergence at* $q = 2k_F$.

The mapping on the problem of fluctuating lines with density n is

$$\begin{cases} k_F = \pi\, n \\ m \longrightarrow \frac{c}{2T} \\ \rho_0 \rightarrow \frac{c}{2\pi^2 T n} \end{cases}$$

BONUS :

• If we come back to the formula for the averaging (10), we see that the length L of the lines play the same role as the inverse temperature for the fermions. This is more clear is one traces over the initial/final positions

$$\langle A(\vec{x}(\tau))\rangle \xrightarrow{\int \mathrm{d}\vec{y}} \frac{\mathrm{Tr}\left\{\mathrm{e}^{-L\,H_N}\,A(\vec{x})\right\}}{\mathrm{Tr}\left\{\mathrm{e}^{-L\,H_N}\right\}} \tag{16}$$

• The temperature of the fermions is mapped onto the inverse of the length $T_{\text{ferm}} = 1/L$ and the Fermi energy $\varepsilon_F = k_F^2/(2m) = \pi^2 n^2 T/c$. The limit of the degenerate gas ($T_{\text{ferm}} \ll \varepsilon_F$) corresponds to a high temperature regime for the lines $T \gg n^2 L/c$.

• In the very begining, we have assumed small distorsions $\partial x/\partial\tau \ll 1$. Velocity is of the order of the Fermi velocity $v_F = k_F/m = 2\pi n T/c$. Small velocity $v_F \ll 1$ requires small temperature for the lines $T \ll c/n$.
We conclude that the validity of the $T_{\text{ferm}} = 0$ calculation is $n^2 L/c \ll T \ll c/n$.

• For finite temperature, we expect that the Kohn anomaly is smothed by the fermion temperature as $\chi(2k_F) \sim -\rho_0\, \ln|\varepsilon_F/T_{\text{ferm}}|$. Using the mapping onto the parameters of the lines we get

$$\chi(q = 2\pi n) \sim -\frac{c}{Tn}\ln\left(n^2 T L/c\right) \tag{17}$$