

Quantum Field Theory in Condensed Matter Physics

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1

QFT: language and goals

Under the calm mask of matter
The divine fire burns.

Vladimir Solovyev

The reason why the terms ‘quantum field theory’ and ‘statistical mechanics’ are used together so often is related to the essential equivalence between these two disciplines. Namely, a quantum field theory of a D -dimensional system can be formulated as a statistical mechanics theory of a $(D + 1)$ -dimensional system. This equivalence is a real godsend for anyone studying these subjects. Indeed, it allows one to get rid of noncommuting operators and to forget about time ordering, which seem to be characteristic properties of quantum mechanics. Instead one has a way of formulating the quantum field theory in terms of ordinary commuting functions, more or less conventional integrals, etc.

Before going into formal developments I shall recall the subject of quantum field theory (QFT). Let us consider first what classical fields are. To begin with, they are entities expressed as continuous functions of space and time coordinates (\mathbf{x}, t) . A field $\Phi(\mathbf{x}, t)$ can be a scalar, a vector (like an electromagnetic field represented by a vector potential (ϕ, \mathbf{A})), or a tensor (like a metric field g_{ab} in the theory of gravitation). Another important thing about fields is that they can exist on their own, i.e. independent of their ‘sources’ – charges, currents, masses, etc. Translated into the language of theory, this means that a system of fields has its own action $S[\Phi]$ and energy $E[\Phi]$. Using these quantities and the general rules of classical mechanics one can write down equations of motion for the fields.

Example

As an example consider the derivation of Maxwell’s equations for an electromagnetic field in the absence of any sources. I use this example in order to introduce some valuable definitions. The action for an electromagnetic field is given by

$$S = \frac{1}{8\pi} \int dt d^3x [\mathbf{E}^2 - \mathbf{H}^2] \quad (1.1)$$

where \mathbf{E} and \mathbf{H} are the electric and the magnetic fields, respectively. These fields are not independent, but are expressed in terms of the potentials:

$$\begin{aligned}\mathbf{E} &= -\nabla\phi + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \\ \mathbf{H} &= \nabla \times \mathbf{A}\end{aligned}\quad (1.2)$$

The relationship between (\mathbf{E}, \mathbf{H}) and (ϕ, \mathbf{A}) is not unique; (\mathbf{E}, \mathbf{H}) does not change when the following transformation is applied:

$$\begin{aligned}\phi &\rightarrow \phi + \frac{1}{c} \frac{\partial \chi}{\partial t} \\ \mathbf{A} &\rightarrow \mathbf{A} + \nabla \chi\end{aligned}\quad (1.3)$$

This symmetry is called *gauge* symmetry. In order to write the action as a single-valued functional of the potentials, we need to specify the gauge. I choose the following:

$$\phi = 0$$

Substituting (1.2) into (1.1) we get the action as a functional of the vector potential:

$$S = \frac{1}{8\pi} \int dt d^3x \left[\frac{1}{c^2} (\partial_t \mathbf{A})^2 - (\nabla \times \mathbf{A})^2 \right] \quad (1.4)$$

In classical mechanics, particles move along trajectories with minimal action. In field theory we deal not with particles, but with configurations of fields, i.e. with functions of coordinates and time $\mathbf{A}(t, \mathbf{x})$. The generalization of the principle of minimal action for fields is that fields evolve in time in such a way that their action is minimal. Suppose that $\mathbf{A}_0(t, \mathbf{x})$ is such a configuration for the action (1.4). Since we claim that the action achieves its minimum in this configuration, it must be invariant with respect to an infinitesimal variation of the field:

$$\mathbf{A} = \mathbf{A}_0 + \delta \mathbf{A}$$

Substituting this variation into the action (1.4), we get:

$$\delta S = \frac{1}{4\pi} \int dt d^3x [c^{-2} \partial_t \mathbf{A}_0 \partial_t \delta \mathbf{A} - (\nabla \times \mathbf{A}_0)(\nabla \times \delta \mathbf{A})] + \mathcal{O}(\delta \mathbf{A}^2) \quad (1.5)$$

The next essential step is to rewrite δS in the following canonical form:

$$\delta S = \int dt d^3x \delta \mathbf{x} \mathbf{A}(t, \mathbf{x}) \mathbf{F}[\mathbf{A}_0(t, \mathbf{x})] + \mathcal{O}(\delta \mathbf{A}^2) \quad (1.6)$$

where $\mathbf{F}[\mathbf{A}_0(t, \mathbf{x})]$ is some functional of $\mathbf{A}_0(t, \mathbf{x})$. *By definition*, this expression determines the function

$$\mathbf{F} \equiv \frac{\delta S}{\delta \mathbf{A}}$$

the *functional* derivative of the functional S with respect to the function \mathbf{A} . Let us assume that $\delta \mathbf{A}$ vanishes at infinity and integrate (1.5) by parts:

$$\delta S = -\frac{1}{4\pi} \int dt d^3x \{ c^{-2} \partial_t^2 \mathbf{A}_0(t, \mathbf{x}) - [(\nabla \times \nabla) \times \mathbf{A}_0(t, \mathbf{x})] \} \delta \mathbf{A}(t, \mathbf{x}) \quad (1.7)$$

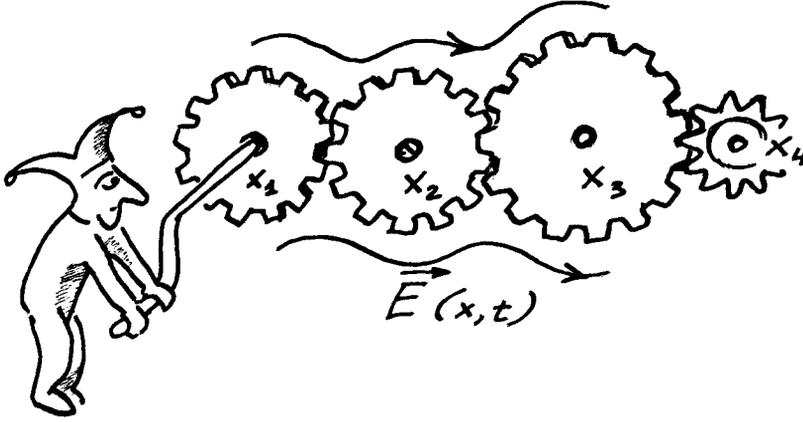


Figure 1.1. Maxwell's equations as a mechanical system.

Since $\delta S = 0$ for any $\delta \mathbf{A}$, the expression in the curly brackets (that is the functional derivative of S) vanishes. Thus we get the Maxwell equation:

$$c^{-2} \partial_t^2 \mathbf{A} - (\nabla \times \nabla) \times \mathbf{A} = 0 \quad (1.8)$$

Thus Maxwell's equations are the Lagrange equations for the action (1.4).

From Maxwell's equations we see that the field at a given point is determined by the fields at the neighbouring points. In other words the theory of electromagnetic waves is a mechanical theory with an infinite number of degrees of freedom (i.e. coordinates). These degrees of freedom are represented by the fields which are present at every point and coupled to each other. In fact it is quite correct to define classical field theory as the mechanics of systems with an infinite number of degrees of freedom. By analogy, one can say that QFT is just the quantum mechanics of systems with infinite numbers of coordinates.

There is a large class of field theories where the above infinity of coordinates is trivial. In such theories one can redefine the coordinates in such a way that the new coordinates obey independent equations of motion. Then an apparently complicated system of fields decouples into an infinite number of simple independent systems. It is certainly possible to do this for so-called linear theories, a good example of which is the theory of the electromagnetic field (1.4); the new coordinates in this case are just coefficients in the Fourier expansion of the field \mathbf{A} :

$$\mathbf{A}(\mathbf{x}, t) = \frac{1}{V} \sum_{\mathbf{k}} \mathbf{a}(\mathbf{k}, t) e^{i\mathbf{k}\mathbf{x}} \quad (1.9)$$

Substituting this expansion into (1.8) we obtain equations for the coefficients, which are just the Newton equations for harmonic oscillators with frequencies $\pm c|\mathbf{k}|$:

$$\partial_t^2 \mathbf{a}_i(\mathbf{k}, t) - (c\mathbf{k})^2 \left(\delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2} \right) \mathbf{a}_j(\mathbf{k}, t) = 0 \quad (1.10)$$

where $\mathbf{a} = (a_1, a_2, a_3)$.

The meaning of this transformation becomes especially clear if we confine our system of fields in a box with linear dimensions L_i ($i = 1, \dots, D$) with periodic boundary conditions. Then our \mathbf{k} -space becomes discrete:

$$k_i = \frac{2\pi}{L_i} n_i$$

(n_i are integer numbers). Thus the continuous theory of the electromagnetic field in real space looks like a discrete theory of independent harmonic oscillators in \mathbf{k} -space. The quantization of such a theory is quite obvious: one should quantize the above oscillators and get a quantum field theory from the classical one. Things are not always so simple, however. Imagine that the action (1.4) has quartic terms in derivatives of \mathbf{A} , which is the case for electromagnetic waves propagating through a nonlinear medium where the speed of light depends on the field intensity \mathbf{E} :

$$c^2 = (c_0^2/n) + \alpha(\partial_t \mathbf{A})^2 \quad (1.11)$$

Then one cannot decouple the Maxwell equations into independent equations for harmonic oscillators.

We have mentioned above that QFT is just quantum mechanics for an infinite number of degrees of freedom. Infinities always cause problems, not only conceptual, but technical as well. In high energy physics these problems are really serious, but in condensed matter physics we are more lucky: here we rarely deal with systems where the number of degrees of freedom is really infinite. Numbers of electrons and ions are always finite though usually very large. If an infinity actually does appear, the first approach to it is to make it countable. We already know how to do this: we should put the system into a box and carry out a Fourier transformation of the fields. In condensed matter problems this box is not imaginary, but real. Another natural way to make the number of degrees of freedom finite is to put the system on a lattice. Again, in condensed matter physics a lattice is naturally present.

Usually QFT is concerned about *universal* features of phenomena, i.e. about those features which are independent of details of the lattice. Therefore QFT describes a continuum limit of many-body quantum mechanics, in other words the limit on a lattice with $a \rightarrow 0$, $L_i \rightarrow \infty$. We shall see that *this limit does not necessarily exist*, i.e. not all condensed matter phenomena have universal features.

Let us forget for a moment about possible difficulties and accept that QFT is just a quantum mechanics of systems of an infinite number of degrees of freedom. Does the word ‘infinite’ impose any additional requirements? It does, because this makes QFT a statistical theory. QFT operates with *statistically averaged quantum averages*. Therefore in QFT we average twice. Let us explain this in more detail. The quantum mechanical average of an operator $\hat{A}(t)$ is defined as

$$\langle \hat{A}(t) \rangle = \int d^N x \psi^*(t, \mathbf{x}) \hat{A}(t) \psi(t, \mathbf{x}) = \sum_q C_q^* C_p \langle q | \hat{A}(t) | p \rangle \quad (1.12)$$

where $|q\rangle$ are eigenstates and the coefficients C_q are not specified. In QFT we usually consider systems in thermal equilibrium, i.e. we assume that the coefficients of the wave

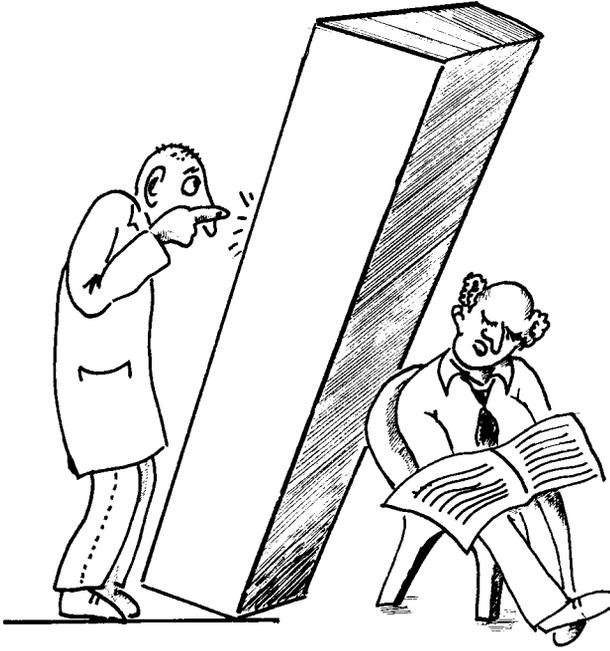


Figure 1.2. Studying responses of a ‘black box’.

functions follow the Gibbs distribution:

$$C_q^* C_p = \frac{1}{Z} e^{-\beta E_q} \delta_{qp} \quad (1.13)$$

where $\beta = 1/T$. In other words, the averaging process in QFT includes quantum mechanical averaging and Gibbs averaging:

$$\langle \hat{A}(t) \rangle_{\text{QFT}} = \frac{\sum_q e^{-\beta E_q} \langle q | \hat{A}(t) | q \rangle}{\sum_q e^{-\beta E_q}} = \frac{\text{Tr}(e^{-\beta \hat{H}} \hat{A})}{\text{Tr}(e^{-\beta \hat{H}})} \quad (1.14)$$

There is also another important language difference between quantum mechanics and QFT. Quantum mechanics expresses everything in terms of wave functions, but in QFT we usually express results in terms of correlation functions or generating functionals of these functions. It is useful to define these important notions from the very beginning. Let us consider a *classical* statistical system first. What is a correlation function? Imagine we have a complicated system where everything is interconnected appearing like a ‘black box’ to us. One can study this black box by its responses to external perturbations (see Fig. 1.2).

A usual measure of this response is a change in the free energy: $\delta F = F[H(\mathbf{x})] - F[0]$. In principle, the functional $\delta F[H(\mathbf{x})]$ carries all accessible information about the system. Experimentally we usually measure derivatives of the free energy with respect to fields taken at different points. The only formal difficulty is that the number of points is infinite. However, we can overcome this by discretizing our space as has been explained above. Therefore we represent our space as an arrangement of small boxes of volume Ω centred

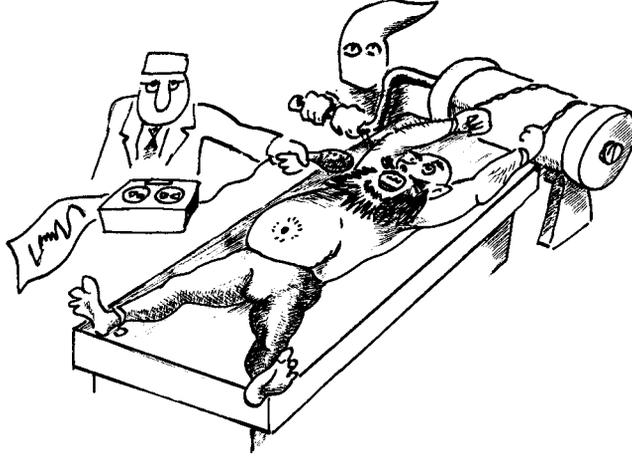


Figure 1.3. Response functions are usually measurable experimentally.

around points \mathbf{x}_n (recall the previous discussion!) assuming that the field $H(\mathbf{x})$ is constant inside each box: $H(\mathbf{x}) = H(\mathbf{x}_n)$. Thus our functional may be treated as a limiting case of a function of a large but finite number of arguments $F[H] = \lim_{\Omega \rightarrow 0} F(H_1, \dots, H_N)$.

Performing the above differentiations we define the following quantities which are called correlation functions:

$$\begin{aligned} \langle M(\mathbf{x}) \rangle &\equiv \frac{\delta F[H]}{\delta H(\mathbf{x})} \\ \langle \langle M(\mathbf{x}_2) M(\mathbf{x}_1) \rangle \rangle &\equiv \frac{\delta^2 F[H]}{\delta H(\mathbf{x}_2) \delta H(\mathbf{x}_1)} \dots \\ \langle \langle M(\mathbf{x}_N) M(\mathbf{x}_{N-1}) \dots M(\mathbf{x}_1) \rangle \rangle &\equiv \frac{\delta^N F[H]}{\delta H(\mathbf{x}_N) \dots \delta H(\mathbf{x}_1)} \dots \end{aligned} \quad (1.15)$$

Recall that the operation $\delta F / \delta H$ thus defined is called a functional derivative. As we see, it is a straightforward generalization of a partial derivative for the case of an infinite number of variables. In general, whenever we encounter infinities in physics we can approximate them by very large numbers, so do not worry much about such things as functional derivatives and path integrals (see below); they are just trivial generalizations of partial derivatives and multiple integrals!

Response functions are usually measurable experimentally, at least in principle (see Fig. 1.3). By obtaining them one can recover the whole functional using the Taylor expansion:

$$\delta F[H(\mathbf{x})] = \sum_n \frac{1}{n!} \int d^D x_1 \dots d^D x_n H(\mathbf{x}_1) \dots H(\mathbf{x}_n) \langle \langle M(x_1) \dots M(x_n) \rangle \rangle \quad (1.16)$$

In which way does the situation in QFT differ from the classical one? First of all, as we have seen, in QFT we average in both the quantum mechanical and thermodynamical sense, but what is more important is that the quantities $M(\mathbf{x})$ are now operators and the result of

averaging depends on their ordering. As we know from an elementary course in quantum mechanics, operators satisfy the Heisenberg equation of motion:

$$i\hbar \frac{\partial \hat{A}}{\partial t} = [\hat{H}, \hat{A}] \quad (1.17)$$

where \hat{H} is the Hamiltonian of the system. This equation has the following solution:

$$\hat{A}(t) = e^{-it\hbar^{-1}\hat{H}} \hat{A}(t=0) e^{it\hbar^{-1}\hat{H}} \quad (1.18)$$

To describe systems in thermal equilibrium we usually use imaginary or the so-called Matsubara time

$$i\tau = t\hbar^{-1}$$

Its meaning will become clear later.

Suppose now that \hat{A} is a perturbation to our Hamiltonian \hat{H} . Then this perturbation changes the energy levels:

$$E_n = E_n^{(0)} + \langle n | \hat{A} | n \rangle + \sum_{m \neq n} \frac{|\langle n | \hat{A} | m \rangle|^2}{E_n - E_m} + \dots \quad (1.19)$$

and therefore changes the free energy:

$$F = -\beta^{-1} \ln \left(\sum_n e^{-\beta E_n} \right)$$

Now I am going to show that in the second order of the perturbation theory these changes in the free energy can be expressed in terms of some correlation function. Let me make some preparatory definitions. Consider an operator $\hat{A}(\mathbf{x})$ and its Hermitian conjugate $\hat{A}^+(\mathbf{x})$. Let us define their τ -dependent generalizations:

$$\begin{aligned} \hat{A}(\tau, \mathbf{x}) &= e^{\tau \hat{H}} \hat{A}(\mathbf{x}) e^{-\tau \hat{H}} \\ \hat{A}^+(\tau, \mathbf{x}) &= e^{\tau \hat{H}} \hat{A}^+(\mathbf{x}) e^{-\tau \hat{H}} \end{aligned} \quad (1.20)$$

where the Matsubara ‘time’ belongs to the interval $0 < \tau < \beta$.

Then we have the following definition of the correlation function of two operators:

$$\begin{aligned} D(1, 2) &\equiv \langle \langle \hat{A}(\tau_1, \mathbf{x}_1) \hat{A}(\tau_2, \mathbf{x}_2) \rangle \rangle \\ &= \begin{cases} \pm \{ Z^{-1} \text{Tr}[e^{-\beta \hat{H}} \hat{A}(\tau_1, \mathbf{x}_1) \hat{A}(\tau_2, \mathbf{x}_2)] - \langle \hat{A}(\tau_1, \mathbf{x}_1) \rangle \langle \hat{A}(\tau_2, \mathbf{x}_2) \rangle \} & \tau_1 > \tau_2 \\ \{ Z^{-1} \text{Tr}[e^{-\beta \hat{H}} \hat{A}(\tau_2, \mathbf{x}_2) \hat{A}(\tau_1, \mathbf{x}_1)] - \langle \hat{A}(\tau_2, \mathbf{x}_2) \rangle \langle \hat{A}(\tau_1, \mathbf{x}_1) \rangle \} & \tau_2 > \tau_1 \end{cases} \end{aligned} \quad (1.21)$$

The minus sign in the upper row appears if \hat{A} is a Fermi operator. Here I have to make the following important remark. The terms Bose and Fermi are used in the following sense. Operators are termed Bose if they create a closed algebra under the operation of commutation, and they are termed Fermi if they create a closed algebra under anticommutation. The phrase ‘closed algebra’ means that commutation (or anticommutation) of operators

of a certain set produces only operators of this set and nothing else. Thus spin operators on a lattice $\hat{S}^a(\mathbf{r})$ ($a = x, y, z$) create a closed algebra under commutation, because their commutator is either zero ($\mathbf{r} \neq \mathbf{r}'$) or a spin operator. One might think that $S = 1/2$ is a special case because the Pauli matrices on one site also satisfy the anticommutation relations:

$$\{\sigma^a, \sigma^b\} = 2\delta_{ab}$$

and it seems that one can choose alternative definitions of their statistics. It is not true, however, because the spin-1/2 operators from different lattice sites always *commute* and, on the contrary, their anticommutator is never equal to zero.

Imagine that we know all the eigenfunctions and eigenenergies of our system. Then we can rewrite the above traces explicitly using this basis. The result is given by

$$D(1, 2) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} |\langle n | \hat{A}(0) | m \rangle|^2 e^{i\mathbf{P}_{mn}\mathbf{x}_{12}} [\pm\theta(\tau_1 - \tau_2)e^{E_{nm}\tau_{12}} + \theta(\tau_2 - \tau_1)e^{E_{nm}\tau_{21}}] \quad (1.22)$$

where $\tau_{12} = \tau_1 - \tau_2$, $\mathbf{x}_{12} = \mathbf{x}_1 - \mathbf{x}_2$. Here we have used the following properties of eigenstates:

$$e^{\tau\hat{H}}|n\rangle = e^{\tau E_n}|n\rangle$$

$$\langle m | \hat{A}(\mathbf{x}) | n \rangle = e^{i(\mathbf{P}_n - \mathbf{P}_m)\mathbf{x}} \langle m | \hat{A}(0) | n \rangle$$

The latter property holds only for translationally invariant systems where the eigenstates of \hat{H} are simultaneously eigenstates of the momentum operator $\hat{\mathbf{P}}$. Now you can check that the change in the free energy can be written in terms of the correlation functions:

$$\beta\delta F = \int_0^\beta d\tau \langle A(\tau) \rangle + \frac{1}{2} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 D(\tau_1, \tau_2) \quad (1.23)$$

Therefore correlation functions are equally important in classical and quantum systems.

Let us continue our analysis of the pair correlation function defined by (1.21) and (1.22). This pair correlation function is often called the Green's function after the man who introduced similar objects in classical field theory. There are two important properties following from this definition. The first is that the Green's function depends on

$$\tau \equiv (\tau_1 - \tau_2)$$

which belongs to the interval

$$-\beta < \tau < \beta$$

The second is that for Bose operators the Green's function is a periodic function:

$$D(\tau) = D(\tau + \beta) \quad \tau < 0 \quad (1.24)$$

and for Fermi operators it is an antiperiodic function:

$$D(\tau) = -D(\tau + \beta) \quad \tau < 0 \quad (1.25)$$

These two properties allow one to write down the following Fourier decomposition of the Green's function:

$$D(\tau, \mathbf{x}_{12}) = \beta^{-1} \sum_{s=-\infty}^{\infty} \int \frac{d^D k}{(2\pi)^D} D(\omega_s, \mathbf{k}) e^{-i\omega_s \tau - i\mathbf{k}\mathbf{x}_{12}} \quad (1.26)$$

where

$$\begin{aligned} D(\omega_s, \mathbf{k}) &= (2\pi)^D Z^{-1} \sum_{n,m} e^{-\beta E_n} (1 \mp e^{\beta - E_{mn}}) |\langle n | \hat{A}(0) | m \rangle|^2 \frac{\delta(\mathbf{k} - \mathbf{P}_{mn})}{i\omega_s - E_{mn}} \\ &\equiv \sum_{n,m} \frac{\rho(n, m)(\mathbf{k})}{i\omega_s - E_{mn}} \end{aligned} \quad (1.27)$$

and

$$\omega_s = 2\pi \beta^{-1} s$$

for Bose systems and

$$\omega_s = \pi \beta^{-1} (2s + 1)$$

for Fermi systems. Thus we get a function defined in the complex plane of ω at a sequence of points $\omega = i\omega_s$. We can continue it analytically to the upper half-plane (for example). Thus we get the function

$$\begin{aligned} D^{(R)}(\omega) &= \sum_{n,m} \frac{\rho(n, m)(\mathbf{k})}{\omega - E_{mn} + i0} \\ \rho(n, m)(\mathbf{k}) &= \frac{(2\pi)^D}{Z} e^{-\beta E_n} (1 \mp e^{\beta - E_{mn}}) |\langle n | \hat{A}(0) | m \rangle|^2 \delta(\mathbf{k} - \mathbf{P}_{mn}) \end{aligned} \quad (1.28)$$

analytical in the upper half-plane of ω . This function has *two wonderful properties*. (a) Its poles in the lower half-plane give energies of transitions E_{mn} which tell us about the spectrum of our Hamiltonian. (b) We can write down our original Green's function in terms of the retarded one:

$$D(\omega_s, \mathbf{k}) = -\frac{1}{\pi} \int dy \frac{\Im m D^{(R)}(y)}{i\omega_s - y} \quad (1.29)$$

This relation is very convenient for practical calculations as will become clear in subsequent chapters.

We see that the quantum case is special due to the presence of the 'time' variable τ . What is specially curious is that the quantum correlation functions have different periodicity properties in the τ -plane depending on the statistics. We shall have a chance to appreciate the really deep meaning of all these innovations in the next chapters.

One should not take away from this chapter a false impression that in QFT we are doomed to deal with this strange imaginary time and are not able to make judgements about real time dynamics. The point is that the τ -formulation is just more convenient; for systems in thermal equilibrium the dynamic (i.e. real time) correlation functions are related to the

thermodynamic ones through the following relationship:

$$D_{\text{dynamic}}(\omega) = \Re e D^{(\text{R})}(\omega) + i \coth\left(\frac{\omega}{2T}\right) \Im m D^{(\text{R})}(\omega) \quad (\text{bosons}) \quad (1.30)$$

$$D_{\text{dynamic}}(\omega) = \Re e D^{(\text{R})}(\omega) + i \tanh\left(\frac{\omega}{2T}\right) \Im m D^{(\text{R})}(\omega) \quad (\text{fermions}) \quad (1.31)$$

The proof of the above relations can be found in any book on QFT and I shall spend no time on it.

These relations are convenient if our calculational procedure naturally provides us with Green's functions in frequency momentum representation. This is not always the case, however. Sometimes we can work only in real space (see the chapters on one-dimensional systems). Then it is better not to calculate $D(i\omega_n)$ first and continue it analytically, but to skip this intermediate step and to express the retarded functions directly in terms of $D(\tau)$. In order to do this, we can use the relationship between the thermodynamic and the retarded Green's functions, which follows from (1.22) and (1.28):

$$\begin{aligned} D(\tau) &= \theta(\tau)D_+(\tau) \pm \theta(-\tau)D_-(\tau) \\ D_+(\tau) &= -\frac{1}{\pi} \int dx \Im m D^{(\text{R})}(x) \frac{e^{-x\tau}}{1 \mp e^{-\beta x}} \\ D_-(\tau) &= -\frac{1}{\pi} \int dx \Im m D^{(\text{R})}(x) \frac{e^{-x\tau}}{e^{\beta x} \mp 1} \end{aligned} \quad (1.32)$$

(the upper sign is for bosons, the lower one for fermions). Then from (1.32) it follows that

$$D_+(\tau) - D_-(\tau) = -\frac{1}{\pi} \int_{-\infty}^{\infty} dx \Im m D^{(\text{R})}(x) e^{-\tau x} \quad (1.33)$$

from which we can recover $\Im m D^{(\text{R})}(\omega)$:

$$\Im m D^{(\text{R})}(\omega) = \frac{1}{2} \int_{-\infty}^{\infty} dt [D_-(it + \epsilon) - D_+(it + \epsilon)] e^{i\omega t} \quad (1.34)$$

If you feel that the discussion of the correlation functions is too abstract, go ahead to the next chapter, where a simple example is provided. This is always the case with new concepts; at the beginning they look like unnecessary complications and it takes time to understand that, in fact, they make life much easier for those who have taken trouble to learn them. In order to make contact with reality easier, I outline below some experimental techniques which measure certain correlation functions more or less directly.

1. *Neutron scattering.* Being neutral particles with spin 1/2, neutrons in condensed matter interact only with magnetic moments. The latter can belong either to nuclei (ions) or to electrons. Thus neutron scattering is a very convenient probe of lattice dynamics and electron magnetism. In experiments on neutron scattering one measures the differential cross-section of neutrons which is directly proportional to the sum of electronic and ionic dynamical structure factors $S_i(\omega, \mathbf{q})$ and $S_{\text{el}}(\omega, \mathbf{q})$. The ionic structure factor is the two-point *dynamical* correlation function of the exponents of ionic displacements \mathbf{u} (see, for

example, Appendix N in the book by Ashcroft and Mermin in the select bibliography):

$$S_i(\omega, \mathbf{q}) = \frac{1}{N} \sum_{\mathbf{r}, \mathbf{r}'} e^{-i\mathbf{q}(\mathbf{r}-\mathbf{r}')} \int \frac{dt}{2\pi} \langle \exp[i\mathbf{q}\mathbf{u}(t, \mathbf{r})] \exp[-i\mathbf{q}\mathbf{u}(0, \mathbf{r}')] \rangle e^{i\omega t} \quad (1.35)$$

(N is the total number of ions in the crystal). In the case when the displacements are *harmonic* the expression for S_i can be simplified:

$$S_i(\omega, \mathbf{q}) = \sum_{\mathbf{r}} \int_{-\infty}^{\infty} \frac{dt}{2\pi} \exp \left\{ \frac{1}{2} q^a q^b [\langle u^a(t, \mathbf{r}) u^b(0, 0) \rangle - \langle u^a(0, 0) u^b(0, 0) \rangle] \right\} e^{i\omega t - i\mathbf{q}\mathbf{r}} \quad (1.36)$$

The electronic structure factor is the imaginary part of the dynamical magnetic susceptibility:

$$\begin{aligned} S_{\text{el}}^{ab}(\omega, \mathbf{q}) &= \frac{1}{e^{\hbar\omega/kT} - 1} \Im m \chi^{(R),ab}(\omega, \mathbf{q}) \\ \chi^{ab}(\omega_n, \mathbf{q}) &= \int d^D r d\tau e^{-i\mathbf{q}\mathbf{r} - i\omega_n \tau} \langle \langle S^a(\tau, \mathbf{r}) S^b(0, 0) \rangle \rangle \end{aligned} \quad (1.37)$$

where $S^a(\mathbf{r})$ is the spin density.

2. *X-ray scattering*. X-ray scattering measures the same ionic structure factor plus several other important correlation functions. In metals, absorption of X-rays with definite frequency ω is proportional to the single-electron density of states $\rho(\omega)$. The latter is equal to

$$\rho(\omega) = \frac{1}{\pi} \sum_{\sigma} \sum_q \Im m G_{\sigma\sigma}^{(R)}(\omega, \mathbf{q}) \quad (1.38)$$

where $G(\omega, \mathbf{q})$ is the single-electron Green's function. One can do even better than this, measuring X-ray absorption at certain angles. The corresponding method is called 'angle resolved X-ray photoemission' (ARPES); it measures $\Im m G_{\sigma\sigma}^{(R)}(\omega, \mathbf{q})$ directly.

3. *Nuclear magnetic resonance and the Knight shift*. A sample is placed in a combination of constant and alternating magnetic fields. Resonance is observed when the frequency of the alternating fields coincides with the Zeeman splitting of nuclei. The magnetic polarization of the electrons changes the effective magnetic field acting on the nuclei and thus changes the Zeeman splitting. The shift of the resonance line (the *Knight shift*) is proportional to the local magnetic susceptibility:

$$\Delta H/H \sim \sum_q F(q) \lim_{\omega \rightarrow 0} \Im m \chi^{(R)}(\omega, q) \quad (1.39)$$

where $F(q) = \sum_a \cos(\mathbf{q}\mathbf{a})$ is the structure factor of the given nuclei. A more detailed discussion can be found in Abrikosov's book *Fundamentals of the Theory of Metals*.

4. *Muon resonance*. This method measures internal local magnetic fields. Therefore it allows one to decide whether the material is in a magnetically ordered state or not. The problem of magnetic order may be very difficult if the order is complex, as in helimagnets or in spin glasses where every spin is frozen along its individual direction.

5. *Infrared reflectivity.* When a plane wave is normally incident from vacuum on a medium with dielectric constant ϵ , the fraction r of power reflected (the reflectivity) is given by

$$r = \left| \frac{1 - \sqrt{\epsilon}}{1 + \sqrt{\epsilon}} \right|^2 \quad (1.40)$$

In order to extract ϵ from the reflectivity one can use the Kramers–Kronig relations. This requires a knowledge of $r(\omega)$ for a considerable range of frequencies, which is a disadvantage of the method. The dielectric function $\epsilon(\omega, \mathbf{q})$ is directly related to the pair correlation function of charge density:

$$\Pi(\omega, \mathbf{q}) = \langle \langle \rho(-\omega, -\mathbf{q}) \rho(\omega, \mathbf{q}) \rangle \rangle \quad (1.41)$$

Its imaginary part is proportional to the electrical conductivity:

$$\Im m \epsilon = \frac{4\pi}{\omega} \Re e \sigma \quad (1.42)$$

Since photons have very small wave vectors $q = \omega/c$, the described method effectively measures values of physical quantities at zero q .

6. *Brillouin and Raman scattering.* In the corresponding experiments a sample is irradiated by a laser beam of a given frequency; due to the nonlinearity of the medium a part of the energy is re-emitted with different frequencies. Therefore a spectral dispersion of the reflected light contains ‘satellites’ whose intensity is proportional to the fourth-order correlation function of dipole moments or spins (light can interact with both). Scattering with a small frequency shift originates from gapless excitations (such as acoustic phonons and magnons) and is referred to as *Brillouin scattering*. For frequency shifts of the order of several hundred degrees the main contribution comes from higher energy excitations such as optical phonons; in this case the process is called *Raman scattering*. The practical validity of this kind of experimental technique is limited by the fact that measurements occur at zero wave vectors.
7. *Ultrasound absorption.* This measures the same density–density correlation function as light absorption, but with the advantage that q is not necessarily small, since phonons can have practically any wave vectors.