

# Statistical Field theory

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# Chapter 1

## Introduction

The material discussed in these notes can also be found in more specialized books. Among them

- Statistical mechanics and functional integrals [1, 2, 3, 4]
- Many body physics [5, 3]

These notes are still in a larval stage. This is specially true for chapters 3 and 7. Despite the attempts to unify the notations and eliminates mistakes, factors of 2 and other errors of signs, it is clear that many of those remain. I'll try to update the notes from time to time. If you find these notes useful and feel like helping to improve them, do not hesitate to email to me ([Thierry.Giamarchi@Physics.UniGE.ch](mailto:Thierry.Giamarchi@Physics.UniGE.ch)) if you have found errors in those notes or simply to let me know if there are parts that you would like to see improved or expanded.



## Chapter 2

# Equilibrium statistical mechanics

### 2.1 Basics; correlation functions

In statistical mechanics one is interested in getting basic quantities such as the partition function. Space is meshed with a network on which some variable describe the state of the system. To be more specific let us consider an Ising model, on a square lattice. On each site  $i$  exists a spin  $\sigma_i = \pm$ . The state of the system is describe by all spin variables  $\sigma_1, \sigma_2, \dots, \sigma_N$ , where  $N$  grows as the volume of the system. The set of all these variables is a configuration that we denote in the following as  $\{\sigma\}$ . To compute physical quantities one needs in addition an Hamiltonian describing the energy of the system for a given configuration. To be specific let us again consider a Ising type Hamiltonian

$$H_0 = - \sum_{i,j} J_{i,j} \sigma_i \sigma_j \quad (2.1)$$

A physical quantity such as the partition function results from the sum over all configurations of the system

$$Z = \sum_{\{\sigma\}} e^{-\beta H_0} = \sum_{\sigma_1 = \pm} \sum_{\sigma_2 = \pm} \dots \sum_{\sigma_N = \pm} e^{-\beta H_0[\{\sigma\}]} \quad (2.2)$$

The difficulty if of course to make the sum over the humongous (thermodynamics) number of variables. From  $Z$  or  $F = -T \log(Z)$  many simple physical quantities can be directly extracted (specific heat, etc.).

In addition to these rather global quantities, one is often interested in correlation functions, measuring thermodynamics averages of local observables or products of local observables. Some examples are

$$\langle \sigma_{i1} \rangle \quad (2.3)$$

$$\langle \sigma_{i1} \sigma_{i2} \rangle \quad (2.4)$$

where the thermodynamics average  $\langle \rangle$  stands for

$$\langle O[\alpha, \dots, \beta] \rangle = \frac{\sum_{\{\sigma\}} O[\sigma_\alpha, \dots, \sigma_\beta] e^{-\beta H_0}}{\sum_{\{\sigma\}} e^{-\beta H_0}} \quad (2.5)$$

Where  $O$  is any operator. Note that the correlation functions depends on the spatial positions  $\alpha, \dots, \beta$ , the average having been made over the microscopic variables  $\sigma$ .

In fact the correlation functions can also be obtained from a partition function. If one adds to the Hamiltonian a source term

$$-\beta H_s = \sum_i h_i O_i \quad (2.6)$$

one introduces the partition function, that now depends on a thermodynamics number of external sources

$$Z[h_1, h_2, \dots, h_N] = \sum_{\{\sigma\}} e^{-\beta[H_0 + H_s]} \quad (2.7)$$

and the associated free energy  $F[h_1, h_2, \dots, h_N]$ . It is then easy to see that

$$\langle [O_\alpha \dots O_\beta] \rangle = \frac{1}{Z[h=0]} \left. \frac{\partial Z[h_1, h_2, \dots, h_N]}{\partial h_\alpha \dots \partial h_\beta} \right|_{\{h\}=0} \quad (2.8)$$

Of course this is a rather formal relation since computing  $Z[h_1, h_2, \dots, h_N]$  is in general a formidable task.

Similar formulas can be derived from the free energy. In particular one can obtain from the free energy

$$\langle O_\alpha \rangle = -\beta \left. \frac{\partial F[h_1, h_2, \dots, h_N]}{\partial h_\alpha} \right|_{\{h\}=0} \quad (2.9)$$

It is easy to see that differentiating the free energy leads to the so-called connected correlations

$$-\beta \left. \frac{\partial F[h_1, h_2, \dots, h_N]}{\partial h_\alpha \partial h_\beta} \right|_{\{h\}=0} = [\langle O_\alpha O_\beta \rangle - \langle O_\alpha \rangle \langle O_\beta \rangle] \quad (2.10)$$

Each time one differentiate an average one gets two terms one coming from the numerator one from the denominator. Thus

$$\partial_{h_\gamma} \langle \dots \rangle = [\langle \dots O_\gamma \rangle - \langle \dots \rangle \langle O_\gamma \rangle] \quad (2.11)$$

It is thus easy to obtain the higher derivatives.

The ingredients that we have illustrated on this example of the Ising model are totally general. It is important to understand that what is generally needed is to be able to perform the sums over the microscopic degrees of freedom.

## 2.2 External field; linear response

Among the various correlation functions some are of special importance. Let us assume that a physical variable of the system can be coupled to an external field, in a way similar to (2.6). In our Ising example this is the case if one puts the system in a magnetic field. The natural variable associated with such a perturbation is the magnetization of the system. One would have two way to compute it. Adding the magnetic field to the Hamiltonian  $H_0$  leads to

$$H_h = -h \sum_i \sigma_i \quad (2.12)$$

From  $H = H_0 + H_h$  one can compute the free energy  $F[h]$ . Standard thermodynamics tells us that the total magnetization  $M$  of the system is simply given by

$$M = -\frac{dF[h]}{dh} \quad (2.13)$$

This relation comes immediately from (2.8) using  $O = -\sum_i \sigma_i$ .  $M$  describes the response of the system to the external field  $h$ . Even for this simple case ( $h$  is space independent) it is quite complicated to get the magnetization.

To generalize this notion of response, let us consider an operator  $O_i$  (that can a priori depend on the position) that couples to an external field  $h_i$  (that can also depend on space) through the Hamiltonian

$$H_p = -\sum_i h_i O_i \quad (2.14)$$

Let us furthermore assume that  $O_i$  is such that in the absence of perturbation  $H_p$  one has  $\langle O_i \rangle_0 = 0$ , where  $\langle \rangle_0$  denotes averages performed with  $H_0$  alone. If it is not the case one can simply subtract the average value from  $O_i$ . In that case one can measure the response of the system, that is given by

$$\mathcal{O}_i[\{h\}] = \langle O_i \rangle \quad (2.15)$$

The notation  $\mathcal{O}_i[\{h\}]$  means that the value  $O_i$  at point  $i$  depends in fact on the value of the external field at all points, i.e. of the whole set of values of  $h$  at each spatial point. For even a simple  $H_0$  it is hopeless to expect to compute the full response  $\mathcal{O}_i$ .

A simpler case, but of considerable interest, is to compute the *linear* response of the system. Indeed if the external field is small one can expand (2.15), in powers of the external field. The lowest order term is linear in the external field (hence the term linear response). One has

$$\mathcal{O}_i[\{h\}] = 0 + a^d \sum_j \chi_{ij} h_j \quad (2.16)$$

which is the most general linear term that one can write. The factor  $a^d$  is here for convenience (see below). At that stage this merely defines  $\chi$ . If we assume in addition that  $H_0$  is invariant by translation, then  $\chi_{ij}$  can only depend on the distance between  $i$  and  $j$  (that we denote symbolically by  $i - j$ ). A more transparent way to write the convolution (2.16) is to go to Fourier space. Let us recall the convention that we use for Fourier transform on the lattice.

$$h_q = a^d \sum_i e^{-iq \cdot r_i} h_i \quad (2.17)$$

$$h_i = \frac{1}{\Omega} \sum_{q=2\pi n/L} e^{iq \cdot r_i} h_q \quad (2.18)$$

where we have introduced a lattice spacing  $a$  ( $a$  can be set to 1 at that stage since it is purely formal). The volume of the system is  $\Omega = Na^d$  and one introduces a distance  $r = ai$ . The sum over  $q$  runs from  $q = -\pi/a$  to  $q = +\pi/a$ , i.e. over  $N$  values of  $n$ . This corresponds to the standard Brillouin zone. In that case

$$\sum_i e^{iq \cdot r_i} = N \delta_{q,0} \quad (2.19)$$

where  $\delta_{i,j}$  is the discrete  $\delta$ . For a continuous system  $r_i \rightarrow r$ , one has the continuous Fourier transform

$$h(q) = \int_{\Omega} d^d r e^{-iq \cdot r} h(r) \quad (2.20)$$

$$h(r) = \frac{1}{\Omega} \sum_{q=2\pi n/L} e^{iq \cdot r} h(q) \quad (2.21)$$

where  $\Omega = L^d$  is the volume of the system. The relation between the lattice variables and the continuous ones is thus

$$h_i \rightarrow h(r) \quad (2.22)$$

$$h_q \rightarrow h(q) \quad (2.23)$$

For the continuous case

$$\int dr e^{iq \cdot r} = \Omega \delta_{q,0} \quad (2.24)$$

still with a discrete  $\delta$ . In the limit where the volume of the system goes to infinity, one can use

$$\frac{1}{\Omega} \sum_q \rightarrow \frac{1}{(2\pi)^d} \int d^d q \quad (2.25)$$

$$\Omega \delta_{q,0} \rightarrow (2\pi)^d \delta(q) \quad (2.26)$$

where  $\delta(q)$  is the Dirac  $\delta$ .

Using these definitions for the Fourier transform one can rewrite (2.16) as

$$\mathcal{O}_q = a^d \frac{1}{N} \sum_{ij} \sum_{q'} e^{-iqr_i + iq'r_j} \chi_{i-j} h_{q'} \quad (2.27)$$

using  $r_i = r_j + r_l$  one has

$$\mathcal{O}_q = a^d \frac{1}{N} \sum_{jl} \sum_{q'} e^{i(q'-q)r_j} e^{-iqr_l} \chi_{r_l} h_{q'} \quad (2.28)$$

$$= a^d \sum_l e^{-iqr_l} \chi_{r_l} h_q \quad (2.29)$$

$$= \chi_q h_q \quad (2.30)$$

Thus in Fourier space the relation between the response and the external field is truly linear, each  $q$  mode being independent. This is a direct consequence of: (i) the invariance by translation of the system which makes the Fourier base diagonal; (ii) the linear approximation for the response. The susceptibility  $\chi_q$  (or in real space  $\chi_{ij}$ ) thus contains all the information we need to get the linear response of the system to any external perturbation. The good point is that  $\chi$  can be computed in the absence of the perturbation  $H_p$  with the much simpler Hamiltonian  $H_0$  and thus we have better chance to obtain it.

Let us get its general expression. To linear order in the perturbation  $H_p$  we get from (2.15)

$$\begin{aligned} \mathcal{O}_i[\{h\}] &\simeq \frac{\sum_{\{\sigma\}} O_i (1 + \beta \sum_j O_j h_j) e^{-\beta H_0}}{\sum_{\{\sigma\}} (1 + \beta \sum_j O_j h_j) e^{-\beta H_0}} \\ &\simeq \langle O_i \rangle_0 + \sum_j \beta [\langle O_i O_j \rangle_0 - \langle O_i \rangle_0 \langle O_j \rangle_0] h_j \end{aligned} \quad (2.31)$$

thus we can identify

$$a^d \chi_{ij} = \beta [\langle O_i O_j \rangle_0 - \langle O_i \rangle_0 \langle O_j \rangle_0] \quad (2.32)$$

which is the so called connected correlation function, i.e. the correlation where the average values have been subtracted. Indeed

$$\langle O_i O_j \rangle - \langle O_i \rangle \langle O_j \rangle = \langle (O_i - \langle O_i \rangle) (O_j - \langle O_j \rangle) \rangle \quad (2.33)$$

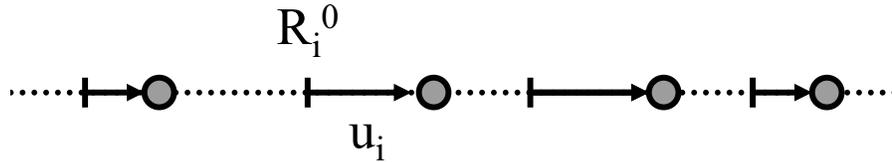


Figure 2.1: Vibrations of a classical lattice. On each site one defines a displacement  $u_i$ .

With our hypothesis  $\langle O \rangle_0 = 0$  the correlation function is equal to its connected part.

Equ. (2.32) is a truly amazing equation. It shows that the *linear response* of the system is totally determined by the *fluctuations* of the same system in the absence of the external perturbation. This result is totally general and its only strong hypothesis is the fact that the system has reached thermal equilibrium. Since the imaginary part of the susceptibility of the system also determine dissipation that can take place in the system (we will come back to this point later), this result is also known as the fluctuation dissipation theorem. It has a crucial importance since it allows to compute properties of the system out of the unperturbed state alone.

As an example, let us apply it to the relatively trivial case of an isolated Ising spin. In that case  $H_0 = 0$ . The response to an external magnetic field (2.12) can be computed exactly for this trivial case

$$m = \frac{e^{\beta h} - e^{-\beta h}}{e^{\beta h} + e^{-\beta h}} = \tanh(\beta h) \quad (2.34)$$

leading to a susceptibility  $\chi = \beta$ . This can be readily obtained from (2.32). Since  $H_0 = 0$

$$\langle \sigma \sigma \rangle_0 = 1 \quad (2.35)$$

Note that the uniform susceptibility (usually denoted simply  $\chi$ ), i.e. the response to a uniform external field  $h_i = h$  is of course the  $q = 0$  Fourier component of the susceptibility. This is simply the integrated correlation function

$$\chi = \sum_j \beta \langle O_i O_j \rangle_0 \quad (2.36)$$

Thus the longer range the correlations, the stronger the response of the system will be. This can be physically understood since a correlated region behaves as a gigantic spin that can respond coherently to the external field.

## 2.3 Continuous systems: functional integral

So far we have delt with systems defined on a lattice. Although all systems in condensed matter exists on some kind of network, it is often very useful to be able to take a continuous limit, remembering the underlying lattice only as an ultraviolet cutoff. How to deal with such cases ?

The first step is to have a variable that varies smoothly enough at the scale of the microscopic lattice so that a continuous variable can be defined. Let us take the very simple example of the vibrations of a classical lattice as shown on Fig. 2.1 On each site one defines a displacement  $u_i$ . The energy is given by

$$H = \sum_{i,z} \frac{k}{2} (u_i - u_{i+z})^2 \quad (2.37)$$

where  $z$  spans the nearest neighbors,  $c$  the elastic constants. At low enough temperatures  $u_i$  varies smoothly at the scale of the lattice  $a$ , thus one can define the continuous variable  $u(r)$  by  $u(r_i) = u_i$ . Since  $u(r)$  is smooth

$$u_{i+z} - u_i = \vec{z} \cdot \vec{\nabla} u(r) \quad (2.38)$$

Thus (2.37) becomes

$$H = \frac{k}{2} \int d^d r \rho_0 \sum_{\alpha\beta} \sum_z z^\alpha z^\beta (\partial_\alpha u(r)) (\partial_\beta u(r)) \quad (2.39)$$

where the  $\alpha, \beta$  at the coordinates  $x, y, \dots$ . This is the standard elastic Hamiltonian. On a square lattice in dimension  $d$ , (2.39) becomes

$$H = \frac{c}{2} \int d^d r (\vec{\nabla}_\alpha u(r)) \cdot (\vec{\nabla}_\beta u(r)) \quad (2.40)$$

with the elastic constant for the continuum  $c = k\rho_0 a^2$ .

Sometimes it is not totally obvious to find the proper continuous limit. For the Ising model for example the spin  $\sigma_i$  is a discrete variable which only takes the values  $\sigma_i = \pm 1$ . This a direct gradient expansion is not possible and one should use another variable to take the continuum limit. This point will be examined in more details in the exercises.

Using the continuous limit, one can thus compute the thermodynamic properties of “continuous” systems. If one keep in mind the original lattice (or artificially introduces one if needed) the partition function and thermodynamics averages are now well defined

$$Z_a = \left( \prod_i \sum_{u_i} \right) e^{-\beta H(\{u\})} \quad (2.41)$$

$$\langle O(r_i)_a \rangle = \frac{1}{Z} \left( \prod_i \sum_{u_i} \right) O(r_i) e^{-\beta H(\{u\})} \quad (2.42)$$

where I have put the index  $a$  to point out that these are the quantities defined for a finite lattice spacing  $a$ . As before the integration should be done on each point of the lattice over all the possible states of the microscopic variables. One can now consider that the partition function and correlations functions of the system in the continuum are quite logically given by

$$Z = \lim_{a \rightarrow 0} Z_a \quad (2.43)$$

$$O(r) = \lim_{a \rightarrow 0} O(r_i)_a \quad (2.44)$$

Depending on the precise normalization, the partition function  $Z$  can contain an infinite constant. This normalization constant correspond to a shift (sometimes infinite) in the entropy. As we will discuss it is much simpler to compute the correlation functions since most normalization factors cancels leaving well defined and unambiguous results directly in the continuum limit.

Let us consider the simple example of the Hamiltonian

$$H = \frac{1}{2} \int \int dr dr' V(r - r') u(r) u(r') \quad (2.45)$$

The discrete partition function is thus

$$Z_a = \left( \prod_i \sum_{u_i} \right) e^{-\frac{1}{2} \beta a^{2d} \sum_{ij} V_{i-j} u_i u_j} \quad (2.46)$$

We thus have to perform Gaussian integrals. Since they will come over and over again (these are mostly the only one one knows how to do !) let us remind the main formulas

$$\int_{-\infty}^{+\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}} \quad (2.47)$$

$$\frac{\int_{-\infty}^{+\infty} e^{-ax^2+bx} dx}{\int_{-\infty}^{+\infty} e^{-ax^2} dx} = e^{\frac{b^2}{4a}} \quad (2.48)$$

$$\frac{\int_{-\infty}^{+\infty} e^{-\frac{1}{2}ax^2} x^2 dx}{\int_{-\infty}^{+\infty} e^{-\frac{1}{2}ax^2} dx} = \frac{1}{a} \quad (2.49)$$

The last formula can easily be obtained by derivating the second one with respect to  $b$ . Here we have the matrix form of these Gaussian integrals

$$\int du_1 \int du_2 \cdots \int du_N e^{-\sum_{ij} u_i M_{ij} u_j} \quad (2.50)$$

where  $M_{ij}$  is an  $N \times N$  real symmetric positive definite matrix. General formula exist for these integrals as well and

$$\int \frac{du_1 du_2 \cdots du_N}{(2\pi)^{N/2}} e^{-\frac{1}{2} \sum_{ij} u_i M_{ij} u_j + \sum_i x_i b_i} = \frac{1}{(\text{Det} M)^{1/2}} e^{\frac{1}{2} \sum_{ij} b_i M_{ij}^{-1} b_j} \quad (2.51)$$

$$\frac{\int du_1 \int du_2 \cdots \int du_N u_k u_l e^{-\frac{1}{2} \sum_{ij} u_i M_{ij} u_j}}{\int du_1 \int du_2 \cdots \int du_N e^{-\frac{1}{2} \sum_{ij} u_i M_{ij} u_j}} = (M^{-1})_{kl} \quad (2.52)$$

and as well for the other ones. But rather than blindly using them, let us see how to obtain them. What complicates the integral (2.50) is the non-diagonal nature of the matrix  $M$ . Let us thus make a change of variables in a basis where the matrix  $M$  is diagonal. It is not a necessity but in general one favors transformations for which the Jacobian is a constant, in order not to have to worry to compute the Jacobian. In the basis, where  $M$  is diagonal (2.50) can just be computed as the product of the integrals (2.47). Since the product of the eigenvalues of the matrix is its determinant we recover (2.51). Note that the correlation function  $G_{ij} = \langle u_i u_j \rangle$  is the solution of the equation  $\sum_{jk} G_{ij} M_{jk} = \delta_{ik}$ .

Let us see some applications. For the Hamiltonian (2.45) one should thus find a basis in which the Hamiltonian is diagonal. The invariance by translation of the Hamiltonian immediately suggests that the Fourier transform is a good basis. Let us check it on the discrete expression (2.46)

$$\begin{aligned} a^{2d} \sum_{ij} V_{i-j} u_i u_j &= \frac{a^d}{N\Omega} \sum_{ij} V_{i-j} \sum_{qq'} e^{i(qr_i + q'r_j)} u_q u_{q'} \\ &= \frac{a^d}{N\Omega} \sum_{lj} V_l \sum_{qq'} e^{i(q+q')r_j} e^{iqr_l} u_q u_{q'} \\ &= \frac{a^d}{\Omega} \sum_l V_l \sum_{qq'} \delta_{q+q',0} e^{iqr_l} u_q u_{q'} \\ &= \frac{a^d}{\Omega} \sum_q \left( \sum_l V_l e^{-iqr_l} \right) u_q u_{-q} = \frac{1}{\Omega} \sum_q V_q u_q u_{-q} \end{aligned} \quad (2.53)$$

Note that this expression is exactly the one that one would have obtained directly from the continuous expression (2.45) and using the Fourier transform in the continuum.

Using (2.53) one can now compute (2.46). Since the  $u_q$  are a priori complex variables, it means that we need the equivalent of the Gaussian integration formulas for complex variables. Let us assume that we have  $u = \text{Re}u + i\text{Im}u$ . We denote the integration over the real and imaginary part symbolically by

$$\int \int \frac{d\text{Re}u d\text{Im}u}{\pi} = \int \int \frac{dud u^*}{2i\pi} \quad (2.54)$$

One has for the Gaussian integrals on the complex variables  $u$  and  $u^*$ .

$$\int \int \frac{dud u^*}{2i\pi} e^{-auu^*} = \frac{1}{a} \quad (2.55)$$

$$\frac{\int \int \frac{dud u^*}{2i\pi} u e^{-\frac{1}{2}auu^*}}{\int \int \frac{dud u^*}{2i\pi} e^{-\frac{1}{2}auu^*}} = 0 \quad (2.56)$$

$$\frac{\int \int \frac{dud u^*}{2i\pi} uu^* e^{-\frac{1}{2}Au u^*}}{\int \int \frac{dud u^*}{2i\pi} e^{-\frac{1}{2}Au u^*}} = \frac{2}{A} \quad (2.57)$$

The fact that  $\int \int dud u^*$  is the correct notation can be checked by using polar coordinates, since using rules for the Jacobians gives the correct result

$$\int \int \frac{dud u^*}{2i\pi} e^{-auu^*} = \int_0^\infty \rho d\rho \int_0^{2\pi} d\theta \frac{e^{-a\rho^2}}{\pi} = \frac{1}{a} \quad (2.58)$$

so we can use all the rules for change of variables in all confidence. One can easily generalize these rules to  $N$  complex variables

$$\left( \prod_i \int \frac{du_i du_i^*}{2i\pi} \right) e^{-\sum_{ij} u_i^* H_{ij} u_j + \sum_i h_i^* u_i + h_i u_i^*} = \frac{e^{\sum_{ij} h_i^* (H^{-1})_{ij} h_j}}{\text{Det}H} \quad (2.59)$$

In order to use the Fourier transform, there is still the problem of the change of variables in the integrals. One starts with  $N$  real values  $u_i$  and we go to  $N$  complex fields  $u_q$ . It thus seems that we have twice as much variables at the end. Of course this is not the case since for real variables the Fourier transform satisfies  $u_{-q} = u_q^*$ . This is fortunate since this ensures that (2.53) is indeed real. We should thus halve the number of allowed values of  $q$  to, let us say positive values. Thus

$$\int \frac{du_1}{\pi^{1/2}} \int \frac{du_2}{\pi^{1/2}} \cdots \int \frac{du_N}{\pi^{1/2}} \rightarrow J \prod_{q>0} \int \int \frac{du_q du_q^*}{2i\pi} \quad (2.60)$$

where  $J$  is the Jacobian of the transformation, which is a constant. Note that the  $q = 0$  mode should be treated with care in (2.60) since  $u_{q=0}$  is real. So either one treats it separately, or simply use formally antiperiodic conditions in the Fourier transform, which shifts all  $q$  by  $\pi/L$ . This shift is totally unimportant in the thermodynamic limit where the number of  $q$  modes becomes large. This ensures that there is no  $q = 0$  mode and (2.60) is totally exact in that case. Of course both methods give the same result. Using these variables (2.53) becomes

$$\frac{1}{2\Omega} \sum_{q>0} (V_q + V_{-q}) [(\text{Re}u_q)^2 + (\text{Im}u_q)^2] \quad (2.61)$$

Note that for all systems for which the potential depends only of the *distance* between two points, i.e. for which  $V(x) = V(-x)$  one has  $V_q = V_{-q}$ . Thus (2.46) becomes

$$Z_a = J \prod_{q \geq 0} \left( \frac{\pi \Omega}{\beta V_q} \right) \quad (2.62)$$

Leading to a partition function

$$F_a = -T\Omega \frac{1}{\Omega} \sum_{q \geq 0} \log \left[ \frac{1}{\beta V(q)} \right] + F_{\text{norm}} \quad (2.63)$$

The factor  $F_{\text{norm}}$  is a shift of the free energy trivially proportional to the temperature and containing all normalization factors. This factor changes the entropy by a simple constant (not normalizing the number of configurations changes the entropy). The rest of the free energy is the important part of the free energy since it depends on the coupling  $V(q)$ . Note that in the limit of large volume  $\frac{1}{\Omega} \sum_q$  is well behaved (see (2.25)). Throwing away the factor  $F_{\text{norm}}$ , the free energy becomes

$$\begin{aligned} F_a &= -T\Omega \frac{1}{\Omega} \sum_{q \geq 0} \log \left[ \frac{1}{\beta V(q)} \right] \\ &\rightarrow -T\Omega \frac{1}{(2\pi)^d} \int d^d q \log \left[ \frac{1}{\beta V(q)} \right] \end{aligned} \quad (2.64)$$

Dealing correctly with the free energy would imply to worry about the normalization of the functional integral. Since this is rather unpleasant and difficult to do directly in the continuum limit, it is simpler to work with the correlation functions. In that case all normalization factors disappears. As an example let us compute

$$\langle [u(r1) - u(r2)]^2 \rangle = \frac{1}{\Omega^2} \sum_{qq'} (e^{iqr1} - e^{iqr2})(e^{iq'r1} - e^{iq'r2}) \langle u_q u_{q'} \rangle \quad (2.65)$$

In  $\langle u_q u_{q'} \rangle$  any normalization factor disappears between the numerator and denominator. Using the expressions (2.53) and (2.49), it is easy to check that  $\langle u_q u_{q'} \rangle = 0$  if  $q \neq q'$ . More precisely

$$\langle u_q u_{q'} \rangle = \delta_{q-q',0} \frac{\Omega}{\beta V_q} \quad (2.66)$$

Thus

$$\begin{aligned} \langle [u(r1) - u(r2)]^2 \rangle &= \frac{1}{\Omega} \sum_q \frac{[2 - 2 \cos(q(r1 - r2))]}{\beta V_q} \\ &\rightarrow \frac{1}{(2\pi)^d} \int d^d q \frac{[2 - 2 \cos(q(r1 - r2))]}{\beta V(q)} \end{aligned} \quad (2.67)$$

Thus both the partition function and correlation can thus be computed by integrating over the infinite number of variables (2.60). Formally this integration is denoted

$$\prod_i \left( \int du_i \right) = \int \mathcal{D}u[r] \quad (2.68)$$

to indicate that one has to integrate over all possible realization of the function  $u(r)$ . Precise normalization is not important provided we stick to correlation functions.

If one had to go systematically to the lattice this would bring little help. However now that we know that the thing can be done let us show how it can be done simply directly in the continuous limit. As mentioned before, in the correlation functions the normalization factors disappear between numerator and denominator, so we do not have to bother about them, or about Jacobians (provided there are constants) when we make a change of variables. Using (2.59), one easily sees that

$$\langle u_i u_j^* \rangle = \frac{1}{Z} \frac{\partial Z}{\partial h_i^* \partial h_j} \Big|_{h, h^* = 0} = H_{i,j}^{-1} \quad (2.69)$$

We can now use this result for each value of  $q > 0$ . Or one can extend the sum over  $q$  to all values keeping in mind that

$$\sum_q V_q u_q u_q^* = \sum_{q>0} [V(q) + V(-q)] u_q u_q^* = \sum_{q>0} 2V(q) u_q u_q^* \quad (2.70)$$

One has thus simply the rule

$$\langle u(q1) u^*(q2) \rangle = \frac{\int \mathcal{D}u[q] u(q1) u^*(q2) e^{-\frac{1}{2} \sum_q A(q) u(q) u^*(q)}}{\int \mathcal{D}u[q] e^{-\frac{1}{2} \sum_q A(q) u(q) u^*(q)}} = \frac{1}{A(q1)} \delta_{q1, q2} \quad (2.71)$$

This is the central result all the rest can be forgotten. Note that this result coincides with the simple result (2.49) for independent real variables. In (2.71)  $q$  is a mere index that denotes any variable, and not necessarily momentum. This is the main message. To deal with functional integration, use your intuition and knowledge of *normal* integrals. Nearly everything works as before, and when in doubt it is usually very easy to go back to the lattice representation to check. Any change of variables (where now the variable is a whole *function*) can be performed, provided one takes care of the Jacobian. In order to avoid this one usually tries to stick to transformations such as shifts  $u(r) + f(r)$  where  $f$  is an arbitrary function or Fourier transforms that have a constant Jacobian. Integrals are then performed using simple rules such as (2.71).

Let us go back to our correlation function, that can be now computed in five seconds, using (2.71) without having to worry any more

$$\begin{aligned} \langle [u(r1) - u(r2)]^2 \rangle &= \frac{1}{\Omega^2} \sum_{qq'} (e^{iqr1} - e^{iqr2})(e^{iq'r1} - e^{iq'r2}) \langle u(q) u(q') \rangle \\ &= \frac{1}{\Omega} \sum_q \frac{[2 - 2 \cos(q(r1 - r2))]}{\beta V(q)} \end{aligned} \quad (2.72)$$

which is the result that we painstakingly obtained going through the lattice (2.67).

Finally, because it will be useful in some occasions let us see how one can derive a functional. Here again things work much like ordinary derivatives, since it is the continuous limit of what we would have for a lattice system. For example

$$\frac{\partial H[u]}{\partial u(r_0)} \quad (2.73)$$

would simply be on the lattice

$$\frac{\partial H[u_1, u_2, u_3, u_4, \dots, u_N]}{a^d \partial u_{r_0}} \quad (2.74)$$

Let us take for example (2.75).

$$H = \int dr mu(r)^2 \quad (2.75)$$

Then we have

$$\begin{aligned} \frac{\partial H[u]}{\partial u(r_0)} &= \frac{\partial a^d \sum_i mu_i^2}{\partial a^d u_{r_0}} \\ &= 2mu_{r_0} = 2mu(r_0) \end{aligned} \quad (2.76)$$

which is the same than we would have obtained directly in the continuum, using standard rules on derivatives, forgetting that  $u$  is a function and ending with the rule

$$\frac{\partial u(r_1)}{\partial u(r_2)} = \delta(r_1 - r_2) \quad (2.77)$$

Another useful rule to compute the derivative is to get it through slight changes in the function, as for standard derivatives. For an arbitrary (but “small” function  $\tilde{u}(r)$ ) one has

$$H[u + \tilde{u}] - H[u] = \int dr \frac{\partial H[u]}{\partial u(r)} \tilde{u}(r) \quad (2.78)$$

which again allows to extract the functional derivative.

## 2.4 Examples: elastic systems

After this very formal section, we will apply this technology to simple and physical examples. The example that will come over and over again in this course is the one of elastic systems. Two main reasons dictate this choice. First, it is simple enough that many results can be derived. Second, and more importantly, it is of crucial importance for a large number of physical systems of considerable current interest, both for classical and quantum systems. Before we embark on the calculations let us see some of the examples of the classical systems that can be described by elastic systems. We will examine the quantum case in the next chapter.

The first example that comes to mind is of course the simple crystals. Beyond the natural crystals, one can make artificial ones where the “atoms” are either colloids, magnetic bubbles, charged spheres (see Fig. 2.2) or even vortices in type II superconductors (see Fig. 2.3 and Fig. 2.4). Magnetic domain walls in magnets are also examples of such elastic structures (see Fig. 2.5).

The basic building brick can thus be quite complicated (a line for vortices). Understanding the physical properties of such systems is a formidable task and a largely open subject. Indeed in addition the effect of thermal fluctuations, these crystals are embedded in an external space and in general, contrarily to normal crystals, subject to disorder. This disorder competes with the natural order of the crystal and lead to many interesting properties, among them glassiness. In addition these systems can in general be subjected to an external force and they will start sliding, leading to quite complicated dynamics. The dynamics is in general of crucial importance. For example in type II superconductors, the motion of the vortices is caused by the presence of a current in the superconductor. Since the vortices are lines of magnetic field, when they move they generate an electric field, opposed to the current. The system is thus not superconducting any more but has a finite resistance. Thus the physics of the vortex lattice has direct consequences on the usefulness of superconductors.

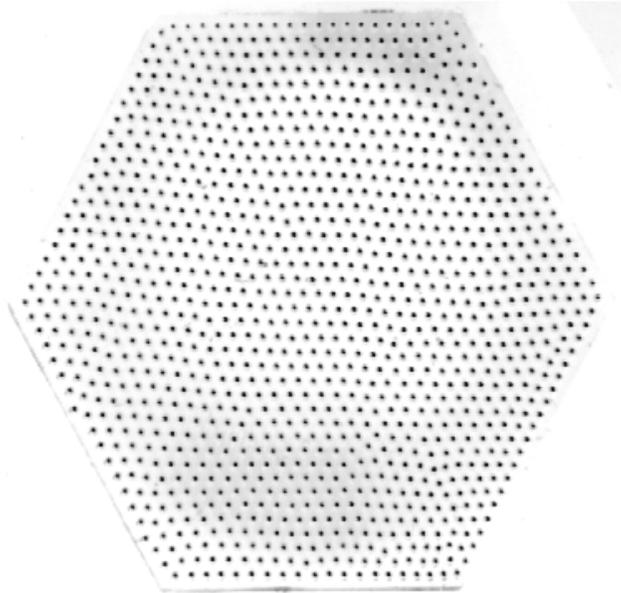


Figure 2.2: The crystal is formed by small charges that repel via Coulomb interaction. The size of the cell is few centimeters [6].

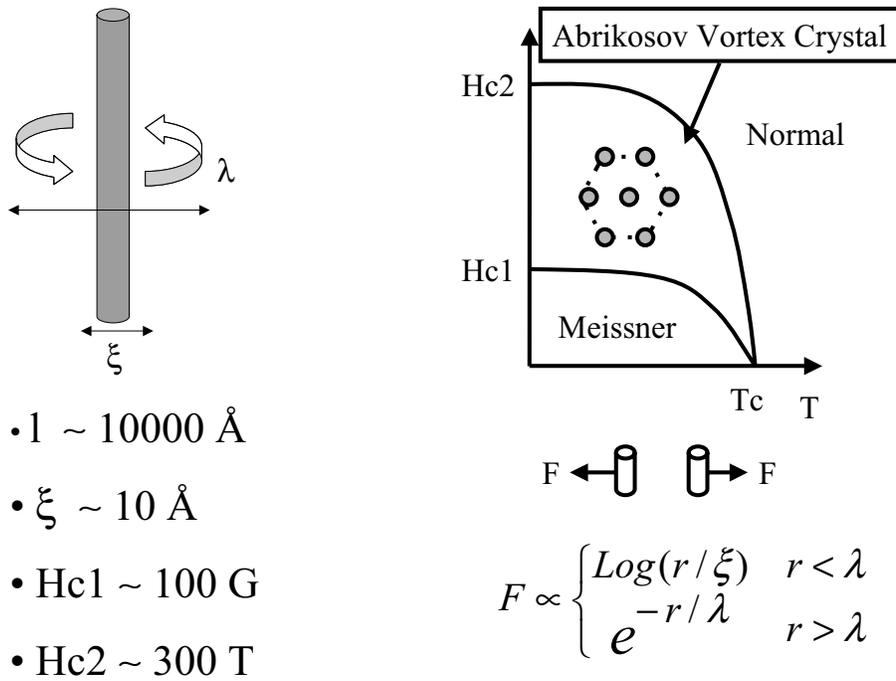


Figure 2.3: In type II superconductors the magnetic field can penetrate as filament of flux surrounded by supercurrent. This form vortices that repel, and lead to a crystal with a lattice spacing controlled by the external magnetic field.

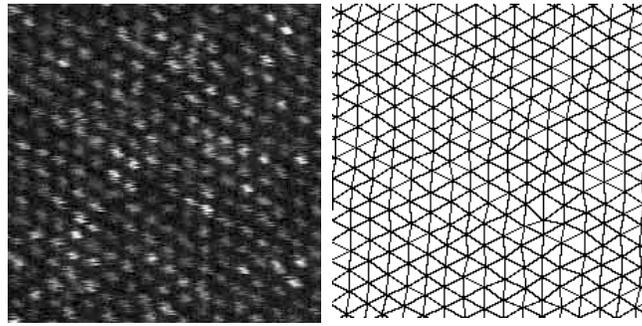


Figure 2.4: The tip of the vortices can be imaged by sprinkling magnetic particles on the compound (Bitter decoration technique). The resulting image [7](left) can then be triangulated to see the positions of the vortice. This is a small part of a very large image ( $\sim 100000$  vortices). Note that the lattice is topologically perfect.

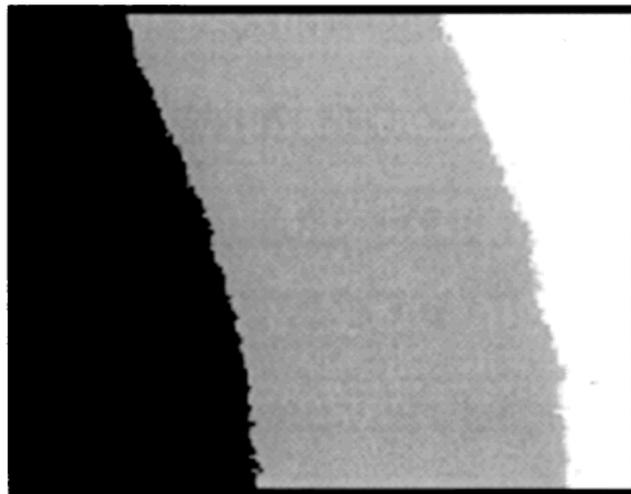


Figure 2.5: A magnetic domain wall between two regions of opposite magnetization in a thin magnetic film is another example of an elastic structure. It is a manifold of internal dimension 1 embedded in a space of dimension 2. Two different domain walls are shown in black and grey [8].

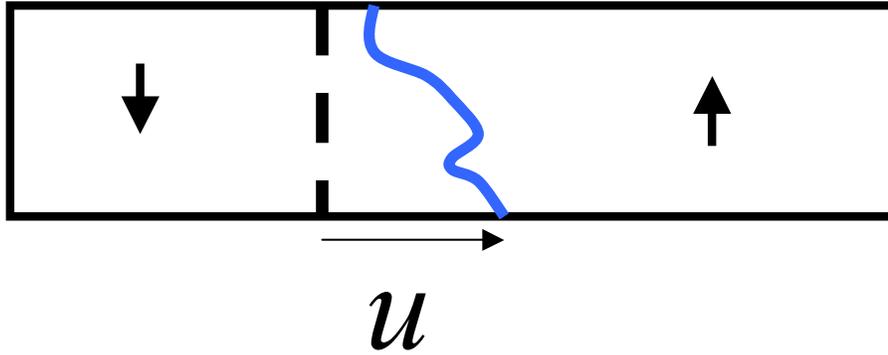


Figure 2.6: A manifold (interface). For the interface  $u(z)$  is the displacement compared to the flat position,  $z$  the interne

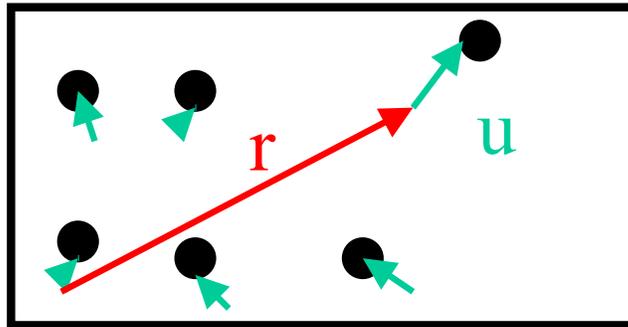


Figure 2.7: The relative displacement correlation function  $B(r)$  measures how the displacement grows as a function of distance. It can be directly observed in decoration experiments such as shown on Fig. 2.4.

We will thus examine in this section the features of the clean classical elastic systems and complicate the problem as we move along this course.

Let us consider a crystal where we denote by  $R_i^0$  the equilibrium position of the particles, and by  $u_i$  the displacements relative to their equilibrium positions. The interaction between the particles of the crystal can be approximated by an elastic Hamiltonian. Although it is possible in principle to stick to the lattice, it is much more convenient to go to the continuum. The Hamiltonian becomes

$$H = \frac{1}{2}c \int d^d r (\nabla u(r))^2 \quad (2.79)$$

where  $c$  is the elastic constant. Of course a true elastic Hamiltonian is more complicated (bulk, tilt and shear) coefficients, but this isotropic elasticity will be enough for our purposes. The elastic approximation assumes that  $|u_{i+1} - u_i| \ll a$ . One can also describes interfaces, such as the one shown on Fig. 2.6 by an elastic energy such as (2.79) the integral being now only on internal variables.

Let us compute various quantities. The simplest one is the relative displacement correlation function

$$B(r) = \langle [u(r1) - u(r2)]^2 \rangle \quad (2.80)$$

which is an indication on how fast the thermal fluctuations disorder the crystal (see Fig. 2.7) In fact

we already computed it in (2.72). Indeed in Fourier space (2.79) is simply

$$H = \frac{c}{2} \frac{1}{\Omega} \sum_q q^2 u(q) u^*(q) \quad (2.81)$$

and thus

$$\begin{aligned} \langle [u(r1) - u(r2)]^2 \rangle &= \frac{1}{\Omega} \sum_q \frac{[2 - 2 \cos(q(r1 - r2))]}{\beta c q^2} \\ &= \frac{T}{(2\pi)^d} \int d^d q \frac{[2 - 2 \cos(q(r1 - r2))]}{c q^2} \end{aligned} \quad (2.82)$$

The expression (2.82) has various interesting features. First, if there are no thermal fluctuations  $T = 0$  one quite naturally finds that the crystal is perfectly ordered. Second, we see that the atoms are less and less perfectly positioned if one looks at larger and larger lengthscale. How (2.82) behaves at large lengthscale tells us whether we have a crystal at all or not. At large lengthscales the cosine oscillates and can be neglected. We thus see that for  $d > 2$  (in practise  $d = 3$ ) the integral is convergent. The correlation function saturates to a finite value. This means that although the thermal displacements put the atoms out of place, they do not wander too much around their equilibrium position. A crystal can thus exist. On the other hand in  $d = 2$  and  $d = 1$  the integral is divergent. This means that the correlation function grows unboundedly as

$$\langle [u(r1) - u(r2)]^2 \rangle \sim T \log[(r1 - r2)/a] \quad d = 2 \quad (2.83)$$

$$\langle [u(r1) - u(r2)]^2 \rangle \sim |r1 - r2| \quad d = 1 \quad (2.84)$$

and there can be no crystal because of the thermal fluctuations. This is another example, albeit devious, of the Mermin-Wagner theorem stating that one cannot break a continuous symmetry (here the translation) in  $d \leq 2$ . The low energy modes (here the phonons) restore the symmetry.

To go further let us express the density of the crystal in the continuum limit. This is a little tricky. Let us first look at the case of the interface, which is simpler. If  $r$  denotes total space, whereas  $z$  is for the internal coordinates,  $x$  the direction along the interface (see Fig. 2.6) the density is

$$\rho(r = (z, x)) = \delta(x - u(z)) \quad (2.85)$$

which can be conveniently expressed as

$$\rho(r = (z, x)) = \int d\lambda e^{i\lambda(x - u(z))} \quad (2.86)$$

For the periodic case equivalently one has

$$\rho(r) = \sum_i \delta(r - R_i^0 - u_i) \quad (2.87)$$

One can wonder why we keep the discrete nature of  $u_i$  in (2.87) while we performed the continuous limit in  $H$ . This is due to the fact that in systems such as the vortex lattice, the lattice spacing is in fact quite large and thus many things (disorder for example) can vary at a lengthscale much shorter than the lattice spacing. It is thus crucial to remember the discrete nature of the lattice to compute the density at a given point  $r$ . On the other hand we know (this is the elastic limit) that  $u$  itself varies

very slowly at the scale of the lattice spacing  $a$  so we can use this fact to simplify (2.87). In order to take the continuum limit, one can introduce a smooth displacement field  $u(r, z)$  by

$$u(r) = \int_{BZ} \frac{d^d r}{(2\pi)^d} e^{iqr} \sum_j e^{-iqR_j} u_j \quad (2.88)$$

such that  $u(R_i) = u_i$  and which has no Fourier components outside of the Brillouin zone (BZ). In terms of the smooth field (2.88) one can introduce the relabeling field

$$\phi(r) = r - u(\phi(r)) \quad (2.89)$$

In the absence of dislocations there is a unique solution of (2.89) giving  $u(r)$  as a function of  $\phi(r)$ .  $\phi$  is a smooth vector field labeling the lines, and which takes an integer-like values at each location of a particle

$$\phi(R_i + u(R_i)) = R_i \quad (2.90)$$

Substituting (2.89) in (2.87) one gets

$$\rho(r) = \sum_i \delta(R_i - \phi(r)) \det[\partial_\alpha \phi_\beta(r)] \quad (2.91)$$

Using the integral representation of the  $\delta$  function, (2.91) becomes

$$\rho(r) = \det[\partial_\alpha \phi_\beta] \int \frac{d^d q}{(2\pi)^d} \rho_0(q) e^{iq\phi(r)} \quad (2.92)$$

where

$$\rho_0(q) = \sum_i e^{iqR_i} \quad (2.93)$$

is the density of the associated perfect system. For the case of a perfect lattice  $\rho_0(q)$  is

$$\rho_0(q) = \rho_0 (2\pi)^d \sum_K \delta(q - K) \quad (2.94)$$

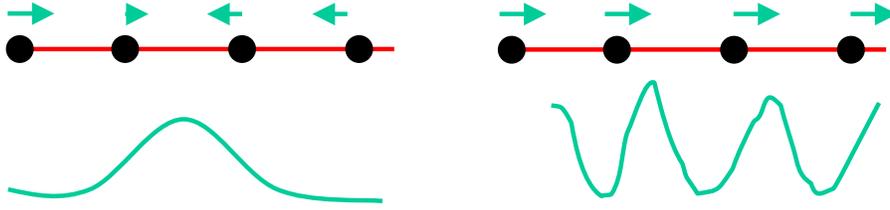
Using (2.94) in (2.92) one gets formula (2.95).

$$\rho(r) = \rho_0 \det[\partial_\alpha \phi_\beta] \sum_K e^{iK \cdot \phi(r)} \quad (2.95)$$

Assuming that we are in the elastic limit  $\partial_\alpha u_\beta \ll 1$  one can expand (2.95) to get

$$\rho(r) \simeq \rho_0 [1 - \partial_\alpha u_\alpha(\phi(r)) + \sum_{K \neq 0} e^{iK(r-u(\phi(r)))}] \quad (2.96)$$

In (2.96) one can replace  $u(\phi(r))$  by  $u(r)$  up to terms of order  $\partial_\alpha u_\beta \ll 1$ . Note that in doing so  $u$  has negligible (suppressed by powers of  $a/\xi$ ) Fourier components outside the Brillouin zone, and thus there is a complete decoupling between the gradient term and higher  $K$  terms. We have realized a sort of Fourier decomposition of the density, separating terms varying at lengthscales much larger than the lattice spacing, to Fourier components varying with harmonics of the periodicity of the lattice. This can be schematically seen on Fig.2.8. Formula (2.96) is quite remarkable and allow to extract many



$$\rho(x) = \rho_0 - \rho_0 \nabla u(x) + \rho_0 \sum_K e^{iK(x-u(x))}$$

Figure 2.8: Eq. (2.96) realizes a Fourier decomposition of the density relative to the wavevectors corresponding to the lattice spacing. It is easy to see physically that the  $q \sim 0$  component is  $\propto \nabla u$ . A variation of the density at the scale of the lattice spacing can be decomposed in  $\cos(K(r - u))$  where a constant (at the scale of the lattice spacing)  $u$  would just shift the peaks of the cos. Putting all harmonics together gives back (2.96)

informations. Note the similarities with the expression for the interface where instead of the discrete sum, we have here an integral. In fact both these expressions can be written as

$$\int dq \rho_0(q) e^{iq(r-u(r))} \quad (2.97)$$

where  $\rho_0(q)$  is the density of the associated *perfect* system

First let us add to the Hamiltonian a field coupling to the density

$$H_\mu = - \int dr \mu(r) \rho(r) \quad (2.98)$$

If this field varies very slowly at the scale of the lattice (we take it constant at the end) only the  $q \sim 0$  matters

$$H_\mu \simeq \int dr \mu(r) \rho_0 \nabla u(r) \quad (2.99)$$

One can thus compute the response of the lattice, i.e. the variation of the density when the external field is applied. Here again only the  $q \sim 0$  component matters

$$\delta \rho(r) \simeq -\rho_0 \langle \nabla u(r) \rangle \quad (2.100)$$

In linear response this is given by (2.32). Thus

$$\begin{aligned} \chi(r) &= \beta \rho_0^2 \langle \nabla u(r) \nabla u(0) \rangle \\ &= \frac{\beta \rho_0^2}{\Omega^2} \sum_{q, q'} (iq)(iq') \langle u_q u_{q'} e^{iqr} \rangle \\ &= \frac{\beta \rho_0^2}{\Omega^2} \sum_q q^2 \frac{\Omega}{\beta q^2 c} e^{iqr} \\ &= \frac{1}{\Omega} \sum_q \frac{\rho_0^2}{c} e^{iqr} \end{aligned} \quad (2.101)$$

Thus  $\chi(q) = \rho_0^2/c$  and we recover directly that the coefficient  $c$  gives the compressibility of the system.

Another important quantity measured in X-ray or neutron experiments is the structure factor

$$S(q) = \langle \rho(q)\rho^*(q) \rangle \quad (2.102)$$

The Fourier transform of the density is given by (this time we look at large  $q$ )

$$\rho(q) = \rho_0 \int dr \sum_K e^{i(K-q)r - iKu(r)} \quad (2.103)$$

Thus quite naturally has peaks around the vectors of the reciprocal lattice. The structure factor is thus given by

$$S(q) = \rho_0^2 \int dr_1 \int dr_2 e^{-iq(r_1-r_2)} \sum_{K_1 K_2} e^{i(K_1 r_1 - K_2 r_2)} \langle e^{i(K_1 u(r_1) - K_2 u(r_2))} \rangle \quad (2.104)$$

We use the standard decomposition in center of mass and relative coordinates  $r_1 = R + r/2$  and  $r_2 = R - r/2$ . The integration over  $R$  can be performed because the  $u$  vary slowly at the scale of the lattice spacing i.e. of  $K^{-1}$ . It gives

$$S(q) = \rho_0^2 \Omega \int dr \sum_K e^{i(K-q)r} \langle e^{i(K(u(r/2) - u(-r/2)))} \rangle \quad (2.105)$$

Thus the shape of the peaks in the structure factor is just given by the Fourier transform of the positional correlation function

$$C_K(z) = \langle e^{iK[u(r) - u(0)]} \rangle \quad (2.106)$$

Clearly the broader the peak the faster the decay of  $C_K(r)$ .  $C_K(r)$  is therefore a direct measure of the degree of translational order that remains in the system. Three possible cases are shown in figure 2.9.  $C(z)$  can easily be computed using functional integrals.

$$\begin{aligned} C(z) &= \frac{1}{Z} \int \mathcal{D}u e^{-\frac{c\beta}{2\Omega} \sum_q q^2 u(q) u^*(q)} e^{iK[u(z) - u(0)]} \\ &= \frac{1}{Z} \int \mathcal{D}u e^{-\frac{c\beta}{2\Omega} \sum_q q^2 u(q) u(-q) + \frac{1}{2} \sum_q (u(q)A(-q) + u(-q)A(q))} \end{aligned} \quad (2.107)$$

with

$$A(-q) = iK \frac{(e^{iqr} - 1)}{\Omega} \quad (2.108)$$

Simply completing the square (that's the magic of functional integrals !) gives

$$C(z) = \frac{1}{Z} \int \mathcal{D}u e^{-\frac{1}{2} \sum_q V(q) [u(q) + \frac{A(q)}{V(q)}] [u(-q) + \frac{A(-q)}{V(-q)}]} e^{\frac{1}{2} \sum_q \frac{A(q)A(-q)}{V(q)}} \quad (2.109)$$

with  $V(q) = \frac{c\beta q^2}{\Omega}$ . Since the change of variable  $u(q) \rightarrow u(q) + A(q)$  is a simple shift the integration on the numerator still cancels exactly with the partition function in the denominator, leading to

$$\begin{aligned} C(z) &= e^{\frac{1}{2} \sum_q \frac{A(q)A(-q)}{V(q)}} \\ &= e^{-\frac{1}{2} \frac{1}{\Omega} \sum_q \frac{[2 - 2 \cos(q(r_1 - r_2))]}{c\beta q^2}} \\ &= e^{-\frac{K^2}{2} \langle [u(z) - u(0)]^2 \rangle} \end{aligned} \quad (2.110)$$

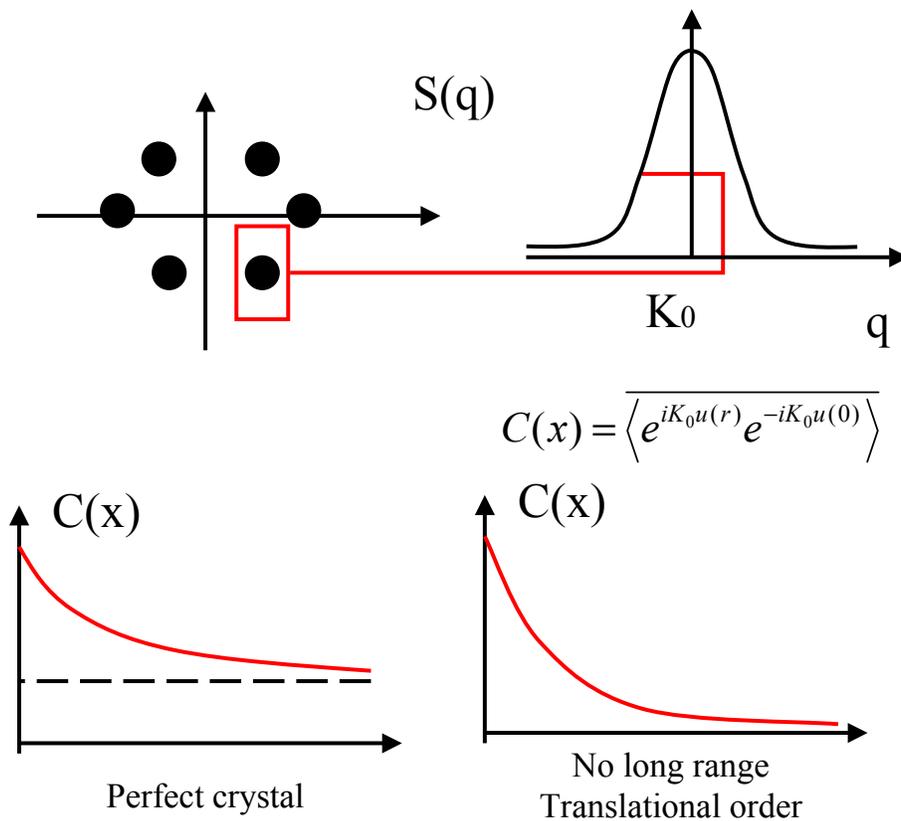


Figure 2.9: The positional correlation function  $C(r)$ , controls the shape of the peaks in the structure factor  $S(q)$ . If  $C(r)$  tends to a constant, one recovers perfect  $\delta$  function peaks, albeit with a reduced weight (the Debye-Waller factor). This is the case for thermal fluctuations in  $d > 2$ . If  $C(r) \rightarrow 0$  perfect translational order is lost. When  $C(r)$  decreases fast enough (exponential like for example) the peaks in  $S(q)$  have a finite height. One can thus extract from  $C(r)$  a characteristic length beyond which translational order is lost (this is the half width of the peaks). If  $C(r)$  decreases as a power law, one can still have divergent peaks, although not perfect  $\delta$ . The system has quasi long range translational order. This is the case of thermal fluctuations in  $d = 2$  (Berezinskii-Kosterlitz-Thouless).

Thus in  $d = 3$  the integral is convergent and thermal fluctuations leave perfect  $\delta$  functions Bragg peaks, but with a weight that is not 1, due to the thermal fluctuations. In  $d = 2$   $B(r)$  is logarithmically divergent.  $C(r)$  behaves as a power law with an exponent that is proportional to the temperature. The Fourier transform is again a power-law. There is no  $\delta$  function any more, sign that there is no perfect crystal, but there are power-law divergent Bragg peaks. In  $d = 1$ ,  $B(r)$  is linear, which Fourier transform is a Lorentzian. The peaks are not divergent any more but have a width proportional to the temperature.

For the case of the interface one has a similar result. The Fourier transform of the density is given by

$$\begin{aligned}\rho(q) &= \int dz dx e^{i(\lambda - q_x)x - i\lambda u(z) - iq_z z} \\ &= (2\pi) \int dz e^{-iq_x u(z) - iq_z z}\end{aligned}\tag{2.111}$$

The structure factor is thus given by

$$\begin{aligned}S(q) &= \int dz \int dz' e^{iq_z(z' - z)} \langle e^{iq_x[u(z') - u(z)]} \rangle \\ &= \Omega \int dz e^{iq_z z} \langle e^{iq_x[u(z) - u(0)]} \rangle\end{aligned}\tag{2.112}$$

An interesting case for this expression is  $d = 1 + 1$ . In that case  $B(z) \sim |z|$  and the structure factor is given by

$$S(q) = \frac{q_x^2 T}{(q_x^2 T)^2 + q_z^2}\tag{2.113}$$

Thus when  $q_x = 0$  the structure factor is the same than for the perfectly straight interface  $S(q) = \delta(q_z)$ . Looking at finite  $q_x$  means than one is more aware of the wandering of the interface in the  $x$  direction. In that case the structure factor is a lorentzian, whose width is controlled by how much wandering there is.

Finally let us look at the real stuff. What happens if we put our periodic (or interface) in a disordered potential. One would have to add to the Hamiltonian a term like

$$H_V = \int dr V(r) \rho(r)\tag{2.114}$$

where  $V$  is some random potential. If one wants to compute some average value, it is now a function of the precise realization of the disorder

$$\langle O \rangle_V = \frac{\int \mathcal{D}u[q] O e^{-\beta(H_0 + H_V)}}{\int \mathcal{D}u[q] e^{-\beta(H_0 + H_V)}}\tag{2.115}$$

Rather than to deal with a specific realization of the disorder one want to have an ensemble average over all possible realizations, in order to have to avoid to deal with a random variable. Of course in doing so one hopes that the system (which only see a single realization of the disorder but which is very large) self-averages the disorder between its different spatial parts, and that the ensemble average coincides with the experimental answers. One thus computes

$$\overline{\langle O \rangle_V} = \int \mathcal{D}V(r) p(V) \frac{\int \mathcal{D}u[q] O e^{-\beta(H_0 + H_V)}}{\int \mathcal{D}u[q] e^{-\beta(H_0 + H_V)}}\tag{2.116}$$

where  $p(V)$  is a functional giving the probability of having a given realization of the disorder. Usually  $p$  is chosen Gaussian and uncorrelated.

$$p(V) = Ce^{-D^{-1} \int dr V(r)^2} \quad (2.117)$$

where  $C$  is the normalization ensuring that  $\int \mathcal{D}V p(V) = 1$ . This ensures that

$$\overline{V(r)V(r')} = D\delta(r - r') \quad (2.118)$$

Even with such a simple  $p(V)$  doing the average over the disorder is tremendously complicated, since one has to average together numerator and denominator. Treating (2.114) is too complicated for these lectures, but there is simplification originally introduced by Larkin. If one assumes that  $u$  is small then the density can be expanded in powers of  $u$  and the disorder replaced by

$$H_f = \int dr f(r)u(r) \quad (2.119)$$

where  $f$  is a random force acting on the particles. This model will eventually break down if the displacements can become large, but it will work at short distance and in any case we can always examine it as a model per se. The advantage is that the model is still quadratic and thus solvable.

One can write

$$H = \frac{1}{\Omega} \sum_q \frac{c}{2} q^2 u(q)u(-q) + \frac{1}{2} [f(-q)u(q) + f(q)u(-q)] \quad (2.120)$$

$$= \frac{1}{\Omega} \left[ \sum_q \frac{c}{2} q^2 \left[ u(q) + \frac{f(q)}{cq^2} \right] \left[ u(-q) + \frac{f(-q)}{cq^2} \right] - \frac{1}{2\Omega} \sum_q \frac{f(q)f(-q)}{cq^4} \right] \quad (2.121)$$

Thus one can define the new variable  $\tilde{u}(q) = u(q) + \frac{f(q)}{cq^2}$ . The correlation function is given by

$$\langle u(q)u(-q) \rangle_f = \langle \tilde{u}(q)\tilde{u}(-q) \rangle_f + \frac{f(q)f(-q)}{(cq^2)^2} \quad (2.122)$$

Because of the form of (2.121) it is easy to see that

$$\langle \tilde{u}(q)\tilde{u}(-q) \rangle_f = \langle u(q)u(-q) \rangle_{f=0} = \frac{\beta\Omega}{cq^2} \quad (2.123)$$

Thus for a given realization of the disorder the correlation function is the sum of two terms. One is the standard thermal fluctuation term, which does *not* depend on the disorder any more. The other is entirely due to the disorder. The average over disorder is easily performed since it is again a Gaussian functional integral, leading to

$$\overline{\langle \tilde{u}(q)\tilde{u}(-q) \rangle} = \frac{\beta\Omega}{cq^2} + \frac{\Delta}{(cq^2)^2} \quad (2.124)$$

The disorder term is thus much more singular than the one due to the thermal fluctuations. Note that it is independent of the temperature. Since the term behaves as  $1/q^4$  it means that below *four* dimensions the displacement correlation function  $B(r)$  will grow unboundedly. Thus in the presence of disorder, however weak, no perfect crystal can exist below four dimensions. Below four dimensions one has

$$B(r) \propto \Delta r^{4-d} \quad (2.125)$$

More details on the physical consequences will be seen as an exercise.



## Chapter 3

# Calculation of Functional Integrals

In the previous examples we examined some theories for which we were lucky to have a quadratic Hamiltonian. In this case the Gaussian integrals are easy to perform and most correlation functions can be computed exactly. However one is rarely so lucky. In this chapter we will examine some simple methods that allow to make progress on more complicated Hamiltonians. Needless to say the list is not exhaustive.

### 3.1 Perturbation theory

Let us assume that we can write our Hamiltonian in the form

$$H = H_0 + H_{\text{pert}} \quad (3.1)$$

where  $H_0$  is a theory we know how to solve exactly (for example a quadratic Hamiltonian) and  $H_{\text{pert}}$  the annoying part. A simple example is given by the well known Ginzburg-Landau energy for which

$$H = \frac{1}{2} \int d^d x [c(\nabla u(x))^2 + mu(x)^2] + \lambda \int d^d x u(x)^4 \quad (3.2)$$

which is a generic energy for most critical phenomena. It is obvious that we can take

$$H_0 = \frac{1}{2} \int d^d x [c(\nabla u(x))^2 + mu(x)^2] \quad (3.3)$$

$$H_{\text{pert}} = \lambda \int d^d x u(x)^4 \quad (3.4)$$

If the perturbation is small one can compute any correlation function by expanding the functional integral in powers of  $H_{\text{pert}}$  (i.e. in powers of  $\lambda$ ). One has thus to compute for any correlation function

$$\langle O_\mu(u) \dots O_\nu(u) \rangle = \frac{\sum_{n=0}^{\infty} \frac{1}{n!} \int \mathcal{D}u e^{-\beta H_0} (-\beta H_{\text{pert}})^n O_\mu(u) \dots O_\nu(u)}{\sum_{n=0}^{\infty} \frac{1}{n!} \int \mathcal{D}u e^{-\beta H_0} (-\beta H_{\text{pert}})^n} \quad (3.5)$$

Since all the terms in the sum have to be computed with the quadratic Hamiltonian  $H_0$  they can be trivially done. One can thus, given some time and effort, compute any correlation function up to a given order in an expansion in powers of  $\lambda$ .

Doing such a calculation brutally would be extremely tedious. Due to the properties of Gaussian integrals tremendous simplifications occur. Indeed let us consider for example a correlation such as

$$\langle u(r_1)u(r_2)u(r_3)u(r_4) \rangle \quad (3.6)$$

where the average is taken with a quadratic Hamiltonian such as  $H_0$ . This correlation function can in principle be obtained by adding source terms to the Hamiltonian in the way explained in Section 2.1.

If the Hamiltonian  $H_0$  is quadratic it can always be written as

$$\beta H_0 = \frac{1}{2} \int dx \int dy u(x) G^{-1}(x-y) u(y) \quad (3.7)$$

such that

$$\langle u(x)u(y) \rangle_0 = G(x-y) \quad (3.8)$$

The “matrix”  $G$  and  $G^{-1}$  are inverse i.e.  $\delta(x_1 - x_2) = \int dx_3 G(x_1 - x_3) G^{-1}(x_3 - x_2)$ . This is the continuous version of the relation (2.52). In presence of the source terms the partition function becomes

$$Z = \int \mathcal{D}u e^{-\frac{1}{2} \int dx dy u(x) G^{-1}(x-y) u(y) + \int dx h(x) u(x)} \quad (3.9)$$

which can be rewritten as

$$Z = \int \mathcal{D}u e^{-\frac{1}{2} \int dx dy (u(x) - \int dz G(x-z) h(z)) G^{-1}(x-y) (u(y) - \int dz G(y-z) h(z))} e^{\frac{1}{2} \int dx dy G(x-y) h(x) h(y)} \quad (3.10)$$

using the change of variable  $\tilde{u}(x) = u(x) - \int dz G(x-z) h(z)$  it is easy to see that

$$Z = Z_{h=0} e^{\frac{1}{2} \int dx dy G(x-y) h(x) h(y)} \quad (3.11)$$

Using (2.8) it is easy to show that

$$\langle u(r_1)u(r_2) \dots u(r_n) \rangle = \left. \frac{\partial e^{\frac{1}{2} \int dx dy G(x-y) h(x) h(y)}}{\partial h(r_1) \partial h(r_2) \dots \partial h(r_n)} \right|_{h=0} \quad (3.12)$$

It is easy to check that

$$\langle u(r_1)u(r_2) \dots u(r_n) \rangle = \sum_{\text{pairings}} G(r_\alpha - r_\beta) G(r_\gamma - r_\delta) \dots G(r_\mu - r_\nu) \quad (3.13)$$

This is known as Wick’s theorem, and is a completely general property of Gaussian integrals. For example for the four points correlation function

$$\langle u(r_1)u(r_2)u(r_3)u(r_4) \rangle = G(r_1 - r_2)G(r_3 - r_4) + G(r_1 - r_3)G(r_2 - r_4) + G(r_1 - r_4)G(r_2 - r_3) \quad (3.14)$$

Wick’s theorem makes the calculation of any order in (3.5) now completely automatic. Another important simplification occurs. Let us illustrate it by computing the two point correlation function at first order in perturbation. (3.5) leads to

$$\begin{aligned} \langle u(r_1)u(r_2) \rangle &= \frac{\int \mathcal{D}u u(r_1)u(r_2) e^{-\beta H_0} (1 - \beta H_{\text{pert}})}{\int \mathcal{D}u e^{-\beta H_0} (1 - \beta H_{\text{pert}})} \\ &= \frac{\langle u(r_1)u(r_2) \rangle_0 - \beta \langle u(r_1)u(r_2) H_{\text{pert}} \rangle_0}{1 - \beta \langle H_{\text{pert}} \rangle_0} \\ &= \langle u(r_1)u(r_2) \rangle_0 - \beta [\langle u(r_1)u(r_2) H_{\text{pert}} \rangle_0 - \langle u(r_1)u(r_2) \rangle_0 \langle H_{\text{pert}} \rangle_0] \end{aligned} \quad (3.15)$$

Thus only the *connected* correlations appear in the expansion. The denominator eliminates all terms that have no connections (contractions) between the operators of the correlation function and the interaction Hamiltonian. Thus when writing all possible contractions at a given order as in (3.14) one should *only* keep the connected ones. This takes care of the denominator in (3.5). One can further simplify the writing of the terms in the perturbation expansion by using the symmetry factors of all possible contractions, and writing pictorially the contractions in terms of diagrams. Each contraction can be written as a line to which the weight  $G(r_1 - r_2)$  is associated. Writing all the terms of the perturbation thus corresponds to writing all possible connected diagrams. This technique known as Feynman diagrams will be examined in more details on examples in the exercises.

## 3.2 Variational method

Let us now examine another method, which can be useful even in the absence of a small parameter in the Hamiltonian. Quite generally one can write

$$\begin{aligned} Z &= \int \mathcal{D}u e^{-\beta H} \\ &= \int \mathcal{D}u e^{-\beta H_0} e^{-\beta(H-H_0)} \\ &= Z_0 \langle e^{-\beta(H-H_0)} \rangle_0 \end{aligned} \tag{3.16}$$

where the index 0 denoted the partition function and the averages with respect of the Hamiltonian  $H_0$ . Here  $H_0$  can be any Hamiltonian. Thus the free energy satisfies

$$F = F_0 - T \log[\langle e^{-\beta(H-H_0)} \rangle_0] \tag{3.17}$$

Given the convexity of the exponential (see e.g. [2]) it is easy to check that one has always

$$\langle e^{-\beta(H-H_0)} \rangle_0 > e^{-\beta\langle(H-H_0)\rangle} \tag{3.18}$$

and thus

$$F \leq F_{\text{var}} = F_0 + \langle H - H_0 \rangle_0 \tag{3.19}$$

The “best”  $H_0$  is obviously  $H$ , i.e. the one for which the variational free energy  $F_{\text{var}}$  is minimum. The idea is to take a simple enough  $H_0$  so that one can compute (for example a quadratic one), and to optimize it to try to get as close as possible of the physics of the original Hamiltonian.

Let us take an example. We start from the so called sine-Gordon Hamiltonian

$$H = \frac{c}{2} \int d^d x (\nabla \phi(x))^2 - g \int d^d x \cos(2\phi(x)) \tag{3.20}$$

with  $g > 0$ . The physical origin of such an Hamiltonian will be seen in exercises. Obviously at  $T = 0$  one can expect  $\phi = 0$  to be the optimal configuration. If the temperature is not too high one can reasonably expect that an approximation where one takes into account harmonic oscillations around this equilibrium position is a good one. Let us thus take for  $H_0$

$$H_0 = \frac{1}{2\Omega} \sum_q G^{-1}(q) \phi(q) \phi(-q) \tag{3.21}$$

and try to optimize by finding the best  $G(q)$ . The variational energy is

$$F_{\text{var}} = -T \sum_{q>0} \log[TG(q)] + \frac{c}{2} T \sum_q q^2 G(q) - g\Omega e^{-\frac{2}{\Omega} \sum_q TG(q)} \quad (3.22)$$

and thus

$$\frac{\partial F_{\text{var}}}{\partial G(q)} = 0 \quad (3.23)$$

leads to

$$G^{-1}(q) = cq^2 + 4ge^{-\frac{2}{\Omega} \sum_q TG(q)} \quad (3.24)$$

which is a self consistent equation for  $G(q)$ . Obviously one can write  $G^{-1}(q) = cq^2 + m$  where the mass  $m$  satisfies

$$m = 4ge^{-\frac{2}{\Omega} \sum_q \frac{T}{cq^2+m}} \quad (3.25)$$

Let us look for example at the two dimensional case. The integral in that case is divergent. One has, putting back an upper cutoff  $\Lambda$

$$\begin{aligned} \frac{1}{(2\pi)^2} \int d^d q \frac{1}{cq^2 + m} &= \frac{1}{(2\pi)} \int_0^\Lambda q dq \frac{1}{cq^2 + m} \\ &\simeq \frac{1}{(4\pi c)} \log\left[\frac{c\Lambda^2}{m}\right] \end{aligned} \quad (3.26)$$

One has thus the selfconsistent equation

$$m = 4g \left( \frac{m}{c\Lambda^2} \right)^{\frac{T}{2\pi c}} \quad (3.27)$$

It is easy to see that for  $T > 2\pi c$  this equation has only  $m = 0$  for solution. The sine-Gordon system behaves thus as a free theory and the cosine potential is irrelevant. On the other hand at low temperatures a non zero mass appears. More examples of the variational method will be seen as exercises.

### 3.3 Saddle point method

Finally let us see a very useful method to evaluate the functional integrals when one can find a parameter such that

$$H = N\tilde{H}[u] \quad (3.28)$$

where  $N \rightarrow \infty$ . Let us illustrate the method on the simple integral

$$\int dx e^{-Nx^2} \quad (3.29)$$

In that simple case it is easy to see that the configuration that will be mostly favored will be the one such that  $\tilde{H}[u]$  is minimal. In the above example this corresponds to  $x = 0$ . All other configurations will acquire exponentially small Boltzman weights in the limit  $N \rightarrow \infty$ . Thus one can make the approximation that

$$\int dx e^{-N\tilde{H}[x]} \sim e^{-N\tilde{H}[x_0]} \quad (3.30)$$

where  $x_0$  is the configuration that minimizes  $\tilde{H}$  i.e. such that

$$\left. \frac{\partial \tilde{H}[x]}{\partial x} \right|_{x_0} = 0 \quad (3.31)$$

In fact quite generally no minimum for real variables exists. However it is generally possible to find for a complex variable  $z$  configurations such that (3.31) is verified. Around this configuration  $z_0$  there are two orthogonal directions in the complex plane, one for which one has a minimum of  $\tilde{H}[z]$  and one for which it is a maximum. In the above mentioned example  $z = 0$  correspond to a minimum of weights along the real axis since  $\tilde{H}[x] = x^2$  whereas it is a maximum along the imaginary axis since  $\tilde{H}[iy] = -y^2$ . Thus quite generally it is impossible to find a minimum, but one is stuck with a saddle point. This does not cause any problem. One can always deform the contour of integration from the real axis to pass through the saddle point configuration  $z_0$  in the direction for which this is a minimum of the energies. It is then easy to check that the formula (3.30) which replaces the sum over all configurations by the single saddle configuration  $z_0$  remains exact. One can thus now compute the various correlation functions using the saddle point configuration only. Formally one can go beyond the saddle point solution (i.e. make an expansion in powers of  $1/N$ ) by integrating over the fluctuations around the saddle point. Since the small deviations around the saddle point are obviously quadratic, such an integration is always possible.

Examples of the saddle point method will be seen as exercises.



## Chapter 4

# Quantum problems; functional integral

Let us now turn to quantum problems. Ultimately we want to understand the problem of many quantum objects coupled together and in equilibrium with a thermal bath. Various methods have been devised to tackle this type of problem (see e.g. [5]). Here we will see how to use functional integrals can help. Before we try the many body problem, let us see the case of a single particle.

### 4.1 Single particle

Let us consider a single quantum object described by a wavefunction  $|\psi\rangle$  and an Hamiltonian  $H$ . Let us denote the pair of conjugate variables  $u$  and  $\Pi$ . These can be the space  $x$  and momentum  $P$ , or other variables. The evolution of the wavefunction is given by the Schroedinger equation

$$H|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \quad (4.1)$$

note that  $H$  can in principle depend explicitly on time (e.g. if the system is in a time dependent external potential). The equation (4.1) defines the evolution operator that brings the system from time  $t_1$  to time  $t_2$  by

$$|\psi(t_2)\rangle = U(t_2, t_1)|\psi(t_1)\rangle \quad (4.2)$$

Knowing the evolution operator allows thus to compute all properties of the system. The evolution operator obeys

$$i\hbar \frac{\partial U(t, 0)}{\partial t} = H(t)U(t, 0) \quad (4.3)$$

with the boundary condition  $U(0, 0) = 1$ . If everything was simple numbers the solution would simply be

$$U(t, 0) = e^{-\frac{i}{\hbar} \int_0^t dt' H(t')} \quad (4.4)$$

but since  $H(t)$  is an operator, in general  $H(t)$  and  $H(t')$  do not commute. If the hamiltonian is time independent one has simply

$$U(t_2, t_1) = e^{-iH(t_2-t_1)} \quad (4.5)$$

More generally the evolution operator obviously verifies, for  $t_1 < t_2 < t_3$

$$U(t_1, t_3) = U(t_1, t_2)U(t_2, t_3) \quad (4.6)$$

One can use this property to split the interval  $t_f, t_i$  in  $N$  segments of length  $\epsilon = (t_f - t_i)/N$  to get

$$U(t_f, t_i) = U(t_f, t_{N-1})U(t_{N-1}, t_{N-2}) \cdots U(t_2, t_i) \quad (4.7)$$

If  $N$  is large enough, even if the Hamiltonian is time dependent one has

$$U(t + \epsilon, t) = e^{-\frac{i}{\hbar}H(t)\epsilon} \quad (4.8)$$

Thus (4.7) and (4.8) allow in principle for a complete calculation of the evolution operator. A more rigorous derivation of the evolution operator can be obtained from the equation (4.3). One can formally solve this equation in powers of  $H$ . Solving iteratively (4.3) gives

$$U(t_f, t_i) = 1 + (-i/\hbar) \int_{t_i}^{t_f} dt_1 H(t_1) + (-i/\hbar)^2 \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 H(t_1)H(t_2) + \cdots \quad (4.9)$$

Notice that in (4.9) the operators are always ordered so that the operator at the later time is on the left. One can formally rewrite this expression by introducing a time ordering operator  $T$  such that it always reorder the operators in this order

$$T(O(t_1)O(t_2)) = \theta(t_1 - t_2)O(t_1)O(t_2) + \theta(t_2 - t_1)O(t_2)O(t_1) \quad (4.10)$$

Using this notation it is easy to see that (4.9) can be rewritten as

$$U(t_f, t_i) = 1 + (-i/\hbar) \int_{t_i}^{t_f} dt_1 H(t_1) + \frac{(-i/\hbar)^2}{2!} \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 T[H(t_1)H(t_2)] + \cdots \quad (4.11)$$

In which one recognize the formal expansion of an exponential

$$U(t_f, t_i) = T[e^{-\frac{i}{\hbar} \int_{t_i}^{t_f} dt H(t)}] \quad (4.12)$$

which of course coincide both with the naive expression (4.4) if the operators commute and also with (4.5) if  $H$  is time independent. It is also easy to show that (4.12) and (4.7) coincide in the large  $N$  limit.

All these expressions of the evolution operator still use operators, which is relatively inconvenient because of their non commutative nature. Let us try to explicitly evaluate (4.8). We consider here only the simple case where the Hamiltonian is totally separated in  $u$  and  $P$ , for example

$$H = H_0(P) + V(u) \quad (4.13)$$

which is a very common case (typically  $H(P) = P^2/(2m)$ ). More complicated cases are analyzed in [3, 4]. We can compute all the matrix elements of the evolution operator  $\langle u_f | U(t_f, t_i) | u_i \rangle$ . Using that  $u$  is a complete basis one has

$$\begin{aligned} \langle u_f | U(t_f, t_i) | u_i \rangle &= \int du_{N-1} \int du_{N-2} \cdots \int du_2 \langle u_f | U(t_f, t_{N-1}) | u_{N-1} \rangle \langle u_{N-1} | U(t_{N-1}, t_{N-2}) | u_{N-2} \rangle \cdots \\ &\quad \langle u_2 | U(t_2, t_i) | u_i \rangle \end{aligned} \quad (4.14)$$

We have thus reduced the calculation of the evolution operator to a functional integral. The building block is the matrix element

$$\langle u_2 | e^{-\frac{i}{\hbar}H(t)\epsilon} | u_1 \rangle \quad (4.15)$$

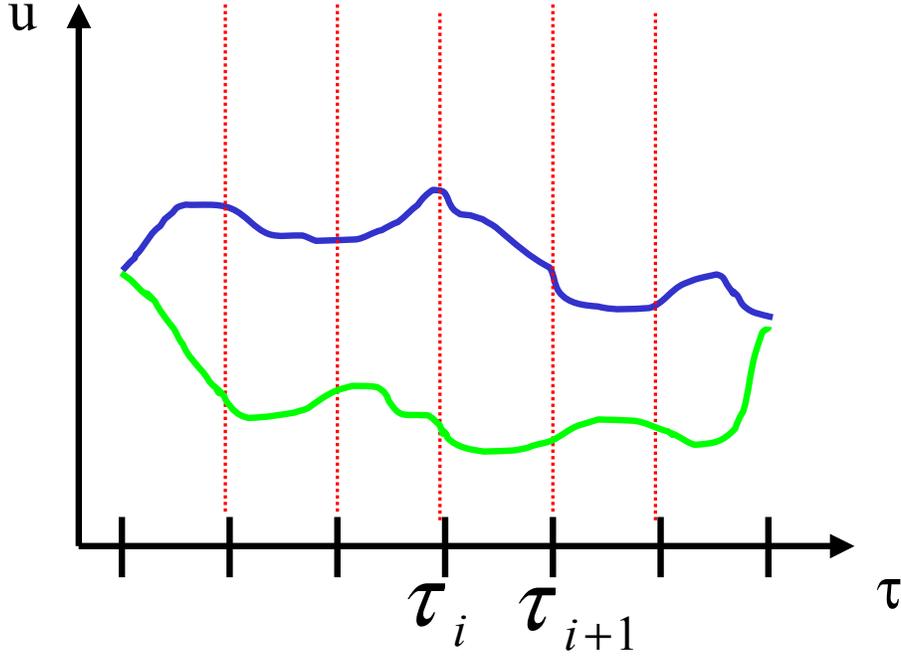


Figure 4.1: . The evolution operator can be defined as a functional integral over all trajectories starting at  $u_i$  at time  $\tau_i$  and ending at  $u_f$  at time  $\tau_f$ .

There are various degrees of rigor with which one can compute (4.15). Of course the calculation should be done only to order  $\epsilon$ , since ultimately one wants to take  $\epsilon \rightarrow 0$ . To order  $\epsilon$

$$e^{-\frac{i}{\hbar}(H_0(P)+V(u))\epsilon} \simeq e^{-\frac{i}{\hbar}H_0(P)\epsilon} e^{-\frac{i}{\hbar}V(u)\epsilon} \quad (4.16)$$

Thus

$$\begin{aligned} \langle u_2 | e^{-\frac{i}{\hbar}H(t)\epsilon} | u_1 \rangle &= \int dp \langle u_2 | e^{-\frac{i}{\hbar}H_0(P)\epsilon} | p \rangle \langle p | e^{-\frac{i}{\hbar}V(u)\epsilon} | u_1 \rangle \\ &= \int dp \langle u_2 | p \rangle \langle p | u_1 \rangle e^{-\frac{i}{\hbar}H_0(p)\epsilon} e^{-\frac{i}{\hbar}V(u_1)\epsilon} \\ &= \int dp \frac{1}{(2\pi)^d} e^{\frac{i}{\hbar}p(u_2-u_1)} e^{-\frac{i}{\hbar}[H_0(p)+V(u_1)]\epsilon} \\ &= \int dp \frac{1}{(2\pi)^d} e^{\frac{i}{\hbar}\epsilon[p\frac{(u_2-u_1)}{\epsilon} - [H_0(p)+V(u_1)]]} \end{aligned} \quad (4.17)$$

Going back to (4.7) we see that we can formally describe the matrix element  $\langle u_f | U(t_f, t_i) | u_i \rangle$  of the evolution operator, by saying that we define an arbitrary trajectory  $u(t)$  starting at  $u_i$  at time  $t_i$  and ending at  $u_f$  at time  $t_f$ . If we discretize the time as in Fig. 4.1,  $u_k$  can be viewed as the value of the variable at time  $t_k$ . In that case

$$\frac{u_{k+1} - u_k}{\epsilon} = \frac{u(t_k + \epsilon) - u(t_k)}{\epsilon} \simeq \left. \frac{du}{dt} \right|_{t_k} \quad (4.18)$$

Let us consider for example the case  $H_0(P) = P^2/(2m)$ . In that case one can easily perform the

integration over  $p$  in (4.17).

$$\langle u_2 | e^{-\frac{i}{\hbar} H(t)\epsilon} | u_1 \rangle = \left( \frac{m}{2\pi i \epsilon \hbar} \right)^{d/2} e^{\frac{i}{\hbar} \left[ \frac{m}{2} \left( \frac{u_2 - u_1}{\epsilon} \right)^2 - V(u_1) \right] \epsilon} \quad (4.19)$$

Thus (4.7) becomes (with the convention  $u_1 = u_i$ ,  $u_f = u_N$ )

$$\begin{aligned} \langle u_f | U(t_f, t_i) | u_i \rangle &= \prod_{j=2}^{N-1} \int \frac{du_j}{A} e^{\frac{i}{\hbar} \sum_{i=1}^N \left[ \frac{m}{2} \left( \frac{u_{j+1} - u_j}{\epsilon} \right)^2 - V(u_j) \right]} \\ &= \int_{u(t_i)=u_i}^{u(t_f)=u_f} \mathcal{D}u[t] e^{\frac{i}{\hbar} \int_{t_i}^{t_f} \left[ \frac{m}{2} \left( \frac{du(t)}{dt} \right)^2 - V(u(t)) \right]} \end{aligned} \quad (4.20)$$

where  $A$  is the normalization defined in (4.19). One recognizes in (4.20) the action  $S$  of the system

$$S = \int dt \mathcal{L}(t) = \int dt \left[ \frac{m}{2} \left( \frac{du(t)}{dt} \right)^2 - V(u(t)) \right] \quad (4.21)$$

where  $\mathcal{L}(t)$  is the Lagrangian. Note that one does not need to perform the integration over  $p$ . An alternative form for (4.20) is

$$\langle u_f | U(t_f, t_i) | u_i \rangle = \int_{u(t_i)=u_i}^{u(t_f)=u_f} \mathcal{D}u[t] \mathcal{D}p[t] e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt \left[ p \left( \frac{du(t)}{dt} \right) - H[t] \right]} \quad (4.22)$$

where one recognizes also the Lagrangian

$$p \left( \frac{du(t)}{dt} \right) - H[t] = \mathcal{L}(t) \quad (4.23)$$

The formula (4.20) is quite remarkable. It shows that the evolution operator can be viewed as the sum over all possible “trajectories” of the particles. The weight of each trajectory is given by  $e^{iS/\hbar}$ . Thus in the classical limit  $\hbar \rightarrow 0$  only the trajectory that minimizes the action survives. This is the classical trajectory. In the quantum case, all trajectories contribute and interfere. (4.20) provides thus a marvelous link between our intuition for classical system and the quantum world. From a practical point of view, (4.20) has replaced the problem of computing the matrix elements of various operators by “simple” integration over numbers, for which we can apply all our knowledge of integrals. It is thus a powerful technique.

Let us examine a direct consequence. Suppose that the system is now in contact with a thermostat. The partition function of the system is given by

$$Z = \text{Tr}[e^{-\beta H}] \quad (4.24)$$

where  $\text{Tr}$  denotes the trace, i.e. the sum over any complete basis of state. Note that here for the system to reach thermal equilibrium the Hamiltonian should be time independent. Using  $u$  as a complete basis, the partition function becomes

$$Z = \int du \langle u | e^{-\beta H} | u \rangle \quad (4.25)$$

One can thus formally split the temperature  $\beta$  into  $N$  segments of size  $\epsilon = \beta/N$  to get for the partition function

$$Z = \int du \int du_{N-1} \cdots \int du_2 \langle u | e^{-\epsilon H} | u_{N-1} \rangle \cdots \langle u_2 | e^{-\epsilon H} | u \rangle \quad (4.26)$$

One thus immediately recognize that (4.26) and (4.7) are identical except for two points: (i)  $u_f = u_i = u$  and one has to integrate over  $u$ ; (ii) more importantly instead of  $e^{-\frac{i}{\hbar}H\epsilon}$  one has  $e^{-H\epsilon} = e^{-\frac{1}{\hbar}H(\epsilon\hbar)}$ . Formally one has thus replaced the *it* in the exponential by a formal time  $\tau$  which in the end will run from 0 to  $\beta\hbar$ . This change is often denoted as going to imaginary time. One can follow the same steps than the one leading to (4.20) to get for the partition function

$$Z = \int du \int_{u(0)=u}^{u(\beta\hbar)=u} \mathcal{D}u(\tau) e^{-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau [\frac{m}{2} (\frac{du(\tau)}{d\tau})^2 + V(u(\tau))]} \quad (4.27)$$

The partition function (4.27) is thus the sum over all closed trajectories over a fictitious (imaginary) time  $\tau$ . Note that the argument in the exponential is indeed the continuation of the action to the imaginary time

$$i \int dt \mathcal{L}(t) \rightarrow \int d\tau \mathcal{L}(it \rightarrow \tau) \quad (4.28)$$

Note that contrarily to the action in real time (4.21), the imaginary time action  $S_\beta$

$$S_\beta = \int_0^{\beta\hbar} d\tau [\frac{m}{2} (\frac{du(\tau)}{d\tau})^2 + V(u(\tau))] \quad (4.29)$$

is a positive form. The integral in imaginary time (4.27) thus does not pose any problem of convergence. This is one of the advantages of the imaginary time.

As for the real time there is an equivalent ‘‘Hamiltonian’’ representation where one does not integrate over  $p$

$$Z = \int \mathcal{D}u(\tau) \mathcal{D}p(\tau) e^{\frac{1}{\hbar} [i \int_0^{\beta\hbar} d\tau p (\frac{du(\tau)}{d\tau}) - \int_0^{\beta\hbar} d\tau H[p(\tau), u(\tau)]]} \quad (4.30)$$

From now on, in order to lighten the notations we will set  $\hbar = 1$ . The  $\hbar$  is the various formulas can be put back by dimensional analysis.

## 4.2 Correlation functions; Matsubara frequencies

We have seen as one can compute the partition function of a *quantum* system through function integrals. The expression (4.27), thus immediately prompts for the question of correlation functions, analogous to (2.5)

$$\langle O(\tau_1) O(\tau_2) \cdots O(\tau_p) \rangle = \frac{\int_{u(0)=u(\beta)} \mathcal{D}u(\tau) e^{-S_\beta} O(\tau_1) O(\tau_2) \cdots O(\tau_p)}{\int_{u(0)=u(\beta)} \mathcal{D}u(\tau) e^{-S_\beta}} \quad (4.31)$$

where the  $O(\tau_i)$  are some functions of the  $u(\tau_i)$ . Note that as for classical systems the correlation function (4.31) can be defined directly through derivative of a partition function as in (2.8). One can already note many similarities between the partition function of a quantum system computed through path integrals and the ones of classical systems. There are indeed deep connections that will be explored in details in Section 4.4

The important question is of course the meaning of such a correlation function (4.31). Note that although we discuss here mostly the imaginary time case, a similar question can be asked for equivalent correlation functions with the real time action. To understand its meaning let us go back to our quantum system. If we start from a certain state  $|\psi(t=0)\rangle$  we can have an operator  $O_1$  acting on the state at time  $t_1$ .

$$O_1 |\psi(t_1)\rangle = O_1 U(t_1, 0) |\psi(t=0)\rangle \quad (4.32)$$

we can let this new state evolve until time  $t_2$  and then apply an operator  $O_2$ . The result is a new state

$$O_2 U(t_2, t_1) O_1 U(t_1, 0) |\psi(t=0)\rangle \quad (4.33)$$

and so on if we want to have  $p$  operators acting at time  $t_1, t_2, \dots, t_p$  (let us limit ourselves to  $p=2$  for this example). Thus (4.33) represent the state starting from  $|\psi(t=0)\rangle$  and whose evolution in time has been modified by the application of the operators  $O_1$  and  $O_2$  at time  $t_1$  and  $t_2$ . We could want to see how this state compares with the evolution of  $|\psi(t=0)\rangle$  at time  $t_2$  in the absence of application of any operator. The result is

$$\begin{aligned} & \langle \psi(t=0) | U^\dagger(t_2, 0) O_2 U(t_2, t_1) O_1 U(t_1, 0) | \psi(t=0) \rangle \\ & \langle \psi(t=0) | U(0, t_2) O_2 U(t_2, t_1) O_1 U(t_1, 0) | \psi(t=0) \rangle \end{aligned} \quad (4.34)$$

An alternative representation for (4.34) is to use the Heisenberg representation, where the states are time independent and the operators evolve with time according to (for a time independent Hamiltonian)

$$\widehat{O}_1(t) = e^{iHt} O_1 e^{-iHt} \quad (4.35)$$

where we denote by  $\widehat{O}_1(t)$  the operator in Heisenberg representation. (4.34) obviously become (for  $t_2 > t_1$ )

$$\langle \psi(t=0) | \widehat{O}_2(t_2) \widehat{O}_1(t_1) | \psi(t=0) \rangle \quad (4.36)$$

Let us consider the analytical continuation to imaginary time of the operators in Heisenberg representation

$$\widetilde{O}_1(\tau) = e^{\tau H} O_1 e^{-\tau H} \quad (4.37)$$

Note that now contrarily to the real time  $[\widetilde{O}(\tau)]^\dagger \neq \widetilde{O}^\dagger(\tau)$ . One could compute

$$\frac{\text{Tr}[e^{-\beta H} \widetilde{O}_2(\tau_2) \widetilde{O}_1(\tau_1)]}{\text{Tr}[e^{-\beta H}]} \quad (4.38)$$

but this expression is unusable since the operators in general do not commute. Let us use again our time ordering operator  $T$ , applied now to imaginary time. Let us assume that all  $\tau \in [0, \beta]$  and define  $T_\tau$  in a similar way than (4.10),

$$T(\widetilde{O}(\tau_1) \widetilde{O}(\tau_2)) = \theta(\tau_1 - \tau_2) \widetilde{O}(\tau_1) \widetilde{O}(\tau_2) + \theta(\tau_2 - \tau_1) \widetilde{O}(\tau_2) \widetilde{O}(\tau_1) \quad (4.39)$$

and compute

$$\frac{\text{Tr}[e^{-\beta H} T_\tau(\widetilde{O}_2(\tau_2) \widetilde{O}_1(\tau_1))]}{\text{Tr}[e^{-\beta H}]} \quad (4.40)$$

The denominator is simply the partition function  $Z$ . Because of the time ordering operator, one can rearrange the operators in (4.40) as

$$\text{Tr}[e^{-(\beta-\tau_2)H} O_2 e^{-(\tau_2-\tau_1)H} O_1 e^{-\tau_1 H}] \quad \tau_2 > \tau_1 \quad (4.41)$$

$$\text{Tr}[e^{-(\beta-\tau_1)H} O_1 e^{-(\tau_1-\tau_2)H} O_2 e^{-\tau_2 H}] \quad \tau_1 > \tau_2 \quad (4.42)$$

Using  $|u\rangle$  as a complete basis one can rewrite (4.41) as (for example for  $\tau_2 > \tau_1$ )

$$\int du \int du_2 \int du_1 \langle u | e^{-(\beta-\tau_2)H} | u_2 \rangle \langle u_2 | O_2 e^{-(\tau_2-\tau_1)H} | u_1 \rangle \langle u_1 | O_1 e^{-\tau_1 H} | u \rangle \quad (4.43)$$

If the operators  $O$  are functions of  $u$

$$O|u\rangle = O(u)|u\rangle \quad (4.44)$$

Thus we can rewrite (4.43) as

$$\int du \int du_2 \int du_1 O_2(u_2) O_1(u_1) \langle u | e^{-(\beta-\tau_2)H} | u_2 \rangle \langle u_2 | e^{-(\tau_2-\tau_1)H} | u_1 \rangle \langle u_1 | e^{-\tau_1 H} | u \rangle \quad (4.45)$$

Now each matrix element in (4.45) can be written as a functional integral as before. For example

$$\langle u_2 | e^{-(\tau_2-\tau_1)H} | u_1 \rangle = \int_{u(\tau_1)=u_1}^{u(\tau_2)=u_2} \mathcal{D}u[\tau] e^{-\int_{\tau_1}^{\tau_2} d\tau \mathcal{L}(\tau)} \quad (4.46)$$

This gives for (4.45)

$$\begin{aligned} I &= \int du \int du_1 \int du_2 O_2(u_2) O_1(u_1) \int_{u(\tau_2)=u_2}^{u(\beta)=u} \mathcal{D}u[\tau] \int_{u(\tau_1)=u_1}^{u(\tau_2)=u_2} \mathcal{D}u'[\tau] \int_{u(0)=u}^{u(\tau_1)=u_1} \mathcal{D}u''[\tau] \\ &\quad e^{-\int_{\tau_2}^{\beta} d\tau \mathcal{L}(u(\tau))} e^{-\int_{\tau_1}^{\tau_2} d\tau \mathcal{L}(u'(\tau))} e^{-\int_0^{\tau_1} d\tau \mathcal{L}(u''(\tau))} \\ &= \int_{u(0)=u(\beta)} \mathcal{D}u[\tau] O_2(u(\tau_2)) O_1(u(\tau_1)) e^{-\int_0^{\beta} d\tau \mathcal{L}(u(\tau))} \end{aligned} \quad (4.47)$$

which is obviously the same as (4.31). Thus the correlation functions obtained through the functional integral have a very natural interpretation in terms of operators. They are the average of the operators acting at time  $\tau_1$ ,  $\tau_2$  etc. The order in which the operators have to be taken is given by the time ordering. The fact that the correspondance between functional integrals and operators has to involve some specification to order is the operator is obvious from the fact that a path integral only involves numbers so that everything is independent of order in the path integral.

The path integrals are thus an extremely convenient way to obtain directly the time ordered correlation functions in imaginary time. Note that similar considerations can be done for the real time, with similar prescription in real time *provided* that the Hamiltonian is time independent. The case of a time dependent Hamiltonian is more complicated, and we will address this issue in Section 7.

The fact that correlation functions computed through functional integral correspond to something in the operator representation is of course good news ! The bad one, is that the said correlation function has absolutely no physical significance. The imaginary time is a purely formal index that has no direct correspondance to the real time. Fortunately as we will see in Section 5.2 the imaginary time correlation functions are easily related to physical objects through an analytical continuation.

Since we have now the correlation functions, let us examine some of their properties. The functional integral sums over all functions  $u$  that satisfies  $u(0) = u(\beta)$ . One can thus view the system as having *periodic* boundary conditions along the imaginary time direction as shown on Figure 4.2 This means that all correlation functions can be also viewed as *periodic* functions on the interval  $[0, \beta]$ . The Fourier transform as a function of time of the correlation functions

$$G(i\omega_n) = \int_0^{\beta} d\tau e^{i\omega_n \tau} G(\tau) \quad (4.48)$$

$$G(\tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} G(i\omega_n) \quad (4.49)$$

is performed over a *discrete* set of frequencies  $\omega_n = 2\pi n/\beta$ . These are called the Matsubara frequencies. The notation  $G(i\omega_n)$  is there to recall that one is working with frequencies associated with imaginary time.

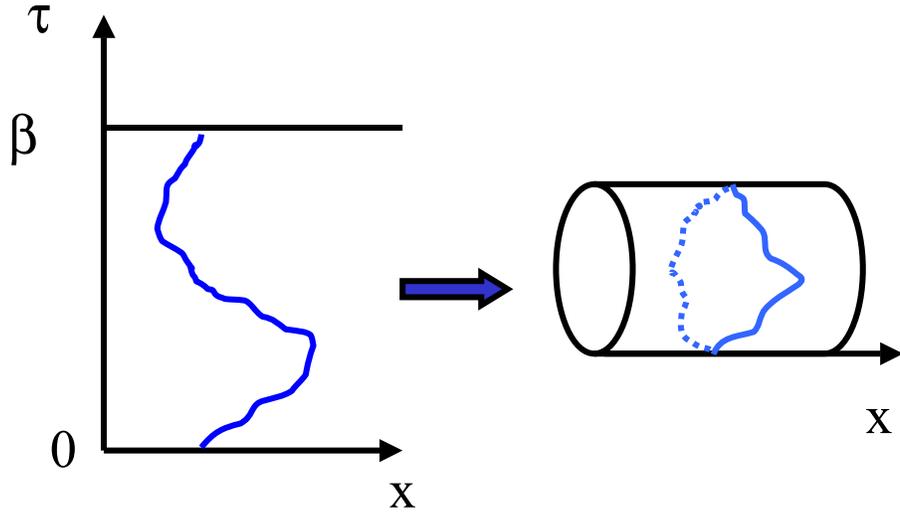


Figure 4.2: Since the functional integral is on periodic trajectories such that  $u(\beta) = u(0)$ , it is equivalent to consider that the system is defined on a torus whose circumference is  $\beta$ .

Even if most of the correlation functions in imaginary time do not have direct physical significance, a notable exception are the correlation functions for  $\omega_n = 0$ . Indeed if one adds to the Hamiltonian a time *independent* perturbation, this give in the lagrangian

$$\mathcal{L}_{\text{pert}} = - \int_0^\beta d\tau \int dx h(x) O(x, \tau) = - \int dx h(x) O(x, \omega_n = 0) \quad (4.50)$$

where  $O$  is as usual some operator of depending on  $u$ . Thus one can perform linear response as in Section 2.2 to find that

$$\langle O(x) \rangle = \int dx' \chi(x, x') h(x') \quad (4.51)$$

It is easy to see that because of the time invariance of the Hamiltonian only the  $\omega_n = 0$  component can be nonzero in (4.51). Since the hamiltonian is time invariant

$$\begin{aligned} \langle O(x) \rangle &= \frac{1}{\beta} \int_0^\beta d\tau \langle O(x, \tau) \rangle \\ &= \frac{1}{\beta} \langle O(x, \omega_n = 0) \rangle \end{aligned} \quad (4.52)$$

Thus the susceptibility is given by

$$\beta \chi(x, x') = \langle O(x, \omega_n = 0) O(x', \omega_n = 0) \rangle - \langle O(x, \omega_n = 0) \rangle \langle O(x', \omega_n = 0) \rangle \quad (4.53)$$

This formula allows for the calculation of most of the thermodynamic properties of the system.

### 4.3 Many degrees of freedom: example of the elastic system

So far we have only considered the case of a single quantum particle. How can we extend the analysis of the previous section to a many body problem. In principle this is very easy, we just introduce a

complete basis for the  $N$  particles  $|u_1, u_2, u_3, \dots, u_N\rangle$ , and repeat all the steps of the previous section. This will obviously lead to the same expressions. In fact there is a catch, although this procedure is obviously correct if the particles are discernables in some way, for the case of indiscernables particles, this will not work. Indeed in that case one should only consider wavefunctions that are either totally symmetric or antisymmetric (depending on whether one has bosons or fermions). Imposing this restriction in first quantization leads to rather untractable expressions, and one has to use second quantization. Establishing the functional integral in that case is more complicated and goes beyond the scope of this course. We will come back to this at the end of this section.

Let us focus to a case where the particles, although quantum are still discernables. A relevant example is again provided by an elastic system. Let us imagine a crystal of quantum particles (either fermions or bosons). If the system can be described by an elastic energy it means that each particle has a label (corresponding to its equilibrium position in the crystal), and is thus discernable. All the results of the previous sections can be applied. The Hamiltonian of the system is (on a lattice)

$$H = \sum_i \left[ \frac{\Pi_i^2}{2M} + \frac{1}{2} k (u_{i+1} - u_i)^2 \right] \quad (4.54)$$

which is the standard phonon Hamiltonian.  $u$  has the dimension of a distance,  $k$  is an energy divided by a distance squared ( $E/L^2$ ).  $\Pi_i$  is the conjugate momentum to  $u_i$ . We go to the continuum limit. We want to keep the dimensions of  $u$  as a distance. Thus  $u_i \rightarrow u(r)$  and  $\Pi_i \rightarrow a^d \Pi(r)$  in order to ensure that the continuum variables  $u(r)$  and  $\Pi(r)$  are canonically conjugate, i.e.

$$[u(r), \Pi(r')] = i\hbar \delta(r - r') \quad (4.55)$$

If we use  $\rho_0 = 1/a^d$  which is the density of particles, the Hamiltonian becomes (using  $\sum_i = \int d^d r \rho_0$ )

$$H = \int d^d r \left[ \frac{\Pi(r)^2}{2M\rho_0} + \rho_0 \frac{1}{2} c (\nabla u(r))^2 \right] \quad (4.56)$$

where  $c = ka^2$  has now the dimension of an energy.  $\Pi(r)$  is a momentum density. This leads to the action in imaginary time

$$S = \int d\tau \int d^d r \rho_0 \left[ \frac{1}{2} M (\partial_\tau u(r, \tau))^2 + \frac{1}{2} c (\partial_r u(\tau, r))^2 \right] \quad (4.57)$$

The action of the system can be written in Fourier space

$$S = \frac{1}{2} \frac{1}{\Omega} \sum_q \frac{1}{\beta} \sum_n \rho_0 [M\omega_n^2 + cq^2] u(q, \omega_n) u^*(q, \omega_n) \quad (4.58)$$

Let us use this formula to compute the compressibility of the quantum system. Using (4.53) it is simply given by

$$\chi = \frac{1}{\Omega\beta} \langle \rho(q, \omega_n = 0) \rho(-q, \omega_n = 0) \rangle \quad (4.59)$$

and using (2.96) this leads to

$$\begin{aligned} \chi &= \frac{\rho_0^2 q^2}{\Omega\beta} \langle u(q, \omega_n = 0) u^*(q, \omega_n = 0) \rangle \\ &= \frac{\rho_0 q^2}{M\omega_n^2 + cq^2} \Big|_{\omega_n=0} \\ &= \frac{\rho_0}{c} \end{aligned} \quad (4.60)$$

Finally, even if we do not treat the case fully let us give some hints of the structure of the functional integral for undiscernable quantum particles. Because of the indiscernable character of the particles it is useful to work directly in second quantization. The Hamiltonian is expressed in term of the creation and destruction operators  $c^\dagger$  and  $c$ . For example

$$K = H - \mu N = \sum_k (\epsilon_k - \mu) b_k^\dagger b_k \quad (4.61)$$

where we work in the presence of a fixed chemical potential  $\mu$ . One would like to build a functional integral similar to the expression (4.22), where we take for  $u$  the destruction operator  $c$ . To find the equivalent of the “conjugate momentum” for the destruction operator we can recall that for bosonic systems

$$[b, b^\dagger] = 1 \quad (4.62)$$

and thus  $b^\dagger$  is essentially, up to a factor of  $i$  the conjugate momentum. Recalling that  $[x, P] = i\hbar$  one can take formally  $P = ib^\dagger$ .

Thus using (4.30), and the expression for  $P$ , the action to put in the functional integral becomes

$$S = \int_0^\beta d\tau \sum_k \eta_k^*(\tau) [-\partial_\tau - (\epsilon_k - \mu)] \eta_k(\tau) \quad (4.63)$$

$$= \sum_{\omega_n, k} (i\omega_n - (\epsilon_k - \mu)) \eta_{k, i\omega_n}^\dagger \eta_{k, i\omega_n} \quad (4.64)$$

The symmetry condition on the bosons wavefunctions imposes again that  $\omega_n = 2\pi n/\beta$ . One can thus easily compute the boson Green’s function out of the functional integral

$$G(k, \tau) = -\langle T_\tau b(\tau) b^\dagger(0) \rangle \quad (4.65)$$

Its Fourier transform is given by

$$G(k, i\omega_n) = \frac{1}{i\omega_n - (\epsilon_k - \mu)} \quad (4.66)$$

Of course the precise demonstration of the above machinery requires more work. In particular one needs to define the eigenstates of the destruction operators (the so called coherent states) and I refer the reader to [3] for more details.

Fermion systems are more complicated since the creation and destruction operator anticommute, and thus the above procedure fails. It is however possible to formally define a similar functional integral if one does not integrate over numbers, but over quantities called Grassman numbers that have the property that two such numbers obey  $ab = -ba$ . Formally the structure remains the same and the “action” of the system is again given by (4.63), and in particular the Green’s function (4.66) is identical. However because of the antisymmetry of the fermionic wave function, one must now ensure that  $\psi(\tau + \beta) = -\psi(\tau)$  thus  $\omega_n = \frac{\pi}{\beta}(2n + 1)$ .

## 4.4 Link with classical problems

As we have already noticed the functional expression for a quantum system in imaginary time looks remarkably similar to the ones for a classical system for which the time  $\tau$  would play the role of an

System	Quantum	Classical
Dimension	$d$	$d+1$
$\beta$	Temperature	Size of system in direction $z$
$\hbar$	quantum fluctuations	Temperature

Table 4.1: Equivalence between a quantum system of dimension  $d$  and a classical system in dimension  $d + 1$ .

extra dimension. This identification allows for a deep connection between the physics of a quantum system in  $d$  dimensions and the one of a classical system in  $d + 1$ . Indeed let us compare for example a quantum system in  $d$  dimension whose Hamiltonian is given by (4.56). Its action is given by (see (4.57) (where we have put back the  $\hbar$ ):

$$S_\beta = \int_0^{\beta\hbar} d\tau \int d^d r \rho_0 \left[ \frac{1}{2} M (\partial_\tau u(r, \tau))^2 + \frac{1}{2} c (\partial_r u(\tau, r))^2 \right] \quad (4.67)$$

and the partition function is given by

$$Z = \int \mathcal{D}u[r, \tau] e^{-\frac{1}{\hbar} S_\beta} \quad (4.68)$$

One easily sees that (4.67-4.68) are exactly identical to the ones of a *classical* system in  $d+1$  dimensions. The extra dimension (which for the classical system we denote  $z$ ) is of a *finite size*  $\beta\hbar$ . The Hamiltonian of the classical system is given by

$$H = \int d^d r d_0^{\beta\hbar} \tau \rho_0 \left[ \frac{1}{2} M (\partial_z u(r, z))^2 + \frac{1}{2} c (\partial_r u(r, z))^2 \right] \quad (4.69)$$

The equivalent of the temperature for the classical system in (4.68) is played by  $\hbar$ . One has thus the correspondance between the classical and quantum system summarized in table 4.1

This remarkable equivalence has several important consequences. Let us mention some of them (the list is only limited by your imagination)

It is sometimes useful, when dealing with a classical or a quantum system to investigate its quantum or classical equivalent. Although the two problems are identical one formalism (classical or quantum) can be more adapted to solve it (or realize that the problem has already been solved by someone else). Very often classical problems are more easy to solve numerically, and one can use the equivalence to obtain from the solution of the associated quantum problem.

We have a good physical intuition of the phase transitions that take place in a classical system. Since the temperature of the classical system is  $\hbar$ , i.e. the degree of quantumness (or equivalently one parameter in the Hamiltonian) of the quantum problem we see that a *quantum* phase transition can also take place in the quantum problem when some parameter is varied in the Hamiltonian. If the quantum Hamiltonian has a continuous symmetry, then since the size in the classical problem in  $z$  is given by  $\beta$  it means that for example a  $d = 2$  quantum problem can have a quantum phase transition only at  $\beta = \infty$  since in that case it corresponds to a classical three dimensional problem. At finite  $\beta$  the classical problem is effectively two dimensional at large lengthscales and no ordered state that breaks a continuous symmetry can exist. Similarly for the breaking of a discrete symmetry a  $d = 1$  quantum system can have a quantum phase transition at  $T = 0$ . At finite temperature no ordered state can exist. We also see that as for classical phase transition, the quantum phase transition will be in general

characterized by a divergent length  $\xi$  and critical exponents. There is however an important difference when compared with classical systems. In classical problems the space is in general isotropic, thus the correlation length should in general have the same critical exponents in *all* spatial directions. For the quantum problem the *time* plays a special role, so that the direction  $z$  in the associated quantum problem has in general a *different* critical exponent than the true spatial directions. So if one assumes that

$$\xi \sim t^{-\nu} \tag{4.70}$$

where  $t = |1 - T/T_c|$  is the deviation to criticality in the classical problem and  $\nu$  the standard critical exponent we can define a divergent length along the  $z$  (or  $\tau$ ) direction as

$$\xi_\tau \sim t^{-\nu z} \tag{4.71}$$

where  $z$  is the so called dynamical exponent. This is the power that allows to relate time and space. For example for the action (4.57) the energy varies as

$$\omega_n^2 + k^2 \tag{4.72}$$

or equivalently  $\omega = ck$  where  $c$  is some velocity. Thus space and time have the same scaling and  $z = 1$ . If we had had an energy such that  $(\nabla u)^2$  was replaced by  $(\nabla u)^4$ . Then  $\omega \sim ck^2$ . In that case  $\tau \sim L^2$  which means that if a length diverges as  $t^{-\nu}$  a time should diverge as  $t^{-2\nu}$  and thus  $z = 2$ . Similarly for the bosonic functional integral (4.63)  $\omega \sim ck^2$  and  $z = 2$ . Except for the introduction of this new exponent, the quantum phase transitions behave quite as their classical equivalents. In particular they obey scaling relations among the exponents.

Finally one can notice that for quantum phase transitions one is naturally led to solve for the problem of systems on a torus as shown in Figure 4.2, for which some of the dimensions are essentially infinite while the time direction is of size  $\beta$ . It would thus be very interesting to know the correlation functions in such a special geometry. If  $\beta = \infty$  the system is infinite in all directions and has in general a critical point, at which the correlation functions decay as power law of the distance. An interesting question is how this power law is modified when one goes to a finite  $\beta$ . Fortunately, for two dimensional classical systems, it is possible to answer this question directly, using the fact that the correlation functions of the infinite system at criticality are in fact invariant not only by rotations and rescaling but by all conformal transformations (i.e. transformations that preserve angles) of the plane. It means that if one knows the correlation function of the infinite system, one can deduce via a conformal transformation the correlation function of the system on a torus. Going into the details of this powerful method would take us too far for this course, and I refer the readers to [9] for more details on that point.

# Chapter 5

## Perturbation; Linear response

### 5.1 Method

Let us now turn for the quantum problem to the same type of questions than we looked at for the classical ones in Section 2.2. We add to the Hamiltonian of the system a perturbation, a priori time and space dependent

$$H_{\text{pert}} = \int dx h(x, t) O(x) \quad (5.1)$$

where  $h(x, t)$  is some external field (magnetic field, electric field, pressure, etc.), and  $O(x)$  the operator to which it couples (magnetization, current, density, etc.). As for the classical systems we choose  $O$  such that in the absence of perturbation its average is zero  $\langle O(x) \rangle = 0$ , since one can always subtract this average value. Since the Schroedinger equation give the time evolution of the quantum system, we are now in a position to compute the response to a *time dependent* perturbation. This was not possible for the statistical problem, since the statistical equilibrium itself does not define the time evolution of a system. We will come back to this point in Section 7.

As for the classical problem computing the full response is hopeless so we will get the linear part of the response.

$$\langle O(x_0, t_0) \rangle \simeq \int dx dt \chi(x_0 - x, t_0 - t) h(x, t) \quad (5.2)$$

Note that here  $t$  denotes the real (true) time of the system.

To compute the response we have first to define what the average means with a time dependent Hamiltonian. To do so we introduce the density matrix  $\rho(t)$  and define the average at time  $t$  as

$$\langle A \rangle_t = \text{Tr}[\rho(t)A] \quad (5.3)$$

If the Hamiltonian is time independent the density matrix is thus just

$$\rho = \frac{1}{Z} e^{-\beta H} \quad (5.4)$$

To determine the time evolution we consider that on an eigenbasis the density matrix is simply given by

$$\rho = \sum_n c_n |n\rangle \langle n| \quad (5.5)$$

if  $|n\rangle$  are the energy eigenstates  $c_n = e^{-\beta E_n} / \sum_n e^{-\beta E_n}$ . We assume that the time evolution is solely given by the evolution of the wavefunctions. This amounts to say that the coefficients  $c_n$  are not

changing as the system is evolving with time, and thus the populations of the levels. The time evolution is thus supposed to be adiabatic. In other words the thermal bath is introduced at a given time when the perturbation does not exist (let us say  $t = -\infty$ ) and the levels are populated according to the (time independent) distribution  $e^{-\beta E_n}$ . The thermal bath is then removed and the perturbation switched on slowly, so that the wavefunction evolves. Using the Schroedinger equation and (5.5) it is easy to show that

$$\frac{\partial \rho(t)}{\partial t} = -i[H(t), \rho(t)] \quad (5.6)$$

To obtain the linear response we consider that  $\rho(t) = \rho_0 + f(t)$  where  $f(t)$  is the part proportional to perturbation  $h$ . Keeping only the linear terms, (5.6) becomes

$$i \frac{\partial f(t)}{\partial t} = [H_0, \rho_0] + [H_0, f(t)] + [H_{\text{pert}}, \rho_0] \quad (5.7)$$

Since  $\rho_0 = \frac{1}{Z_0} e^{-\beta H_0}$ , one has  $[H_0, \rho_0] = 0$ . One can transform (5.7) into

$$e^{-iH_0 t} \left[ i \frac{\partial}{\partial t} \left( e^{iH_0 t} f(t) e^{-iH_0 t} \right) \right] e^{iH_0 t} = [H_{\text{pert}}(t), \rho_0] \quad (5.8)$$

One can introduce, the Heisenberg representation of the operators

$$\hat{A} = e^{iH_0 t} A e^{-iH_0 t} \quad (5.9)$$

Using this representation (5.8) becomes

$$i \frac{\partial}{\partial t} \left( e^{iH_0 t} f(t) e^{-iH_0 t} \right) = [\hat{H}_{\text{pert}}(t), \rho_0] \quad (5.10)$$

Beware that since  $H_{\text{pert}}$  is already time dependent the time dependence in  $\hat{H}$  has two origins. (5.10) is easily integrated, using the fact that the perturbation is absent at time  $t = -\infty$  and thus  $f(-\infty) = 0$  to give

$$f(t) = -i e^{-iH_0 t} \int_{-\infty}^t dt' [\hat{H}_{\text{pert}}(t'), \rho_0] e^{iH_0 t'} \quad (5.11)$$

Note that because of the explicit time dependence of  $H_{\text{pert}}$

$$e^{-iH_0 t} \hat{H}_{\text{pert}}(t') e^{iH_0 t} \neq \hat{H}_{\text{pert}}(t' - t) \quad (5.12)$$

Using (5.11) we can now compute the average values

$$\langle A(t) \rangle = \text{Tr}[(\rho_0 + f(t))A] \quad (5.13)$$

Let us choose for simplicity an operator whose average value in the absence of perturbation is zero (otherwise one can simply subtract the average value). In that case

$$\begin{aligned} \langle A(t) \rangle &= \text{Tr}[A f(t)] \\ &= -i \text{Tr} \left[ \int_{-\infty}^t dt' e^{-iH_0 t} [\hat{H}_{\text{pert}}(t'), \rho_0] e^{iH_0 t} A \right] \end{aligned} \quad (5.14)$$

Using the cyclic invariance of the Trace  $\text{Tr}[ABC \cdots D] = \text{Tr}[BC \cdots DA]$  one obtains

$$\begin{aligned} \langle A(t) \rangle &= -i\text{Tr}\left[\int_{-\infty}^t dt' [\hat{H}_{\text{pert}}(t'), \rho_0] e^{iH_0 t} A e^{-iH_0 t'}\right] \\ &\quad -i\text{Tr}\left[\int_{-\infty}^t dt' [\hat{H}_{\text{pert}}(t'), \rho_0] \hat{A}(t)\right] \end{aligned} \quad (5.15)$$

Using (5.1) one gets

$$\langle A(t) \rangle = -i\text{Tr}\left[\int_{-\infty}^t dt' \int dx' [\hat{O}(t', x'), \rho_0] \hat{A}(t) h(x', t')\right] \quad (5.16)$$

Using

$$\text{Tr}[[A, B]C] = \text{Tr}[ABC - BAC] = \text{Tr}[B[C, A]] \quad (5.17)$$

one can rewrite (5.16) as

$$\begin{aligned} \langle A(t) \rangle &= -i\text{Tr}[\rho_0 \int_{-\infty}^t dt' \int dx' [\hat{A}(t), \hat{O}(t', x')]] h(x', t') \\ &= -i \int_{-\infty}^t dt' \int dx' \langle [\hat{A}(t), \hat{O}(t', x')] \rangle_0 h(x', t') \end{aligned} \quad (5.18)$$

where  $\langle \rangle_0$  denotes averages taken with the unperturbed Hamiltonian  $H_0$ . It is thus convenient to define a so called retarded correlation function (quite generally we take a space dependent operator  $A(x)$ )

$$G_{A,O}^{\text{ret}}(x - x', t - t') = -i\theta(t - t') \langle [\hat{A}(t, x), \hat{O}(t', x')] \rangle_0 \quad (5.19)$$

Quite generally one thus has for the susceptibility (5.2)

$$\chi(x - x', t - t') = G_{A,O}^{\text{ret}}(x - x', t - t') \quad (5.20)$$

The *retarded* correlation (also called Green's) function is thus the one that is physically observable. The  $\theta$  function is due to the causality and expresses the fact that a measure at time  $t$  can only depend on the perturbation at anterior times. Rather than working in space time, it is better to go to Fourier space. Indeed since  $H$  is time independent the Fourier transform of (5.2) will be diagonal

$$\langle O(q, \omega) \rangle = \chi(q, \omega) h(q, \omega) \quad (5.21)$$

with

$$\chi(q, \omega) = \int d^d r dt e^{-i(qr - \omega t)} \chi(r, t) \quad (5.22)$$

Using (5.19) gives

$$\begin{aligned} \chi(q, \omega) &= \int d^d r \int dt G_{A,O}^{\text{ret}}(r, t) e^{i\omega t - iqr} \\ &= -i \int d^d r \int_0^{+\infty} dt e^{i\omega t - iqr} \langle [\hat{A}(t, r), \hat{O}(0, 0)] \rangle_0 \end{aligned} \quad (5.23)$$

## 5.2 Analytical continuation

The retarded Green's functions are thus the one that one wants to compute since they describe the physical response of the system to an external perturbation. Unfortunately there is no systematic way of computing them directly. As we have seen in section 4.2 the correlation functions that have a simple expression in term of a functional integral (and thus that can be computed systematically, at least perturbatively) are the time ordered correlation functions. Fortunately, the two are easily related.

To see this let us express formally the correlation functions using the eigenstates of  $H$  that we denote  $|n\rangle$ . If we introduce the time ordered correlation function (see (4.40))

$$G(\tau) = -\langle T_\tau A(\tau) O(0) \rangle \quad (5.24)$$

(note that  $A$  and  $O$  can be dependent of  $r$  but that we will not write it explicitly to keep the notations simple). We can express it formally as (for e.g.  $\tau > 0$ )

$$\begin{aligned} G(r, \tau) &= -\frac{1}{Z} \sum_{n,m} \langle n | e^{-\beta H} A(\tau) | m \rangle \langle m | O(0) | n \rangle \\ &= -\frac{1}{Z} \sum_{n,m} \langle n | e^{-\beta H} e^{\tau H} A e^{-\tau H} | m \rangle \langle m | O | n \rangle \\ &= -\frac{1}{Z} \sum_{n,m} e^{-\beta E_n} e^{\tau(E_n - E_m)} \langle n | A | m \rangle \langle m | O | n \rangle \end{aligned} \quad (5.25)$$

The Fourier transform with Matsubara frequencies gives

$$\begin{aligned} G(i\omega_p) &= \int_0^\beta d\tau G(\tau) \\ &= -\frac{1}{Z} \sum_{n,m} e^{-\beta E_n} \langle n | A | m \rangle \langle m | O | n \rangle \frac{e^{\beta(i\omega_p + E_n - E_m)} - 1}{i\omega_p + E_n - E_m} \\ &= \frac{1}{Z} \sum_{n,m} \langle n | A | m \rangle \langle m | O | n \rangle \frac{e^{-\beta E_n} - e^{-\beta E_m}}{i\omega_p + E_n - E_m} \end{aligned} \quad (5.26)$$

A similar representation can be used with the retarded Green's functions

$$\begin{aligned} G^{\text{ret}}(t) &= -i\theta(t) \langle [\hat{A}(t), \hat{O}(0)] \rangle \\ &= -i\theta(t) \sum_n \langle n | e^{-\beta H} [\hat{A}(t), \hat{O}(0)] | n \rangle \\ &= -i\theta(t) \sum_{n,m} \langle n | e^{-\beta H} \hat{A}(t) | m \rangle \langle m | \hat{O}(0) | n \rangle - \langle n | e^{-\beta H} \hat{O}(0) | m \rangle \langle m | \hat{A}(t) | n \rangle \\ &= -i\theta(t) \sum_{n,m} e^{-\beta E_n} e^{it(E_n - E_m)} \langle n | A | m \rangle \langle m | O | n \rangle - e^{-\beta E_n} e^{it(E_m - E_n)} \langle n | O | m \rangle \langle m | A | n \rangle \\ &= -i\theta(t) \sum_{n,m} \langle n | A | m \rangle \langle m | O | n \rangle e^{it(E_n - E_m)} [e^{-\beta E_n} - e^{-\beta E_m}] \end{aligned} \quad (5.27)$$

The Fourier transform is

$$G^{\text{ret}}(\omega) = \int dt G^{\text{ret}}(t) e^{i\omega t} \quad (5.28)$$

Because of the  $\theta(t)$  factor in  $G^{\text{ret}}(t)$  the integral is effectively from  $t = 0$  to  $t = \infty$ . Because of the integration to  $t = \infty$  one has to make sure that the integral is convergent at large time. One way to do this is to add a small convergence factor to the fourier transform

$$G^{\text{ret}}(\omega) = \int_0^{+\infty} dt G^{\text{ret}}(t) e^{i(\omega+i\delta)t} \quad (5.29)$$

where  $\delta = 0^+$ . Note that this convergence factor has a physical interpretation. As we saw in order to compute the time dependence of the density matrix the way we did, we had to apply the perturbation adiabatically from  $t = -\infty$ . Thus  $h(t)$  was changed into  $h(t)e^{-\delta|t|}$  in order to ensure that the perturbation vanishes at  $t = -\infty$ . Thus the linear response relation (5.2) becomes

$$\begin{aligned} \langle O(x_0, t_0) \rangle &\simeq \int dx dt \chi(x_0 - x, t_0 - t) e^{\delta t} h(x, t) \\ &\simeq e^{\delta t_0} \int dx dt \chi(x_0 - x, t_0 - t) e^{-\delta(t_0-t)} h(x, t) \end{aligned} \quad (5.30)$$

One thus recovers an adiabatic response in which the susceptibility contains the factor  $e^{-\delta(t_0-t)}$  which is exactly the convergence factor that we used. Using (5.29) and (5.27) one gets

$$\begin{aligned} G^{\text{ret}}(\omega) &= -i \sum_{n,m} \langle n|A|m\rangle \langle m|O|n\rangle [e^{-\beta E_n} - e^{-\beta E_m}] \int_0^{+\infty} dt e^{i(\omega+i\delta)t} e^{it(E_m-E_n)} \\ &= \sum_{n,m} \langle n|A|m\rangle \langle m|O|n\rangle [e^{-\beta E_n} - e^{-\beta E_m}] \frac{1}{(\omega + i\delta + E_n - E_m)} \end{aligned} \quad (5.31)$$

Comparing (5.31) and (5.26) one easily sees that the Matsubara and retarded Green's functions are related through the analytic continuation

$$G^{\text{ret}}(\omega) = G^{\text{Matsubara}}(i\omega_n \rightarrow \omega + i\delta) \quad (5.32)$$

This is a quite remarkable formula since it allows us to compute physical observable directly from the path integral formulation. Note that it is quite natural to go from back from the imaginary time  $\tau = it$  by such a kind of analytic continuation. What is not obvious is the fact that the time ordered function give a correlation with a commutator in real time. The  $\omega + i\delta$  is not arbitrary and is due to the causality of the retarded correlation functions. Using (5.31) it is easy to show, since the eigenvalues  $E_{n,m}$  are real, that for a complex variable  $z$  the Green's function verifies the relation

$$G(z) = \frac{-1}{\pi} \int d\omega \frac{1}{z - \omega} \text{Im} G^{\text{ret}}(\omega) \quad (5.33)$$

In particular taking  $z = \omega + i\delta$  and the relation

$$\frac{1}{x + i\delta} = \mathcal{P} \frac{1}{x} - i\pi\delta(x) \quad (5.34)$$

where  $\mathcal{P}$  is the principal part, one gets the Kramers-Kroenig relation

$$\text{Re} G^{\text{ret}}(\omega) = \frac{-1}{\pi} \int d\omega' \mathcal{P} \frac{1}{\omega - \omega'} \text{Im} G^{\text{ret}}(\omega') \quad (5.35)$$

The causality and analytical properties of the Green's function thus imposes very strong constraints, and the knowledge of either the real or imaginary part is enough to completely determine the function. Such relations are useful since some experiments measure one or the other, but it is rare to be able to have the full function.

One also notes from (5.31) and (5.35) that when  $O = A^\dagger$  (which is usually the correlation function one is interested in),  $\text{Im}G(\omega)$  is an odd function of  $\omega$  whereas  $\text{Re}G(\omega)$  is an even function.

### 5.3 Fluctuation dissipation theorem

To get a complete physical understanding of the meaning of the susceptibility  $\chi$  let us examine the change of energy of the system. In the absence of an external perturbation the energy is conserved. This is not the case any more when the system is subject to a time dependent external potential, and some energy is injected in the system. The energy of the system at time  $t$  is given by

$$E(t) = \text{Tr}[\rho(t)H(t)] \quad (5.36)$$

and thus the change of energy is

$$\frac{dE(t)}{dt} = \text{Tr}[\rho(t)\frac{dH(t)}{dt}] + \text{Tr}[\frac{d\rho(t)}{dt}H(t)] \quad (5.37)$$

Using the equation of evolution (5.6) for  $\rho(t)$  one can rewrite the second term in (5.37) as

$$-i\text{Tr}[[H(t), \rho(t)]H(t)] = -i\text{Tr}[\rho(t)[H(t), H(t)] = 0 \quad (5.38)$$

using the cyclic invariance of the trace. Thus

$$\frac{dE(t)}{dt} = \text{Tr}[\rho(t)\frac{dH(t)}{dt}] = \langle \frac{dH(t)}{dt} \rangle \quad (5.39)$$

Let us consider a simple sinusoidal perturbation of the form

$$H_{\text{pert}} = Ohe^{i\omega t} + O^\dagger h^* e^{-i\omega t} \quad (5.40)$$

In that case

$$\frac{dE(t)}{dt} = i\omega[\langle O \rangle_t h e^{i\omega t} - \langle O^\dagger \rangle_t h^* e^{-i\omega t}] \quad (5.41)$$

Using linear response one has

$$\langle O(t) \rangle = \int dt' \chi_{OO}(t-t') h e^{i\omega t'} + \chi_{OO^\dagger}(t-t') h^* e^{-i\omega t'} \quad (5.42)$$

Rather than compute the change in energy at a given time, since we deal here with a sinusoidal perturbation we can average over one period (we assume  $\omega > 0$ )

$$\overline{\frac{dE(t)}{dt}} = \frac{1}{T} \int_0^{T=2\pi/\omega} dt \frac{dE(t)}{dt} \quad (5.43)$$

Using (5.41) and (5.42) one gets

$$\begin{aligned} \overline{\frac{dE(t)}{dt}} &= i\omega[\chi_{OO^\dagger}(\omega) - \chi_{O^\dagger O}(-\omega)] h h^* \\ &= \omega i[\chi_{OO^\dagger}(\omega) - \chi_{O^\dagger O}(-\omega)] h h^* \end{aligned} \quad (5.44)$$

Using the definition (5.23) one obtains

$$\begin{aligned} \chi(\omega)^* &= +i \int_0^{+\infty} dt \langle [O(t), O^\dagger(0)] \rangle^* e^{-i\omega t} \\ &= -i \int_0^{+\infty} dt \langle [O^\dagger(t), O(0)] \rangle e^{-i\omega t} \\ &= \chi(-\omega) \end{aligned} \quad (5.45)$$

as it should be for an hermitian operator. Thus (5.44) becomes

$$\begin{aligned}\frac{\overline{dE(t)}}{dt} &= \omega i h h^* [\chi_{OO^\dagger}(\omega) - \chi_{OO^\dagger}(\omega)^*] \\ &= -2\omega h h^* \text{Im} \chi_{OO^\dagger}(\omega)\end{aligned}\quad (5.46)$$

Thus the imaginary part of the susceptibility controls the dissipation of energy in the system. Using (5.31) one can write for the imaginary part

$$\begin{aligned}\text{Im} \chi_{OO^\dagger}(\omega) &= -\pi \sum_{n,m} \langle n|O|m\rangle \langle m|O^\dagger|n\rangle [e^{-\beta E_n} - e^{-\beta E_m}] \delta(\omega + E_n - E_m) \\ &= -\pi \sum_{n,m} |\langle n|O|m\rangle|^2 e^{-\beta E_n} (1 - e^{-\beta \omega}) \delta(\omega + E_n - E_m)\end{aligned}\quad (5.47)$$

Thus the imaginary part is always negative for  $\omega > 0$  leading to a positive dissipation as it should be.

Thus (5.23) relates the response of the system to an external perturbation (and thus the dissipation of the energy brought by this perturbation) to a correlation function of the system in equilibrium. This relation is known as the fluctuation-dissipation theorem. It is the analogous of what we saw for classical systems. It is a very strong relation since it relies on two quite general assumptions: (i) that we restrict to linear response; (ii) more importantly that the system is in thermodynamic equilibrium. Compared to the case we saw for classical systems, since here we have the equation of motion (the Schroedinger equation) and not just the condition for thermodynamic equilibrium, we are able to deal with time dependent perturbation as well.

## 5.4 Kubo formula

We already saw the example of the compressibility, given by the density-density correlation function. Another famous example is the conductivity of a system. Two ways can be used to compute it. The simplest derivation, far from being rigorous is to add to the Hamiltonian a perturbation similar to the one we used for the compressibility

$$H_{\text{pert}} = \int d^d r V(r, t) \delta \rho(r) \quad (5.48)$$

where  $\delta \rho = \rho - \rho_0$  is the density where we have subtracted the average value in the absence of the perturbation  $V$ . We can compute in linear response

$$\langle \delta \rho(q, \omega) \rangle = \chi(q, \omega) V(q, \omega) \quad (5.49)$$

where  $\chi(q, \omega)$  is the Fourier transform of the retarded Green's function

$$\langle \delta \rho(r, t); \delta \rho(0, 0) \rangle_{\text{ret}} = -i \theta(t) \langle [\delta \rho(r, t), \delta \rho(0, 0)] \rangle \quad (5.50)$$

As usual we compute first the correlation function in Matsubara frequencies and then perform the analytical continuation. If the Hamiltonian is invariant by translation, then it cannot couple different values of  $q$  and  $\omega$  and it is easy to see that the only non-zero component is

$$\langle \delta \rho(q, i\omega_n) \delta \rho(-q, -i\omega_n) \rangle \quad (5.51)$$

We will perform in section 6.1 the full calculation of the compressibility for the crystal case. For now let us focuss on the conductivity. This is the quantity giving the relation between the current  $j$  and the electric field  $E$  inside the system. The electric field is simply given by  $E = -\nabla V$ . To obtain the current one can use the continuity equation

$$\frac{\partial \rho(r, t)}{\partial t} + \nabla_r \cdot j(r, t) = 0 \quad (5.52)$$

This implies, when written in term of the Fourier transforms

$$i\omega \rho(q, \omega) = iq \cdot j(q, \omega) \quad (5.53)$$

The problem with this derivation is that  $j$  is a vector, but for the moment let us assume that  $j$  and  $q$  are aligned, in that case we can get from (5.49)

$$\begin{aligned} \langle j(q, \omega) \rangle &= \frac{\omega}{q} \chi(q, \omega) V(q, \omega) \\ &= \frac{\omega}{q} \chi(q, \omega) \frac{1}{-iq} E(q, \omega) \end{aligned} \quad (5.54)$$

This could be expressed in a more convenient way, using again the relation (5.53) as

$$\langle j(q, \omega) \rangle = \frac{i}{\omega} \langle j(q, \omega); j(-q, -\omega) \rangle_{\text{ret}} E(q, \omega) \quad (5.55)$$

The conductivity is thus simply given by the current-current correlation function.

The derivation given above is simple but suffers from various imprecisions. Let us now give a more rigorous derivation. Instead of adding a potential  $V$  to the Hamiltonian let us now consider the addition of a vector potential  $\mathcal{A}$ . For a time dependent potential vector

$$E(r, t) = -\frac{\partial \mathcal{A}(r, t)}{\partial t} \quad (5.56)$$

The vector potential is put in the Hamiltonian via the minimal substitution  $\Pi \rightarrow \Pi - qA$ , where  $A$  is the operator corresponding to the applied potential vector. The current is given by the functional derivative ( $\alpha = x, y, z$ )

$$j_\alpha(r, t) = -\frac{\partial H}{\partial \mathcal{A}_\alpha(r, t)} \quad (5.57)$$

For example for a single particle with a kinetic energy  $\Pi^2/(2M)$  the Hamiltonian in presence of the potential vector is

$$\frac{1}{2M} \sum_\alpha (\Pi_\alpha - q \int d^d r \mathcal{A}_\alpha(r, t) |r\rangle \langle r|)^2 \quad (5.58)$$

and the  $\alpha$  ( $\alpha = x, y, z$ ) component of the current is given by

$$j_\alpha(r, t) = \frac{q}{2M} [\Pi |r\rangle \langle r| + |r\rangle \langle r| \Pi] - \frac{q^2}{M} \mathcal{A}_\alpha(r, t) |r\rangle \langle r| \quad (5.59)$$

which is the standard quantum mechanical extension of  $j = q\rho v$  with  $v = (P - qA)/m$ . Thus the current itself contains the potential vector  $\mathcal{A}$ . If one wants the linear response in  $\mathcal{A}$  one should thus

expand both the current and the Hamiltonian. Let us call  $j^0 = j(A = 0)$ , i.e. the current in the absence of vector potential. For the quadratic kinetic energy (5.58) this is

$$j_\alpha^0(r, t) = \frac{q}{2M} [\Pi|r\rangle\langle r| + |r\rangle\langle r|\Pi] \quad (5.60)$$

At linear order in the vector potential, the average value of the current is thus given by

$$\langle j_\alpha(r, t) \rangle = \sum_\beta \int dr' dt' \frac{\partial \langle j_\alpha(r, t) \rangle}{\partial \mathcal{A}_\beta(r', t')} \mathcal{A}_\beta(r', t') \quad (5.61)$$

The derivative contains two terms, the explicit dependence of the current operator with the potential vector and the fact that in the average value the Hamiltonian contains the potential vector. The second contribution can be computed in linear response, since

$$H = H[A = 0] - \int dr \sum_\alpha j_\alpha^0(r) \mathcal{A}(r, t) \quad (5.62)$$

at linear order in  $\mathcal{A}$ . Thus

$$\langle j_\alpha(r, t) \rangle = \sum_\beta \int dr' dt' \left[ \left\langle \frac{\partial j_\alpha(r, t)}{\partial \mathcal{A}_\beta(r', t')} \right\rangle_{H[A=0]} - \langle j_\alpha^0(r, t); j_\beta^0(r', t') \rangle_{\text{ret}} \right] \mathcal{A}_\beta(r', t') \quad (5.63)$$

which can be rewritten

$$\langle j_\alpha(r, t) \rangle = \sum_\beta \int dr' dt' \left[ - \left\langle \frac{\partial^2 H}{\partial \mathcal{A}_\alpha(r, t) \partial \mathcal{A}_\beta(r', t')} \right\rangle_{A=0} - \langle j_\alpha^0(r, t); j_\beta^0(r', t') \rangle_{\text{ret}} \right] \mathcal{A}_\beta(r', t') \quad (5.64)$$

Since  $H$  is a function of  $\Pi - qA$  only differentiating with respect to  $A$  is the same than with respect to  $\Pi$ . One thus has

$$\left. \frac{\partial^2 H}{\partial \mathcal{A}_\alpha(r, t) \partial \mathcal{A}_\beta(r', t')} \right|_{A=0} = q^2 \frac{\partial^2 H}{\partial \Pi^2} \delta(r - r') \delta(t - t') \delta_{\alpha\beta} \quad (5.65)$$

As usual it is simpler to go to Fourier space. One has

$$\mathcal{A}_\alpha(q, \omega) = \frac{1}{i\omega} E_\alpha(q, \omega) \quad (5.66)$$

In fact since the perturbation is applied adiabatically, all  $\omega$  should be  $\omega + i\delta$  once again, but we will stick to the notation  $\omega$  to keep the notation simple. Thus the full conductivity matrix  $\sigma_{\alpha\beta}(q, \omega)$  relating the current to the electric field through

$$j_\alpha(q, \omega) = \sum_\beta \sigma_{\alpha\beta}(q, \omega) E_\beta(q, \omega) \quad (5.67)$$

is given by

$$\sigma_{\alpha\beta}(q, \omega) = \frac{1}{i\omega} [-\chi_{j_\alpha, j_\beta}(q, \omega) - e^2 \delta_{\alpha\beta} \langle \frac{\partial^2 H}{\partial \Pi^2} \rangle] \quad (5.68)$$

where the first term is the Fourier transform of the retarded current current correlation function

$$\chi_{j_\alpha, j_\beta}(r, t) = -i\theta(t) \langle [j_\alpha(r, t), j_\beta(0, 0)] \rangle \quad (5.69)$$

The second term is purely imaginary. It is called the diamagnetic term. For a simple quadratic Hamiltonian the diamagnetic term is simply

$$-\frac{ne^2}{i\omega M} \quad (5.70)$$

whereas if the kinetic energy comes from a tight binding Hamiltonian  $\epsilon(k) = -t \cos(k)$  one would have

$$\frac{1}{i\omega} \langle T \rangle \quad (5.71)$$

i.e. the average value of the Kinetic energy itself. The equation (5.68) is known as the Kubo formula. It is a very important special case of linear response since it allows to compute a transport property of the system. Because of the  $i\omega$  in the denominator the dissipation is now given by the real part of  $\sigma$ . The real part of the conductivity is thus totally given by the current-current correlation function. In order to get the uniform conductivity, one should first take the limit  $q \rightarrow 0$  keeping  $\omega$  finite. Then one can take the  $\omega \rightarrow 0$  limit to get the static conductivity. Note that this is a quite different procedure than the one used to obtain the thermodynamic response of the system. In that case it is important to take first  $\omega \rightarrow 0$  to have a static perturbation. This perturbation can have any wavevector  $q$ . This difference of limit is quite crucial, since as we just saw both the conductivity and the compressibility are given, up to factors of  $q$  and  $\omega$  by the same correlation function (i.e. density density or current current).

When the current commutes with the Hamiltonian the conductivity is easily computed. Physically this means that the current is conserved, and thus one naively expects the conductivity to be infinite. Because the current commutes with  $H$ , one has  $J(r, t) = J(r, 0)$ . Thus the commutator

$$\int dr [j_\alpha(r, t), j_\beta(0, 0)] = \int dr [j_\alpha(r, 0), j_\beta(0, 0)] = 0 \quad (5.72)$$

and thus the conductivity is totally given by the diamagnetic term. It is of the form

$$\sigma_{\alpha\beta}(q, \omega) = -\delta_{\alpha\beta} \frac{\mathcal{D}}{i(\omega + i\delta)} \quad (5.73)$$

where I have put back the small convergence factor in  $\omega$ . The conductivity is thus given by

$$\sigma_{\alpha\beta}(\omega) = \delta_{\alpha\beta} \mathcal{D} [\pi\delta(\omega) - i\mathcal{P}(\frac{1}{\omega})] \quad (5.74)$$

It is thus purely imaginary at any finite frequency and the static conductivity is infinite. Note that in that case one has obviously

$$\int_{-\infty}^{+\infty} \text{Re}\sigma_{\alpha\beta}(\omega) = \pi e^2 \langle \frac{\partial^2 H}{\partial \Pi^2} \rangle \quad (5.75)$$

This identity known as a sum rule is in fact true quite generally, even if the current does not commute with the Hamiltonian. It rest only on the fact that except for the kinetic energy the rest of the hamiltonian is a function of the density only (and not on  $\Pi$ ). It can be proven by looking at the spectral representation for the conductivity.

## 5.5 Scattering, Memory function

For a system for which the current commutes with the Hamiltonian, the conductivity is thus trivial. The difficulty is of course to compute it when there is some source of scattering present in the system and the current is not conserved any more. Ways of solving this problem depend on the particular nature of the problem and there is no general method. Naively one could imagine to try naive perturbation theory in the scattering coupling constant. However it is easy to see that the conductivity does not have any simple perturbative expansion in the scattering. Indeed the conductivity is infinite in the absence of scattering and expected to be finite when the scattering is finite, which is obviously non perturbative. Looking at the Drude result for the conductivity  $\sigma = ne^2\tau/m$  where  $\tau$  is the lifetime strongly suggest that the *resistivity* should have a well defined perturbation theory in the scattering. However no Kubo formula for the resistivity exists which makes it difficult to compute perturbatively.

An approximation to compute the conductivity tries to use this idea of a perturbative expansion for the resistivity. The idea is to notice that in a presence of a finite lifetime one would expect a conductivity of the form (Drude form)

$$\sigma(\omega) = \frac{iCste}{\omega + i/\tau} \quad (5.76)$$

One will thus rewrite the Kubo formula in this way. If the conductivity is non-infinite at zero frequency the Kubo formula (5.68) can be rewritten as

$$\sigma(\omega) = \frac{i}{\omega} [-\chi(\omega = 0) + \chi(\omega)] \quad (5.77)$$

where  $\chi$  is the retarded current-current correlation function which can be rewritten as

$$\sigma(\omega) = \frac{i\chi(0)}{\omega + M(\omega)} \quad (5.78)$$

with

$$M(\omega) = \frac{\omega\chi(\omega)}{\chi(0) - \chi(\omega)} \quad (5.79)$$

$M$  is known as the memory function. So far the transformation is exact. The approximation consist in computing  $M$  perturbatively in the scattering. If the scattering is zero,  $\chi(\omega) = 0$  for  $\omega$  finite. Thus at lowest order in the scattering *and* at *finite* frequency

$$\chi(0) - \chi(\omega) \sim \chi(0) \quad (5.80)$$

which is just the diamagnetic term. The numerator can be shown to be at least of order two in the scattering. Indeed integrating by part twice in  $\chi(\omega)$  leads to

$$-\omega\chi(\omega) = [\langle F; F \rangle_\omega - \langle F; F \rangle_{\omega=0}]/\omega \quad (5.81)$$

where the  $F$  operators take into account that the current is not a conserved quantity  $F = [j, H]$  and  $\langle F; F \rangle_\omega^0$  stands for the retarded correlation function of the operator  $F$  at frequency  $\omega$ . Since the  $F$  operators are proportional to the scattering, at the lowest order in the scattering the averages can be computed with the Hamiltonian  $H_0$  *in the absence* of scattering. Thus the memory function can be perturbatively computed as

$$M(\omega) = \frac{[\langle F; F \rangle_\omega^0 - \langle F; F \rangle_{\omega=0}^0]/\omega}{-\chi(0)} \quad (5.82)$$

Since the Hamiltonian in the absence of scattering is usually simple the averages can now be done. It is important to note that the expansion is perfectly controlled for a fixed frequency, when the scattering becomes small. The (uncontrolled) hope, is that the result will remain well behaved even in the opposite limit which is the one important experimentally, namely fixed scattering constant and frequency going to zero. Although it is of course not always the case, check on many examples shows that the method, which corresponds to a sort of hydrodynamics approximation is quite reliable.

# Chapter 6

## Examples

Now that we have the whole machinery working, let us try to apply it to some concrete situations.

### 6.1 Compressibility

To warm up we go back to the compressibility of the crystal, that we already computed in section 4.3. We start with the crystal Hamiltonian (4.56). The first step is to write the action in imaginary time. This was already done in (4.57) and (4.58). We want the compressibility, which is the response to the addition of

$$\delta H = - \int d^d r \mu(r) \delta \rho(r) \quad (6.1)$$

Given the conventions taken for the perturbation for the linear response (compare (6.1) with (5.1)), the compressibility will be given by minus the retarded density-density correlation function.

To obtain the retarded correlation function, we have first to compute the density-density correlation function in imaginary time (note the minus sign needed to obtain the proper analytical continuation as explained in Section 5.2).

$$\begin{aligned} \chi_{\rho\rho}(r, \tau) &= -\langle T_\tau \delta \rho(r, \tau) \delta \rho(0, 0) \rangle \\ &= -\frac{1}{(\Omega\beta)^2} \sum_{q_1, \omega_{n1}, q_2, \omega_{n2}} e^{i(q_1 r - \omega_{n1} \tau)} \langle \delta \rho(q_1, \omega_{n1}) \delta \rho(q_2, \omega_{n2}) \rangle \end{aligned} \quad (6.2)$$

Thus the Fourier transform is simply given by

$$\chi_{\rho\rho}(q, \omega_n) = -\frac{1}{(\Omega\beta)} \sum_{q_2, \omega_{n2}} \langle \delta \rho(q, \omega_n) \delta \rho(q_2, \omega_{n2}) \rangle \quad (6.3)$$

We ultimately want the uniform (i.e.  $q \rightarrow 0$ ) compressibility, thus we can use for the variation of the density

$$\delta \rho(r, t) = \rho(r, t) - \rho_0 = -\rho_0 \nabla u(r, t) \quad (6.4)$$

and thus

$$\delta \rho(q, \omega) = -\rho_0 (iq) u(q, \omega) \quad (6.5)$$

Using (2.71) and (4.58) one obtains

$$\langle u(q, \omega_n) u^*(q_2, \omega_{n2}) \rangle = \frac{\beta \Omega}{\rho_0 (M \omega_n^2 + c q^2)} \delta_{q, q_2} \delta_{\omega_n, \omega_{n2}} \quad (6.6)$$

And thus

$$\chi_{\rho\rho}(q, \omega_n) = -\frac{\rho_0 q^2}{M\omega_n^2 + cq^2} \quad (6.7)$$

To obtain the retarded function we now make the analytical continuation. The susceptibility is

$$\chi(q, \omega) = -\chi_{\rho\rho}^{\text{ret}}(q, \omega) = -\chi_{\rho\rho}(q, i\omega_n)|_{i\omega_n \rightarrow \omega + i\delta} \quad (6.8)$$

This gives

$$\chi(q, \omega) = \frac{\rho_0 q^2}{-M(\omega + i\delta)^2 + cq^2} \quad (6.9)$$

In order to get the compressibility one has first to take the  $\omega = 0$  limit and thus one recovers

$$\kappa = \frac{\rho_0}{c} \quad (6.10)$$

which is the static compressibility and is identical to the value (4.60) we obtained directly from the Matsubara calculation

But the formula (6.9) contains much more information. In particular it gives the response of the system to a time and space dependent potential. Let us assume that we excite the system with a sinusoidal potential. We readily see that there is a divergent response for the system if

$$\omega^2 = \frac{c}{M}q^2 \quad (6.11)$$

This means that this modes can exist even if the external potential is infinitesimally small. These are thus collective modes of the system. In that case one recognize the acoustic phonons. Since the imaginary part is infinitesimal these modes can propagate without damping. Let us look at what would happen if one added a long range interaction in the system. The Hamiltonian would get an additional part

$$\begin{aligned} H_L &= \frac{1}{2} \int dr dr' V(r - r') \delta\rho(r) \delta\rho(r') \\ &= \frac{1}{2\Omega} \sum_q \rho_0^2 V(q) q^2 u(q) u^*(q) \end{aligned} \quad (6.12)$$

In fact the short range elasticity corresponds to  $V(r) = \delta(r)$ , i.e. to a constant  $V(q)$ . If one has a Coulomb potential  $V(r) \sim 1/r$ . Thus the Fourier transform behaves as

$$\begin{aligned} V(q) &\sim \frac{1}{q^2} & d = 3 \\ V(q) &\sim \frac{1}{|q|} & d = 2 \\ V(q) &\sim \log(1/|q|) & d = 1 \end{aligned} \quad (6.13)$$

The eigenmodes of the system becomes in this case

$$M\omega^2 = q^2 [c + \rho_0 V(q)] \quad (6.14)$$

Leading at small  $q$  and  $\omega$  to modes behaving as

$$\begin{aligned} \omega(q)^2 &\sim C + q^2 & d = 3 \\ \omega(q)^2 &\sim |q| & d = 2 \\ \omega(q)^2 &\sim q^2 \log(1/|q|) & d = 1 \end{aligned} \quad (6.15)$$

One recognizes here the plasmon modes.

## 6.2 Conductivity of quantum crystals; Hall effect

Let us now move to the transport properties. As we saw the conductivity is given by the current current correlation function. In order to determine the current in the crystal we can use again the continuity equation (5.52). Since we are interested in the current for small  $q$ , we can use (6.4) to obtain

$$-\rho_0 \frac{\partial \sum_{\beta} \nabla_{\beta} u_{\beta}(r, t)}{\partial t} + \sum_{\beta} \nabla_{\beta} j_{\beta}(r, t) = 0 \quad (6.16)$$

an obvious solution to this equation is simply

$$j_{\beta}(r, t) = \rho_0 \partial_t u_{\beta}(r, t) \quad (6.17)$$

and thus the charge current is

$$j_{\beta}(r, t) = e \rho_0 \partial_t u_{\beta}(r, t) \quad (6.18)$$

where  $e$  is the charge of the carriers. A physical way to understand this relation is to look at the higher harmonics of the density. The density can be viewed as a wave

$$\rho(x, t) = \rho_0 \cos(K(x - u(x, t))) \quad (6.19)$$

thus the maxima of the wave are at  $x = u(x, t)$  and thus the wave move with a velocity  $\partial_t u(r, t)$ . This is an handwaving derivation but the continuity equation shows that this answer is correct.

To compute the conductivity we thus have to look in imaginary time to the correlation function

$$\chi_{\alpha\beta}(r, t) = -\langle T_{\tau} \partial_{\tau} u_{\alpha}(r, \tau) \partial_{\tau} u_{\beta}(0, 0) \rangle \quad (6.20)$$

Normally we would just proceed with the calculation. However in the case of the crystal there is a slight simplification that is worth mentioning. If we look at the Fourier transform, and integrate by part (I have made apparent the time difference  $\tau - \tau'$ )

$$\begin{aligned} \chi(q, i\omega_n) &= -\int_0^{\beta} d\tau e^{+i\omega_n(\tau-\tau')} \langle T_{\tau} \partial_{\tau} u_{\alpha}(q, \tau) \partial_{\tau'} u_{\beta}(-q, \tau') \rangle \\ &= -\int_0^{\beta} d\tau e^{+i\omega_n(\tau-\tau')} \theta(\tau - \tau') \langle \partial_{\tau} u_{\alpha}(q, \tau) \partial_{\tau'} u_{\beta}(-q, \tau') \rangle + \theta(\tau' - \tau) \langle \partial_{\tau'} u_{\beta}(-q, \tau') \partial_{\tau} u_{\alpha}(q, \tau) \rangle \\ &= -\int_0^{\beta} d\tau e^{+i\omega_n(\tau-\tau')} i\omega_n [\theta(\tau - \tau') \langle u_{\alpha}(q, \tau) \partial_{\tau'} u_{\beta}(-q, \tau') \rangle + \theta(\tau' - \tau) \langle \partial_{\tau'} u_{\beta}(-q, \tau') u_{\alpha}(q, \tau) \rangle] \\ &\quad + \langle [u_{\alpha}(q, \tau), \partial_{\tau} u_{\beta}(-q, \tau)] \rangle \\ &= -\int_0^{\beta} d\tau e^{+i\omega_n(\tau-\tau')} \omega_n^2 [\theta(\tau - \tau') \langle u_{\alpha}(q, \tau) \partial_{\tau'} u_{\beta}(-q, \tau') \rangle + \theta(\tau' - \tau) \langle \partial_{\tau'} u_{\beta}(-q, \tau') u_{\alpha}(q, \tau) \rangle] \\ &\quad + \langle [u_{\alpha}(q, \tau), \partial_{\tau} u_{\beta}(-q, \tau)] \rangle + \langle [u_{\alpha}(q, \tau), u_{\beta}(-q, \tau)] \rangle \\ &= -\int_0^{\beta} d\tau e^{+i\omega_n(\tau-\tau')} \omega_n^2 \langle T_{\tau} u_{\alpha}(q, \tau) u_{\beta}(-q, \tau') \rangle + \langle [u_{\alpha}(q, \tau), \partial_{\tau} u_{\beta}(-q, \tau)] \rangle \end{aligned} \quad (6.21)$$

In (6.21) the first term is simply the correlation function of the  $u$ . The  $\omega_n^2$  in front comes from the time derivative in the current. Using the fact that

$$\frac{\partial_{\tau} u(\tau)}{\partial \tau} = [H, u(\tau)] \quad (6.22)$$

the second term can be rewritten as

$$\langle [u_\alpha(q, \tau), [H, u_\beta(-q, \tau)]] \rangle \quad (6.23)$$

Using the crystal Hamiltonian (4.58) one sees that (6.23) is exactly identical to the diamagnetic term. The fact that the time derivative act on the  $T_\tau$  product thus compensate exactly here the diamagnetic term, leaving for the *full* conductivity

$$\sigma_{\alpha\beta}(q, \omega) = e^2 \rho_0^2 \frac{1}{\Omega\beta} \frac{i}{\omega} \left[ \omega_n^2 \langle u_\alpha(q, i\omega_n) u_\beta^*(q, i\omega_n) \rangle \right]_{i\omega_n \rightarrow \omega + i\delta} \quad (6.24)$$

where we have put back the small convergence factor in the frequency. Note that this form is identical to (5.54) that one would obtain with the continuity equation. Using again the correlation function for the  $u$

$$\langle u_\alpha(q, i\omega_n) u_\beta^*(i\omega_n) \rangle = \frac{\delta_{\alpha\beta} \Omega \beta}{\rho_0 (M\omega_n^2 + cq^2)} \quad (6.25)$$

one obtains for the conductivity  $\sigma(\omega) = \sigma(q = 0, \omega)$

$$\sigma_{\alpha\beta}(\omega) = \frac{\delta_{\alpha\beta} e^2 \rho_0 i}{(\omega + i\delta)} = \delta_{\alpha\beta} \mathcal{D}[\pi\delta(\omega) + i\mathcal{P}(\frac{1}{\omega})] \quad (6.26)$$

Thus we recover a perfect conductivity. Physically the crystal can slide when submitted to an external potential.

The above derivation was essentially using the operator form of the current. Let us show that one can recover the same result directly from the functional integral. We will show it for simplicity in one dimension to avoid carrying out the axis index  $\alpha$  but of course the result and method are quite general. We will use a reparametrization of the elastic Hamiltonian in term of the “phase”  $\phi(x) = \pi u(x)/a$  and its conjugate variable  $\Pi(x)$  such that  $[\phi(x), \Pi(x')] = i\hbar\delta(x - x')$ . We rewrite the Hamiltonian

$$H = \frac{\hbar}{2\pi} \int dx \left[ \frac{1}{\hbar^2} v K (\pi \Pi(x))^2 + \frac{v}{K} (\partial_x \phi(x))^2 \right] \quad (6.27)$$

where  $v$  has the dimension of a velocity and  $K$  is dimensionless. This parametrization is quite useful in term of fermionic problems but The system density is simply

$$\rho(x) = \rho_0 - \frac{1}{\pi} \partial_x \phi(x) + \rho_0 \sum_p e^{ip[\frac{2\pi}{a}x - 2\phi(x)]} \quad (6.28)$$

where  $p$  is a relative integer. Using the expression of the current  $j(r, t) = \frac{e}{\pi} \partial_t \phi(r, t)$  from the continuity equation and the Heisenberg equation for an operator

$$\partial_t O(t) = \frac{i}{\hbar} [H, O(t)] \quad (6.29)$$

it is easy to see that the current *operator* is

$$j(r, t) = \frac{e}{\hbar} (vK) \Pi(r, t) \quad (6.30)$$

Thus the current-current correlation function in imaginary time is

$$\chi(\tau - \tau') = -\left(\frac{evK}{\hbar}\right)^2 \langle \Pi(x, \tau) \Pi(x', \tau') \rangle_S \quad (6.31)$$

This correlation can be computed by functional integration

$$\langle \Pi(x, \tau) \Pi(x', \tau') \rangle_S = \frac{\int \mathcal{D}\Pi \int \mathcal{D}\phi e^{-S/\hbar} \Pi(x, \tau) \Pi(x', \tau')}{\int \mathcal{D}\Pi \int \mathcal{D}\phi e^{-S/\hbar}} \quad (6.32)$$

Since the Hamiltonian is quadratic in  $\Pi$  it is easy to perform the  $\Pi$  integration explicitly. One gets

$$\langle \Pi(x, \tau) \Pi(x', \tau') \rangle_S = -\frac{\hbar^2}{(\pi v K)^2} \langle \partial_\tau \phi(x, \tau) \partial_{\tau'} \phi(x', \tau') \rangle_S + \mathcal{D} \quad (6.33)$$

The second term exactly cancels the diamagnetic term, whereas the first one is exactly the one we already computed in (6.24). Once again the functional integration avoids to have to deal with the time ordering operators and such nasty complications linked with the operators.

Now that we know the full conductivity tensor we can study the effect of other external perturbations. Before we embark on the effects of scattering let us look at the simple effect of putting an external magnetic field on the system. Let us assume that we have a two dimensional crystal in the  $x - y$  plane and that we put a magnetic field along the  $z$  direction. In that case  $B = \nabla \wedge A$  is realized if we take for example  $A = (-By/2, Bx/2, 0)$ . The elastic Hamiltonian in the presence of the external field, and taking into account that we have two components for the displacement field becomes

$$\frac{1}{2} \left[ \int d^2r \sum_\alpha \frac{1}{\rho_0 M} (\Pi_\alpha - a A_\alpha)^2 + \rho_0 \sum_{\alpha\beta} c (\nabla_\alpha u_\beta(r))^2 \right] \quad (6.34)$$

where we have assumed isotropic elasticity. The operator  $A$  needs to be made more precise. To do so let us go back to the expression for the current of a single particle. In that case

$$H_{\text{kin}} = \frac{1}{2M} (\Pi - \int dr \mathcal{A}(r) |r\rangle \langle r|)^2 \quad (6.35)$$

leading to the current (5.59). For many particles one has

$$H_{\text{kin}} = \sum_i \frac{1}{2M} (\Pi_i - \int dr \dot{A}(r) |r\rangle \langle r|)^2 \quad (6.36)$$

and the current becomes

$$j_\alpha(r, t) = \frac{q}{2M} \sum_i [\Pi_i |r\rangle \langle r| + |r\rangle \langle r| \Pi_i] - \sum_i \frac{q^2}{M} \mathcal{A}_\alpha(r, t) |r\rangle \langle r| \quad (6.37)$$

Since one wants the long wavelength part of the current one has to understand the current at point  $r$  as an average of the current operator on a volume large compared to the lattice spacing and centered around point  $r$ . Since the wavefunctions of a given site are essentially zero above the lattice spacing

$$\int_{r_0} dr |r\rangle \langle r| \sim 1 \quad (6.38)$$

for the particles around the site  $r_0$ . Thus (6.37) becomes

$$\begin{aligned} j_\alpha(r, t) &= \frac{q}{M} [\Pi_{r_i=r} \rho_0] - \frac{q^2}{M} \mathcal{A}_\alpha(r, t) \rho_0 \\ &= \frac{q}{M} [\Pi(r)] - \frac{q^2}{M} \mathcal{A}_\alpha(r, t) \rho_0 \end{aligned} \quad (6.39)$$

which is the result that we derived directly from the continuity equation and the expression of the density operator in the continuum limit.

In the presence of the magnetic field, one can proceed in a similar way. The operator projecting the particle  $i$  at point  $r$  is (is it easy to check that they have the same matrix elements)

$$|r\rangle\langle r| = \delta(r - R_i^0 - u_i) \quad (6.40)$$

and thus for all the particles

$$|r\rangle\langle r| = \sum_i \delta(r - R_i^0 - u_i) \quad (6.41)$$

The Hamiltonian becomes

$$\begin{aligned} H_{\text{kin}} &= \sum_i \frac{1}{2M} (\Pi_i - \int dr \dot{A}(r) \sum_i \delta(r - R_i^0 - u_i))^2 \\ &= \sum_i \frac{1}{2M} (\Pi_i - \dot{A}(R_i^0 + u_i))^2 \\ &= \int d^d r \frac{1}{2M\rho_0} (\Pi(r) - \rho_0 \dot{A}(r + u_i))^2 \end{aligned} \quad (6.42)$$

We can write it in a more convenient form noting that  $\mathcal{A}_\alpha = -\epsilon_{\alpha\beta} r_\beta B/2$  where  $\epsilon_{\alpha\beta}$  is the antisymmetric tensor  $\epsilon_{xy} = -\epsilon_{yx} = 1$  and  $\epsilon_{xx} = \epsilon_{yy} = 0$ . Thus the potential vector part in (6.42) reads

$$A_\alpha = -\frac{B}{2} \epsilon_{\alpha\beta} (r_\beta + u_\beta(r, t)) \quad (6.43)$$

We can go from the Hamiltonian to the action by performing the integration on  $\Pi$ , using (4.30). The action will be given by

$$\sum_\alpha \int d^2 r \int_0^\beta d\tau i \Pi \partial_\tau u_\alpha(r, \tau) - H(\Pi, u) \quad (6.44)$$

The integration over  $\Pi$  can be done easily doing first the shift  $\Pi \rightarrow \Pi - qA$  leading to the action

$$\sum_{\alpha\beta} \int d^2 r \int_0^\beta d\tau [i \frac{-eB}{2} \epsilon_{\alpha\beta} \rho_0 (r_\beta + u_\beta(r, t))] (\partial_\tau u_\alpha(r, \tau)) + \sum_\alpha \rho_0 \frac{1}{2} [M (\partial_\tau u_\alpha(r, \tau))^2 + c (\nabla_\beta u_\alpha(r, \tau))^2] \quad (6.45)$$

One can easily see that the term containing  $\int_0^\beta d\tau r \partial_\tau$  is a total derivative over time and thus vanishes due to the periodicity in time. The action is thus given by

$$\sum_{\alpha\beta} \int d^2 r \int_0^\beta d\tau [i \frac{-eB\rho_0}{2} \epsilon_{\alpha\beta} u_\beta(r, t)] (\partial_\tau u_\alpha(r, \tau)) + \sum_\alpha \rho_0 \frac{1}{2} [M (\partial_\tau u_\alpha(r, \tau))^2 + c (\nabla_\beta u_\alpha(r, \tau))^2] \quad (6.46)$$

The second part in (6.46) is the standard elastic action. The first term is easy to identify. If we consider the Lorentz force it is simply given by  $qv \wedge B$  where  $v$  is the velocity. Here  $v = \partial_\tau u$ . The energy associated to the work of the Lorentz force is simply  $fu$  and one recovers the expression in (6.46). One can easily rewrite the action in Fourier space. It is convenient to use a matrix representation

$$\frac{1}{2\beta\Omega} \sum_{q, \omega_n} (u_x^*(q, i\omega_n), u_y^*(q, i\omega_n)) \begin{pmatrix} \rho_0 [M\omega_n^2 + cq^2] & +\omega_n B e \rho_0 \\ -\omega_n B e \rho_0 & \rho_0 [M\omega_n^2 + cq^2] \end{pmatrix} \begin{pmatrix} u_x(q, i\omega_n) \\ u_y(q, i\omega_n) \end{pmatrix} \quad (6.47)$$

It is important to note that although we used a matrix to show the coordinates  $x, y$ , they are nothing more than another indices and do not play a special role compared to  $r$  or  $\tau$ . We have to diagonalize the actions. We know how to do that for  $r$  and  $\tau$  by using the Fourier transform. Because the correlations in  $q, \omega_n$  are diagonal we only have to invert the resulting  $2 \times 2$  matrix to obtain the correlation functions  $\langle u_\alpha(q, \omega) u_\beta^*(q, \omega) \rangle$ . If we denote

$$G^{-1}(q, \omega_n) = \rho_0 \begin{pmatrix} M\omega_n^2 + cq^2 & +\omega_n Be \\ -\omega_n Be & M\omega_n^2 + cq^2 \end{pmatrix} \quad (6.48)$$

Then the conductivity is simply given by

$$\sigma_{\alpha\beta} = -e^2 \rho_0^2 i(\omega + i\delta) G_{\alpha\beta}(q, i\omega_n \rightarrow \omega + i\delta) \quad (6.49)$$

Let us first look at the effect on the conductivity. The longitudinal conductivity is given by

$$\begin{aligned} \sigma_{xx}(\omega, q=0) &= \sigma_{yy}(\omega, q=0) = \frac{-ie^2 \rho_0 (\omega + i\delta) M \omega_n^2}{M^2 \omega_n^4 + B^2 e^2 \omega_n^2} \Big|_{i\omega_n \rightarrow \omega + i\delta} \\ &= \frac{-ie^2 \rho_0 (\omega + i\delta) M}{M^2 \omega_n^2 + B^2 e^2} \Big|_{i\omega_n \rightarrow \omega + i\delta} \\ &= \frac{-ie^2 \rho_0 \omega M}{-M^2 (\omega + i\delta)^2 + B^2 e^2} \end{aligned} \quad (6.50)$$

Thus the static conductivity is now zero at zero frequency. The conductivity is however infinite at a frequency

$$\omega_c = eB/M \quad (6.51)$$

which is known as the cyclotron frequency. Physically this traduces the fact that the electrons in the presence of the magnetic field describe circular orbits.

We can also look for the Hall resistance. It is defined in a geometry where no current can flow along the  $y$  direction. One has a current flowing along  $x$ . The Hall resistance is defined as  $R_H = V_y/I_x$ . Using the relation between the current and the field

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix} \begin{pmatrix} J_x \\ J_y \end{pmatrix} \quad (6.52)$$

and between the field and the current

$$\begin{pmatrix} J_x \\ J_y \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \end{pmatrix} \quad (6.53)$$

shows that the resistivity and conductivity tensor are invert of one another. The Hall resistance can be deduced from (6.52) by imposing that  $J_y = 0$ , and using  $E_y = -V_y/L_y$ . In that case one has  $E_y/J_x = \rho_{yx}$ . We could compute  $\sigma$  and then deduce  $\rho$  but we can save some time. Since the conductivity tensor is given (up to a factor  $\omega$ ) by the matrix  $G$ , the resistivity tensor is simply

$$\rho_{\alpha\beta} = \frac{i}{e^2 \rho_0^2 (\omega + i\delta)} [G^{-1}]_{\alpha\beta} \quad (6.54)$$

One can thus read directly the Hall resistance from the action

$$\rho_{yx} = \frac{-i\omega_n eB}{(\omega + i\delta)e^2 \rho_0} \Big|_{i\omega_n \rightarrow \omega + i\delta} = \frac{-B}{e\rho_0} \quad (6.55)$$

The Hall resistance is thus equal to its classical value, unaffected by the interactions among the particles in the crystal and the quantum fluctuations. Note that quite remarkably this result would remain valid for the crystal even if one add scattering provided it is isotropic, i.e. it acts only on the *diagonal* elements of the action.

### 6.3 Commensurate systems

Let us now move to more complicated systems. One particular case of interest is when the crystal is put in an external potential. This can be due for example to the periodic potential of the atoms of the underlying microscopic system in which the quantum crystal is created. One has thus to add to the elastic Hamiltonian a term

$$H = \int d^d r V(r) \rho(r) \quad (6.56)$$

where  $V(r)$  is a potential. Once again we can use the decomposition of the density. If  $V(r)$  has only Fourier component at a wavelength large compared to the lattice spacing, then (6.59) becomes

$$H = -\rho_0 \int d^d r V(r) \nabla u(r) \quad (6.57)$$

It is then easy to see that the potential  $V(r)$  can be trivially absorbed by the change of variables

$$u(r) \rightarrow u(r) - \frac{1}{M} \int^r d^d r' V(r') \quad (6.58)$$

Such a redefinition of  $u$  will of course affect the correlation functions, but since the current is given by  $\partial_\tau u$ , the current, and hence all transport properties, will be unaffected.

We thus have to take into account higher harmonics of the potential. If we consider a potential which is periodic with a periodicity close to the one (let us say with a wavevector  $K_0$ ) of the crystal we will get from (6.59)

$$H = -\rho_0 \int d^d r V_0 \cos(K_0 u(r)) \quad (6.59)$$

we thus recover that a periodic external potential leads to a sine Gordon type Hamiltonian.

Such an Hamiltonian is not exactly solvable but we can try to get the transport properties using the variational approach introduced in Section 3.2. Let us focuss for simplicity to the case of a one-dimensional quantum system at  $T = 0$  and use again the notations of Section 3.2. In that case because of the time direction we have to deal with a two dimensional classical system. As we analyzed in Section 3.2, there are two possible phases, depending on the parameter  $K$ . If  $K > K_c = 2$  the periodic potential is irrelevant. The variational solution is  $G = G^0$ . The conductivity is thus the one of a perfect crystal with a Drude peak at  $\omega = 0$ . On the other hand for  $K < K_c$  a mass appears in the propagator. The conductivity would become in the variational approximation

$$\sigma(\omega) = \frac{e^2 v K}{\pi} \frac{i}{\omega + i\delta} \frac{\omega_n^2}{\omega_n^2 + m} \Big|_{i\omega_n \rightarrow \omega + i\delta} \quad (6.60)$$

when the mass  $m$  is zero one recovers the standard result. For a finite mass the conductivity would have a delta function peak at a frequency  $\sqrt{m}$  and thus be zero at  $\omega = 0$ . This traduces the fact that the crystal is pinned by the periodic potential and cannot slide when a small external force is applied. The fact that the conductivity is non zero only at a single frequency is obviously an artefact of the variational approximation that has replaced the original problem where all modes are coupled by a single Harmonic one. We will see a better expression for the conductivity, using a memory function approach, in the exercises.



# Chapter 7

## Out of equilibrium classical systems

In the previous sections we have focussed on systems that are in thermodynamic equilibrium. However, in many situations it is interesting to know what happens when the system is pushed out of equilibrium. This can be the case when the perturbation that one applies is too strong to use linear response.

Obviously such problems are much more difficult to treat since we lose most of our theoretical tools. I will illustrate on the simple case of classical systems some of the techniques that can be used to tackle this kind of problems.

### 7.1 Overdamped dynamics

Instead of dealing with the equilibrium of the system, let us now focus on the dynamics of a classical system. We thus have to solve the equation of motion

$$ma = \sum F \quad (7.1)$$

where  $a$  is the acceleration of the system and  $F$  all the forces. Since we are dealing with a macroscopic system we expect them to reach some kind of stationary state even when they are out of equilibrium, and thus we will focus here on systems that have overdamped dynamics. The equation of motion becomes

$$\eta \frac{du}{dt} = \sum F \quad (7.2)$$

where  $u$  is some internal coordinate of the system and  $\eta$  a friction coefficient. It is easy to see that even if one added the inertial term it would not affect the low frequency properties if the system reaches some stationary state. Indeed it would be proportional to  $\omega^2 u$  whereas the damping is  $\omega u$ , and thus always negligible at small  $\omega$ . We will thus drop this term completely from now on. If the system can be described by an Hamiltonian  $H$  the forces are given by  $-\partial H/\partial u$ . Thus the equation of motion is quite generally given by

$$\eta \frac{\partial u}{\partial t} = -\frac{\partial H[u]}{\partial u} + F_{\text{other}} \quad (7.3)$$

where  $F_{\text{other}}$  describes the force that does not derive from a potential energy and that can drive the system out of equilibrium. For example this can be for a crystal and an externally applied constant force  $F$  that will make the crystal slide. For example if one takes a crystal with an elastic energy the equation of motion would be

$$\eta \frac{\partial u(r, t)}{\partial t} = \partial_r^2 u(r, t) + F_{\text{ext}} \quad (7.4)$$

If we could solve this equation, given the initial configuration  $u(t_0)$  we could compute all properties of the system. For example if one takes the case of the driven crystal. An obvious solution is  $u(r, t) = u_0 + \frac{F}{\eta}t$  which describes the fact that the crystal move uniformly with the velocity  $F/\eta$ . In general of course solving the equation (7.3) is an incredibly complicated task.

## 7.2 Link with thermodynamics

Before we embark on a way to rewrite the equation (7.3) in a more convenient form, let us see how one can recover the case of a system in equilibrium with a thermostat at temperature  $T$ . If one consider a system whose state can be described by a random variable  $u_p$ , with a certain probability  $P(u)$ , one can define an evolution law (known as a Markov chain), that gives the variable  $u_{p+1}$  as a function of the variable  $u_p$ . We want the successions of random variables  $u_p$  to sample a given distribution that we call  $e^{-S(u)}$  (in practice for us this will be the Boltzmann distribution), i.e. that is one averages the sequence of variables one get the results according to the distribution  $S$

$$\frac{1}{N} \sum_p f(u_p) = \int du f(u) e^{-S[u]} \quad (7.5)$$

for  $N$  becoming large enough.

In order to reach that goal it is sufficient that (i) the evolution law that transform the variable  $x$  into the variable  $y$  allow to reach any configuration; (ii) that the rule of transformation satisfies the reversibility condition

$$e^{-S[x]} P(x \rightarrow y) = e^{-S[y]} P(y \rightarrow x) \quad (7.6)$$

Indeed it is easy to see that if (7.6) is satisfied the distribution  $e^{-S[x]}$  is stationary. The probability to have the variable  $y$  is indeed given, if  $x$  is distributed along  $e^{-S[x]}$  by

$$\begin{aligned} P(y) &= \int dx e^{-S[x]} P(x \rightarrow y) \\ &= \int dx e^{-S[y]} P(y \rightarrow x) \\ &= e^{-S[y]} \end{aligned} \quad (7.7)$$

by normalization of  $P(x \rightarrow y)$ . In addition *any* initial distribution will converge to the equilibrium distribution. If we define the distance of the distribution  $M_p(x)$  at “time”  $p$  as

$$D_p = \int |M_p(x) - e^{-S[x]}| dx \quad (7.8)$$

then at time  $p + 1$  the distance is

$$\begin{aligned} D_{p+1} &= \int dy \left| \int dx M_p(x) P(x \rightarrow y) - e^{-S[y]} \right| \\ &= \int dy \left| \int dx (M_p(x) - e^{-S[x]}) P(x \rightarrow y) \right| \\ &\leq \int dy \int dx |(M_p(x) - e^{-S[x]}) P(x \rightarrow y)| \\ &\leq \int dx |M_p(x) - e^{-S[x]}| = D_p \end{aligned} \quad (7.9)$$

the equality being obviously only reached at equilibrium. Thus if we have a way to construct such an evolution in “time” we see that simply performing averages of the variables will allow us to reach thermal equilibrium distributions. For the hamiltonian  $H$  this can be done by adding to the equation (7.3) a “thermal” noise.

$$\eta \frac{\partial u}{\partial t} = -\frac{\partial H[u]}{\partial u} + \zeta(r, t) \quad (7.10)$$

Let us take this thermal noise uncorrelated from different sites and different times.

$$\langle \zeta(r, t) \zeta(r', t') \rangle = \Gamma \delta(r - r') \delta(t - t') \quad (7.11)$$

It thus obeys the probability distribution

$$P(\zeta) = e^{-\frac{1}{2\Gamma} \int dr dt \zeta^2(r, t)} \quad (7.12)$$

where  $\Gamma$  is a coefficient we will determine. If one discretize (7.10) one gets

$$\eta(u_{t+dt} - u_t) = -\frac{\partial H[u_t]}{\partial u_t} + \zeta(r, t) \quad (7.13)$$

Thus the probability to go from the variable  $u_t$  to  $u_{t+dt}$  is equal to the probability to find a  $\zeta(r, t)$  that satisfies (7.13). One has thus

$$\begin{aligned} \frac{P(x \rightarrow y)}{P(y \rightarrow x)} &= \frac{\prod_r P(\zeta(r, t) = \eta \partial_t u(r, t)|_{u_t} + \frac{\partial H[u_t]}{\partial u_t})}{\prod_r P(\zeta(r, t) = -\eta \partial_t u(r, t)|_{u_{t+dt}} + \frac{\partial H[u_{t+dt}]}{\partial u_t})} \\ &= e^{-\frac{1}{\Gamma} \int dr \int_t^{t+dt} dt \eta \partial_t u \frac{\partial H[u_t]}{\partial u_t}} \\ &= e^{-\frac{\eta}{\Gamma} [H[u(t+dt)] - H[u(t)]]} \end{aligned} \quad (7.14)$$

This gives back the Boltzmann distribution provided that one takes for the thermal noise  $\Gamma = \eta T$ . The equation (7.10) is known as a Langevin equation. It allows to directly recover the equilibrium solution out of a dynamical solution. Let us consider for example the case of the crystal. In that case one can easily solve the equation in Fourier space

$$(-i\eta\omega + cq^2)u(q, \omega) = \zeta(q, \omega) \quad (7.15)$$

In order to recover the thermal average one would have to perform the average over time of

$$I = \langle u(q, t) u^*(q, t) \rangle \quad (7.16)$$

where  $\langle \rangle$  denotes the average over the thermal noise. If we choose the initial time at which the thermal noise is applied at  $t = -\infty$  then the correlations become invariant by translation in time and thus the time average is not necessary ((7.16) is at equal time). The correlation function is thus just given by

$$\begin{aligned} I &= \int d\omega_1 (2\pi) \int d\omega_2 (2\pi) \frac{\langle \zeta(q, \omega_1) \zeta(-q, \omega_2) \rangle}{(-i\eta\omega_1 + cq^2)(-i\eta\omega_2 + cq^2)} \\ &= \int d\omega (2\pi) \frac{\eta T}{(-i\eta\omega + cq^2)(i\eta\omega + cq^2)} \\ &= \frac{T}{cq^2} \end{aligned} \quad (7.17)$$

which is just the thermal propagator.

### 7.3 MSR Formalism

Dealing with the Langevin equation (7.10) is thus very convenient since it allows to solve both for equilibrium and non-equilibrium situations. Unfortunately dealing with an equation is not very convenient. So we will rewrite the equation as an integral. Indeed all correlation functions can be computed by averaging over all configurations  $u$  that satisfy the equation of motion. In other word we have to compute averages with

$$\int \mathcal{D}u \delta(\eta \partial_t u = \sum F) \quad (7.18)$$

It is easy to rewrite this constraint in an exponential form by introducing a second field.

$$\int \mathcal{D}u(r, t) \mathcal{D}\hat{u}(r, t) e^{-i\hat{u}(r, t)(\eta \partial_t u - \sum F)} \quad (7.19)$$

We have now reduced our problem to a functional integral. The price to pay to deal with the dynamics is that this integral now contains two independent fields instead of one, for the case of equilibrium. This formalism is known as the Martin-Siggia-Rose formalism. It is in fact the application to the classical case to a more ancien (but more heavy formulation) formalism to deal with the out of equilibrium quantum systems, known as the Keldysh technique. (7.19) can be further simplified since the integration over the thermal noise can be explicitly performed. We thus end up with the following measure

$$\int \mathcal{D}u(r, t) \mathcal{D}\hat{u}(r, t) e^{-S[u(r, t), \hat{u}(r, t)]} \quad (7.20)$$

with

$$S = \int dr dt i[\hat{u}(r, t)(\eta \partial_t u + \frac{\partial H[u_t]}{\partial u_t} - F_{\text{other}})] - \eta T \int dr dt (i\hat{u}(r, t))(i\hat{u}(r, t)) \quad (7.21)$$

Since one has two fields, there are now several correlation functions that can be computed. Let us illustrate the various correlation functions by taking the action corresponding to a crystal. In that case the action can be written

$$S = \begin{pmatrix} u(-q, -\omega) & \hat{u}(-q, -\omega) \end{pmatrix} \begin{pmatrix} 0 & \frac{i}{2}[i\eta\omega + cq^2] \\ \frac{i}{2}[-i\eta\omega + cq^2] & \eta T \end{pmatrix} \begin{pmatrix} u(-q, -\omega) \\ \hat{u}(-q, -\omega) \end{pmatrix} \quad (7.22)$$

This can be easily inverted to lead to

$$\langle u(q, \omega) u(-q, -\omega) \rangle = \frac{2\eta T}{(\eta\omega)^2 + (cq^2)^2} \quad (7.23)$$

$$\langle u(q, \omega) \hat{u}(-q, -\omega) \rangle = \frac{i}{-i\eta\omega + cq^2} \quad (7.24)$$

$$\langle \hat{u}(q, \omega) \hat{u}(-q, -\omega) \rangle = 0 \quad (7.25)$$

What is the meaning of each of these correlation function. The  $\langle uu \rangle$  one is the usual correlation. It is easy to check that  $\langle \hat{u}\hat{u} \rangle$  will always be zero. To understand  $\langle u\hat{u} \rangle$ , let us add to the Hamiltonian a small perturbation linearly coupled to the field  $u$

$$\delta H = - \int dr f(r) u(r) \quad (7.26)$$

It is easy to see that this will give rise to a term  $f(r)$  in the action (7.21). Thus if one computes the *reponse* of the field  $u$  to the perturbation the response will be given by

$$R = \langle u(r, t) \rangle_f \quad (7.27)$$

and thus at linear order the response to the field  $f$  is simply given by

$$R = i\langle u(r, t)\hat{u}(r', t')\rangle \quad (7.28)$$

We see that contrarily to the equilibrium case where correlation and response were trivially related by the fluctuation dissipation theorem, here they correspond to two different entities. This is natural since for out of equilibrium systems the fluctuation dissipation theorem will not hold in general. One thus need to different fields for the two different objects that are the correlation and the response in such systems. Of course in equilibrium, i.e. when no external forces are present the fluctuation dissipation theorem will hold and correlation and response will be trivially related.

As an example let us look at our elastic system In that case the correlation  $C$  and the response  $R$  are given by

$$C_{q\omega} = \frac{2\eta T}{(cq^2)^2 + (\eta\omega)^2} \quad C_{qt} = T \frac{e^{-cq^2|t|/\eta}}{cq^2} \quad (7.29)$$

$$R_{q\omega} = \frac{1}{cq^2 - i\eta\omega} \quad R_{qt} = \frac{\theta(t)}{\eta} e^{-cq^2 t/\eta} \quad (7.30)$$

They are related by the fluctuation-dissipation theorem  $TR_{rt} = -\theta(t)\partial_t C_{rt}$ . The  $\theta(t)$  is there to ensure causality.

This formalism has several advantages, in particular when dealing with disordered systems. More examples will be seen in the exercises.



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