

Chapter 1

Introduction

The concept of quasiparticles is of major importance in the theory of condensed matter. This concept can be rigorously justified within the Green's function formalism, which a long time ago became the main working tool of all modern approaches to many particle systems. The method of Green's functions allows to formulate criteria for the existence of quasiparticles in specific models of interacting particles, as well as constitutes the universal method of practical calculations of arbitrary physical properties of many particle systems with the account of different types of interactions. This method originated in quantum field theory, where quite effective and convenient approach, based on the use of *Feynman diagrams* appeared for the first time. The following transfer of these methods to the theory of many particle systems, in fact, lead to the formulation of the modern theory of condensed matter [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963); Lifshits E.M., Pitaevskii L.P. (1980)].

In this lecture course we do not present step by step derivation of the Green's function formalism itself, our aim is to teach how to use this method for solution of concrete physical problems. It is assumed that the basic principles of construction of Feynman diagrams for different types of interactions are already known, both for the case of zero temperature $T = 0$, as well as for finite temperatures (Matsubara formalism) [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963)]. The structure of the course is clear from the Contents. Separate chapters are devoted to the analysis of different types of interactions, which are studied within the electronic theory of the solid state, and also to a number of major electronic instabilities (phase transitions). At first, in each chapter we formulate the rules of diagram technique, appropriate for the interaction under study, then we analyze different problems, in most cases presenting all the details of

calculations, or at least giving all the information necessary to reproduce the results. Practically everywhere in these lectures we tried to adhere to the rules and major notations used in “AGD” book [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963)], though due to rather “informal” style of our presentation, we can not guarantee the absence of some “randomness” in notations between different sections. In fact, each chapter can be used as the introduction to the problems of the appropriate part of the solid state theory. In this sense the chapters can be read independently of each other, but it should be noted that all the problems under discussion has much in common and are, in fact, deeply connected to each other. Bibliography is in no sense complete, we quote only the sources, from which we have taken the material used in our presentation, limiting ourselves mainly to textbooks or reviews. Accordingly, there are practically no references to original papers and no discussion of priorities, in most important cases we just quote the name of the author (with an approximate year, when the result was obtained). Some of the material of these lectures is based on personal exercises by the author, no specific references are given in most of such cases.

The main idea of diagrammatic approach in the theory of condensed matter reduces in fact to the summation of an infinite series of Feynman diagrams for the single-particle or many-particle (in most cases two-particle) Green’s functions (and (or) appropriate vertex parts, describing multi-particle interactions). Usually it is possible to perform a certain *partial* summation of some classes (types) of diagrams of perturbation series, which are “dominating” over some physical parameter (e.g. dimensionless coupling constant, density of particles, or some other combination of parameters, characteristic for the problem under discussion). In most cases, such dominating classes of diagrams were determined already during the initial stages of the development of diagrammatic approaches to different kinds of interactions [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963); Lifshits E.M., Pitaevskii L.P. (1980)], and we shall consider a number of such typical cases and physical results obtained. In some (very) rare cases and for (mostly) oversimplified model cases, it is possible to perform a *complete* summation of *all* Feynman diagrams. These cases (problems) are much less known, but mostly are quite important and instructive. We shall consider a number of such problems, both to illustrate technical aspects and also to analyze nontrivial conclusions, such as the “destruction” of the concept of quasiparticles itself, which being quite useful certainly has its limits. Here we shall move closer to most modern aspects of the theory.

Practically everywhere in these lectures we use the natural units with $\hbar = c = 1$, “restoring” \hbar and c only in some final expressions and estimates. Boltzmann’s constant is always taken as $k_B = 1$.

1.1 Quasiparticles and Green’s functions

Though we shall not be presenting any systematic derivation of diagrammatic approach to many-particle systems, let us start with some short introduction of some elementary concepts and definitions, just for coherence of presentation and to remind a reader basic physical ideas behind the application of Green’s functions in condensed matter theory .

Consider first the case of temperature $T = 0$, i.e. the system at its ground state. Let us start from the elementary problem of a *single* quantum particle moving in some time-independent external potential (or field), and described by the usual (time-dependent) Schrödinger equation with appropriate Hamiltonian H :

$$i \frac{\partial \psi(\mathbf{r}, t)}{\partial t} - H\psi(\mathbf{r}, t) = 0 \quad (1.1)$$

Instead of solving this equation directly (with some initial condition for the wave-function) we introduce the Schrödinger-like equation for the *Green’s function* $G(\mathbf{r}, t; \mathbf{r}', t')$, depending on *two* values of time and coordinate:

$$i \frac{\partial G}{\partial t} - HG = i\delta(\mathbf{r} - \mathbf{r}')\delta(t - t') \quad (1.2)$$

with initial condition $G(\mathbf{r}, t + 0; \mathbf{r}', t) = \delta(\mathbf{r} - \mathbf{r}')$. Physically, Green’s function represents the *probability amplitude* for a particle transition from (initial) point \mathbf{r}' at the moment of time t' to the some point \mathbf{r} at the moment t . Squared modulus of this amplitude gives the probability of such transition. This is easily checked expressing ψ -function at the moment $t + \tau$ via ψ -function at the moment t as:

$$\psi(\mathbf{r}, t + \tau) = \int d\mathbf{r}' G(\mathbf{r}, t + \tau; \mathbf{r}' t) \psi(\mathbf{r}', t) \quad (1.3)$$

It is easily seen that this expression for $\psi(\mathbf{r}, t + \tau)$ satisfies the Schrödinger equation (1.1), and for $\tau \rightarrow 0$ it coincides with $\psi(\mathbf{r}, t)$ due to the initial condition $G(\mathbf{r}, t + 0; \mathbf{r}', t) = \delta(\mathbf{r} - \mathbf{r}')$. Obviously, we have to assume $G = 0$ for $\tau < 0$ to guarantee causality.

Let us now introduce some set of eigenfunctions of the stationary Schrödinger equation:

$$H\varphi_\lambda(\mathbf{r}) = \varepsilon_\lambda\varphi_\lambda(\mathbf{r}) \quad (1.4)$$

Depending on the problem at hand, the quantum numbers λ can have different physical meaning. If our problem (Hamiltonian) is translation invariant $\lambda \rightarrow \mathbf{p}$, e.g. the momentum of a free particle, for the system in an external magnetic field λ represents the set of Landau quantum numbers, for a particle moving in some arbitrary (or random) potential, these may be some (in general unknown to us) quantum numbers of the states diagonalizing the Hamiltonian.

Consider the simple case of a particle moving in some potential:

$$H = \frac{p^2}{2m} + V(\mathbf{r}) \quad (1.5)$$

Any solution of the Schrödinger equation (1.1) can be expanded using the complete system of eigenfunctions of (1.4):

$$\psi(\mathbf{r}, t) = \sum_\lambda c_\lambda(t)\varphi_\lambda(\mathbf{r}) \quad (1.6)$$

Then we can write (1.3) as an equation for the coefficients of this expansion:

$$c_\lambda(t + \tau) = \sum_{\lambda'} G_{\lambda\lambda'}(\tau)c_{\lambda'}(t) \quad (1.7)$$

and obtain:

$$G_{\lambda\lambda'}(\tau) = \int d^3r d^3r' G(\mathbf{r}, \mathbf{r}'\tau)\varphi_\lambda^*(\mathbf{r})\varphi_{\lambda'}(\mathbf{r}') \quad (1.8)$$

– the Green's function in the representation of quantum numbers λ . As φ_λ is an exact stationary state of the (time-independent) Hamiltonian H , there are no transitions to another states, so that $c_\lambda(t + \tau) = e^{-i\varepsilon_\lambda\tau}c_\lambda(t)$, i.e.

$$G_{\lambda\lambda'}(\tau) = G_\lambda(\tau)\delta_{\lambda\lambda'} = e^{-i\varepsilon_\lambda\tau}\theta(\tau) \quad (1.9)$$

where $\theta(\tau) = 1$ for $\tau \geq 0$ and $\theta(\tau) = 0$ for $\tau < 0$. Consider now the Fourier transform¹:

$$G_\lambda(\varepsilon) = \frac{1}{i} \int_{-\infty}^{\infty} d\tau e^{i\varepsilon\lambda\tau} G_\lambda(\tau) \quad (1.10)$$

$$G_\lambda(\tau) = i \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} e^{-i\varepsilon\lambda\tau} G_\lambda(\varepsilon) \quad (1.11)$$

Then, after elementary integration we get:

$$G_\lambda(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_\lambda + i\delta}, \quad \delta \rightarrow +0 \quad (1.12)$$

The sign of $\delta \rightarrow 0$ is chosen to guarantee $G_\lambda(\tau) = 0$ for $\tau < 0$. In fact we have:

$$\begin{aligned} G_\lambda(\tau) &= i \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \frac{e^{-i\varepsilon\tau}}{\varepsilon - \varepsilon_\lambda + i\delta} \\ &= \begin{cases} e^{-i\varepsilon_\lambda\tau} & \text{for } \tau > 0 \\ 0 & \text{for } \tau < 0 \end{cases} \end{aligned} \quad (1.13)$$

To convince yourself note, that the integrand here has a pole at $\varepsilon = \varepsilon_\lambda - i\delta$. Then for $\tau > 0$ we can close the integration contour in the lower half-plane of complex variable ε (as the factor $e^{-i\varepsilon\tau}$ guarantees the exponential damping of the integrand at the semicircle at infinity in the lower half-plane), then the pole of the integrand is inside the contour of integration and using Cauchy theorem we obtain the result given in Eq. (1.13). For $\tau < 0$, to guarantee the zero contribution from the semicircle, we have to close integration contour in the upper half-plane of ε . Then there is no pole inside the contour and the integral reduces to zero.

In a mixed $(\mathbf{r}, \varepsilon)$ representation we obtain:

$$\begin{aligned} G(\mathbf{r}, \mathbf{r}', \varepsilon) &= \sum_{\lambda, \lambda'} G_{\lambda\lambda'}(\varepsilon) \varphi_\lambda(\mathbf{r}) \varphi_{\lambda'}^*(\mathbf{r}') \\ &= \sum_{\lambda} \frac{\varphi_\lambda(\mathbf{r}) \varphi_\lambda^*(\mathbf{r}')}{\varepsilon - \varepsilon_\lambda + i\delta} \end{aligned} \quad (1.14)$$

¹Note the additional factor i which we introduced in (1.10), (1.11) and below in (1.19) which guarantees correspondence with standard notations of ‘‘AGD’’. Usually this factor is just added in the definition of Green’s function [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963)].

Here the sum over λ includes summation over all bound states and integration over the continuous part of the spectrum. We can see that $G(\mathbf{r}, \mathbf{r}', \varepsilon)$ possesses poles at the values of ε equal to ε_λ , i.e. at the energies of bound states, and the cut (continuum of the poles) on the part of the real axis of ε , corresponding to the continuous part of the spectrum.

Consider now the many-particle system. Let us limit discussion only to the case of (many) Fermions. Similar analysis can be given for the system of Bose particles, but we skip it referring the reader to the general courses [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963); Lifshits E.M., Pitaevskii L.P. (1980)]. Consider first the case of non-interacting Fermions (Fermi-gas). Elementary excitations in this case are pairs of excited particles (above the Fermi surface) and holes (below the Fermi surface).

Let us determine Green's function for a particle excitation $G_{\lambda\lambda'}(\tau)$, i.e. the transition amplitude of a particle from some state λ to a state λ' (for the case of non-interacting Fermions). We have to take into account limitations due to Pauli principle, i.e. exclude transitions to occupied states. This can be achieved by an additional factor $(1 - n_\lambda)$ in the definition of the Green's function, where

$$n_\lambda = \begin{cases} 1 & \text{for } \varepsilon_\lambda \leq \varepsilon_F \\ 0 & \text{for } \varepsilon_\lambda > \varepsilon_F \end{cases} \quad (1.15)$$

is just the particle number in a state λ (Fermi distribution for $T = 0$). Thus we obtain:

$$G_{\lambda\lambda'}^+(\tau) = (1 - n_\lambda)\delta_{\lambda\lambda'} \begin{cases} e^{-i\varepsilon_\lambda\tau} & \text{for } \tau > 0 \\ 0 & \text{for } \tau < 0 \end{cases} \quad (1.16)$$

Let us now find similar expression for holes. As the number of available states for holes at the state λ is just n_λ , we get:

$$G_{\lambda\lambda'}^-(\tau) = n_\lambda\delta_{\lambda\lambda'} \begin{cases} e^{i\varepsilon_\lambda\tau} & \text{for } \tau > 0 \\ 0 & \text{for } \tau < 0 \end{cases} \quad (1.17)$$

where we have taken into account also that the hole energy (with respect to the Fermi level) is opposite in sign to the particle energy.

It is convenient to introduce Green's function $G_\lambda(\tau)$, defined both for $\tau > 0$ and $\tau < 0$:

$$G_\lambda(\tau) = \begin{cases} G_\lambda^+(\tau) & \text{for } \tau > 0 \\ -G_\lambda^-(-\tau) & \text{for } \tau < 0 \end{cases} \quad (1.18)$$

Fourier transform of this function is easily calculated as:

$$\begin{aligned} G_\lambda(\varepsilon) &= -i(1 - n_\lambda) \int_0^\infty d\tau e^{-i\varepsilon_\lambda\tau + i\varepsilon\tau} + in_\lambda \int_{-\infty}^0 d\tau e^{i\varepsilon_\lambda\tau + i\varepsilon\tau} \\ &= \frac{1 - n_\lambda}{\varepsilon - \varepsilon_\lambda + i\delta} + \frac{n_\lambda}{\varepsilon - \varepsilon_\lambda - i\delta} \end{aligned} \quad (1.19)$$

where it is necessary to introduce $\delta \rightarrow +0$ to guarantee convergence. It is convenient to rewrite this expression as:

$$\begin{aligned} G_\lambda(\varepsilon) &= \frac{1}{\varepsilon - \varepsilon_\lambda + i\delta \text{sign}\varepsilon_\lambda} \\ &= \begin{cases} \frac{1}{\varepsilon - \varepsilon_\lambda + i\delta} & \text{for } \varepsilon_\lambda > \varepsilon_F \\ \frac{1}{\varepsilon - \varepsilon_\lambda - i\delta} & \text{for } \varepsilon_\lambda < \varepsilon_F \end{cases} \end{aligned} \quad (1.20)$$

where we have introduced sign-function: $\text{sign}(x) = 1$ for $x > 0$ and $\text{sign}(x) = -1$ for $x < 0$. Note that the Fourier transform of this Green's function has a pole at ε equal to a particle (hole) energy.

Consider now the system of *interacting* Fermions. Single-particle Green's function in a system of interacting Fermions can be defined as:

$$G^+(\mathbf{r}\mathbf{t}; \mathbf{r}'\mathbf{t}')_{t > t'} = \langle 0 | \hat{\psi}(\mathbf{r}\mathbf{t}) \hat{\psi}^+(\mathbf{r}'\mathbf{t}') | 0 \rangle \quad (1.21)$$

where $|0\rangle$ is an exact ground state ("vacuum") of our system, corresponding to the filled Fermi-sphere, $\hat{\psi}(\mathbf{r}\mathbf{t})$ is second quantized operator of a Fermi field in Heisenberg representation [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963)]:

$$\hat{\psi}(\mathbf{r}\mathbf{t}) = e^{iHt} \hat{\psi}(\mathbf{r}) e^{-iHt} \quad (1.22)$$

with H – the Hamiltonian of our many-particle (interacting) system. Operator $\hat{\psi}(\mathbf{r})$ can be expressed in a standard way via annihilation operators a_λ of a particle in λ -states (while $\hat{\psi}^+$ is similarly expressed via creation operators a_λ^+):

$$\hat{\psi}(\mathbf{r}) = \sum_\lambda a_\lambda \varphi_\lambda(\mathbf{r}) \quad (1.23)$$

Eq. (1.21) obviously gives us the transition amplitude for a particle propagating from $(\mathbf{r}'\mathbf{t}')$ to $(\mathbf{r}\mathbf{t})$.

Similar expression can be written for propagating hole:

$$G^-(\mathbf{r}\mathbf{t}; \mathbf{r}'\mathbf{t}')_{t > t'} = \langle 0 | \hat{\psi}^+(\mathbf{r}'\mathbf{t}') \hat{\psi}(\mathbf{r}\mathbf{t}) | 0 \rangle \quad (1.24)$$

where it is taken into account that annihilation of a particle in a given point is equivalent to creation of a hole.

Both expressions (1.21) and (1.24) are defined for $t > t'$. It is convenient to can write down a single expression, which for $t > t'$ describes propagating particle, while for $t < t'$ – propagating hole (similarly to Eq. (1.18)):

$$G(\mathbf{r}t; \mathbf{r}'t') = \begin{cases} G^+(\mathbf{r}t; \mathbf{r}'t') & \text{for } t > t' \\ -G^-(\mathbf{r}'t'; \mathbf{r}t) & \text{for } t < t' \end{cases} \quad (1.25)$$

Another way to write this is²:

$$G(x, x') = \langle 0 | T \hat{\psi}(x) \hat{\psi}^+(x') | 0 \rangle \quad (1.26)$$

where we have denoted $x = (\mathbf{r}t)$, and the symbol of T -ordering means that all the operators standing to the right of T are placed in order over time arguments, with those corresponding to later moments standing to the left from those corresponding to earlier times, with the account of a sign change due to permutations of Fermion operators (necessary to place operators in the “right” order in time arguments). Formal definition of T -ordering taken from the quantum field theory is given by:

$$T \{F_1(t_1)F_2(t_2)\} = \begin{cases} F_1(t_1)F_2(t_2) & \text{for } t_1 > t_2 \\ -F_2(t_2)F_1(t_1) & \text{for } t_1 < t_2 \end{cases} \quad (1.27)$$

for Fermion operators and

$$T \{B_1(t_1)B_2(t_2)\} = \begin{cases} B_1(t_1)B_2(t_2) & \text{for } t_1 > t_2 \\ B_2(t_2)B_1(t_1) & \text{for } t_1 < t_2 \end{cases} \quad (1.28)$$

for Boson operators. Green’s function defined by Eq. (1.26) is usually called Feynman or causal (T -ordered)³.

²Standard definition of “AGD” differs by an additional factor of $-i$, which we have taken into account in Fourier transforms above.

³Note that this definition does not coincide with that of the so called two-time Green’s function introduced by Bogoliubov and Tyablikov and used in the theory of linear response [Zubarev D.N. (1974)], even if we go there to the limit of zero temperature. The advantage of introducing Feynman’s functions is in the availability of diagram technique, giving the universal method to calculate these Green’s functions via perturbation theory. There is no (convenient) diagram technique for Green’s functions of Bogoliubov and Tyablikov. There are a number of exact relations and methods, allowing to express the Green’s functions of linear response theory via Feynman’s functions for $T = 0$ and appropriate generalizations for the case of finite temperatures (Matsubara formalism) which we shall use below [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963); Lifshits E.M., Pitaevskii L.P. (1980)].

If we deal with an infinite homogeneous (translation invariant) system we have $G(\mathbf{r}t; \mathbf{r}'t') = G(\mathbf{r} - \mathbf{r}', t - t')$ and it is convenient to perform Fourier transformation both in $t - t'$ and $\mathbf{r} - \mathbf{r}'$:

$$G(\mathbf{p}\tau) = \int d^3r G(\mathbf{r}\tau) e^{-i\mathbf{p}\mathbf{r}} \quad (1.29)$$

where

$$G(\mathbf{p}\tau) = \begin{cases} \langle 0 | a_{\mathbf{p}} e^{-iH\tau} a_{\mathbf{p}}^{\dagger} | 0 \rangle e^{iE_0\tau} & \tau > 0 \\ - \langle 0 | a_{\mathbf{p}}^{\dagger} e^{iH\tau} a_{\mathbf{p}} | 0 \rangle e^{-iE_0\tau} & \tau < 0 \end{cases} \quad (1.30)$$

where E_0 is the ground state energy (in our case just equal to Fermi energy E_F).

Quasiparticles can be a viable concept if the single-particle Green's function of a system under consideration can be expressed as ($\tau > 0$):

$$G(\mathbf{p}\tau) \approx Z e^{-i\xi(\mathbf{p})\tau - \gamma(\mathbf{p})\tau} + \dots \quad \text{and} \quad \gamma(\mathbf{p}) \ll \xi(\mathbf{p}) \quad (1.31)$$

where $\xi(\mathbf{p}) = \varepsilon(\mathbf{p}) - E_F$, i.e. it contains a contribution of the form similar to that of the Green's function of the free (non-interacting) Fermi gas. Eq. (1.31) means the presence (with amplitude Z in the ground state $|0\rangle$) of a wave-packet, corresponding to a quasiparticle with energy $\xi(\mathbf{p})$ and *damping* $\gamma(\mathbf{p})$. We have to require that $\gamma(\mathbf{p}) \ll \xi(\mathbf{p})$, i.e. the weakness of damping to make quasiparticles "well defined"⁴. In a similar way, for $\tau < 0$ we can define the Green's function for a quasihole. Finally, in a system with well defined quasiparticles the Fourier transform of the Green's function (1.26) can be written as:

$$\begin{aligned} G(\mathbf{p}\varepsilon) &= Z \left\{ \frac{1 - n_{\mathbf{p}}}{\varepsilon - \xi(\mathbf{p}) + i\gamma(\mathbf{p})} + \frac{n_{\mathbf{p}}}{\varepsilon - \xi(\mathbf{p}) - i\gamma(\mathbf{p})} + G_{reg}(\mathbf{p}\varepsilon) \right\} \\ &= \frac{Z}{\varepsilon - \xi(\mathbf{p}) + i\gamma(\mathbf{p}) \text{sign}(p - p_F)} + G_{reg}(\mathbf{p}\varepsilon) \end{aligned} \quad (1.32)$$

We see that the poles of this expression define the quasiparticle spectrum and damping. This is a general property of Green's functions, allowing to determine the quasiparticle spectrum in many-particle system. The value of G_{reg} in (1.32) is determined by the contribution of many-particle excitations, and in most cases is of no special importance. However, in systems with strong correlations (interactions) we may meet with situation, when

⁴This condition, as we shall see below, is satisfied in Landau theory of Fermi liquids, where close to the Fermi surface we have: $\xi(\mathbf{p}) \approx v_F(|\mathbf{p} - p_F|)$, while $\gamma(\mathbf{p}) \sim (|\mathbf{p} - p_F|)^2$ (v_F is Fermi velocity).

there is actually no quasiparticle poles in the Green's function, so that there is no single-particle excitations at all and everything is actually determined by G_{reg} , making the studies of the properties of such systems much more complicated.

Why do we need Green's functions at all? First they give us the general method to study the spectrum of excitations in many-particle (interacting) systems. It happens also, that the knowledge of Green's functions allows to calculate ground state ($T = 0$) averages of arbitrary physical characteristics of many-particle systems. Let us consider simple examples. Using the introduced *single-particle* Green's function we may calculate the ground state averages of operators which can be written as a sum of single-particle contributions (one-particle operators) [Bogoliubov N.N. (1991a); Sadovskii M.V. (2003a)]:

$$\hat{A} = \sum_i \hat{A}_i(x_i, \mathbf{p}_i) \quad (1.33)$$

where x_i represents e.g. both spatial and spin variables, while \mathbf{p}_i are the momenta (operators!) of separate particles of our system. Typical examples are:

$$n(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \quad (1.34)$$

– operator of the particle density at the point \mathbf{r} ,

$$\mathbf{j}(\mathbf{r}) = \frac{e}{m} \sum_i \mathbf{p}_i \delta(\mathbf{r} - \mathbf{r}_i) \quad (1.35)$$

– current density at \mathbf{r} etc.

Operator \hat{A} in second quantized form can be written as:

$$\hat{A} = \int dx \psi^\dagger(x) A(x, \mathbf{p}) \psi(x) \quad (1.36)$$

Consider Green's function (1.25), (1.26) at $t = t' - 0$:

$$G(x, x', \tau)|_{\tau \rightarrow -0} = - \langle 0 | \psi^\dagger(x') \psi(x) | 0 \rangle \quad (1.37)$$

Then the average value of \hat{A} in the ground state can be written as:

$$\langle A \rangle = \int dx A(x, \mathbf{p}) G(x, x', \tau = -0)|_{x=x'} = -SpAG|_{\tau=-0} \quad (1.38)$$

Thus, the value of $G|_{\tau=-0}$ up to a sign coincides with single-particle density matrix at $T = 0$:

$$\rho(x', x) = \langle 0 | \psi^+(x') \psi(x) | 0 \rangle = -G|_{\tau=-0} \quad (1.39)$$

To determine the average values of two-particle operators:

$$\hat{B} = \sum_{ik} B_{ik}(x_i \mathbf{P}_i; x_k \mathbf{P}_k) \quad (1.40)$$

we have to calculate *two-particle* Green's function, defined usually as:

$$G_2(1, 2; 3, 4) = \langle 0 | T \psi(1) \psi(2) \psi^+(3) \psi^+(4) | 0 \rangle \quad (1.41)$$

etc. Thus, the problem of finding the average values of multi-particle operators, requires the knowledge of appropriate density matrices [Bogoliubov N.N. (1991a)], which can be expressed via corresponding multi-particle Green's functions.

1.2 Diagram technique. Dyson equation

Feynman diagrams give an elegant graphical representation of arbitrary contributions to perturbation series for Green's functions. The standard way to obtain specific diagram rules for a given interacting system reduces to the study of (scattering) S -matrix perturbation expansion and the use of the Wick's theorem [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963); Lifshits E.M., Pitaevskii L.P. (1980)]. Typical graphic elements of any diagram technique are Green's functions *lines* and interaction *vertices*, which are combined into Feynman diagrams of a certain "topology", depending on the nature of interaction under consideration. Below we shall formulate these rules explicitly [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963)] for different kinds of interactions, which will be studied in these lectures.

Wonderful aspect of Feynman diagram technique is the possibility to perform *graphical summation* of infinite (sub)series of diagrams. Consider the simplest (and actually most important!) example of such summation, leading to the derivation of the so called Dyson's equation [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963); Lifshits E.M., Pitaevskii L.P. (1980)]. Let us denote an *exact* Green's function by a "fat" (or "dressed" line), and a free-particle Green's function via "thin" line. Full transition

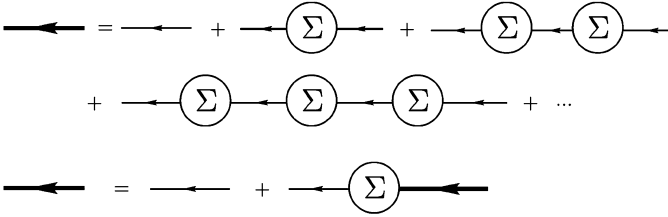


Fig. 1.1 Diagrammatic derivation of the Dyson equation.

amplitude (Green's function) of a transition from point 2 to point 1 is obviously equal to the sum of all possible transition amplitudes, appearing at all orders of perturbation theory, i.e. to the sum of all possible Feynman diagrams for the Green's function. Let us classify diagrams in the following way. First of all separate the only graph (line), corresponding to the propagation of a free particle. The remaining diagrams has the following form: up to some point the particle is propagating freely, then some scattering occurs, resulting in creation and annihilation of a number of particles and holes (or the particle is just scattered by the other particles, belonging to the Fermi "sea", below the Fermi level), then again we have a freely propagating particle, then scattering processes (interactions) are repeated etc. Let us denote as Σ the sum of all diagrams, which can not be separated in two parts by *cutting a single Fermion line*, this "block" Σ is called the irreducible *self-energy* of a particle (Fermion). Now we can easily convince ourselves that the full Green's function is determined by the Dyson equation, graphically shown in Fig. 1.1. In analytic form it is an integral equation:

$$G(1, 2) = G_0(1, 2) + \int d\tau_3 d\tau_4 G_0(1, 3) \Sigma(3, 4) G(4, 2) \quad (1.42)$$

Iterating this equation we obtain the full perturbation series for the Green's function. After Fourier transformation Dyson equation is reduced to the algebraic one:

$$G(\mathbf{p}\varepsilon) = G_0(\mathbf{p}\varepsilon) + G_0(\mathbf{p}\varepsilon) \Sigma(\mathbf{p}\varepsilon) G(\mathbf{p}\varepsilon), \quad (1.43)$$

which is easily solved:

$$G(\mathbf{p}\varepsilon) = \frac{1}{\varepsilon - \varepsilon(\mathbf{p}) - \Sigma(\mathbf{p}\varepsilon)} \quad (1.44)$$

where we have taken into account the explicit form of $G_0(\mathbf{p}\varepsilon)$. It is clear that the self-energy $\Sigma(\mathbf{p}\varepsilon)$ represents in a compact form all changes in a particle motion as a result of its interaction with other particles of a system. In general case, self-energy is complex, i.e. consists of real and imaginary parts (that is the reason why in (1.44) we have dropped an infinitesimal imaginary term of the free particle $i\delta\text{sign}(\varepsilon - \varepsilon_F)$). Solving Dyson equation in some approximation (or, in rare cases, exactly) allows us to analyze the energy (excitation) spectrum of many-particle interacting systems.

1.3 Green's functions at finite temperatures

Green's functions formalism is almost directly generalized for the case of finite temperatures T [Abrikosov A.A., Gorkov L.P., Dzyaloshinskii I.E. (1963)]. To remind the reader the essence of this (Matsubara) formalism we again restrict ourselves mainly to the case of Fermions. So called thermodynamic (or Matsubara) Green's function is defined as:

$$\mathcal{G}(\mathbf{p}, \tau_2 - \tau_1) = -i \langle T_\tau a_{\mathbf{p}}(\tau_2) a_{\mathbf{p}}^+(\tau_1) \rangle \quad (1.45)$$

where we use "interaction" representation for operators in the following form:

$$a_{\mathbf{p}}(\tau) = e^{(H - \mu N)\tau} a_{\mathbf{p}} e^{-(H - \mu N)\tau} \quad (1.46)$$

where Matsubara "time" $0 < \tau_1, \tau_2 < \beta = \frac{1}{T}$ and μ is the chemical potential, while angular brackets denote the averaging over grand canonical Gibbs ensemble, which is conveniently written as:

$$\langle A \rangle = \frac{Sp \rho A}{Sp \rho} \quad \text{where} \quad \rho = e^{-\beta(H - \mu N)} \quad (1.47)$$

with $Z = Sp \rho$.

The reason why Matsubara Green's functions \mathcal{G} can be expanded in (almost) the same diagrammatic expansion, as quantum mechanical Green's functions G in the case of $T = 0$, is as follows. We have seen that diagrammatic expansion for G directly follows from the time dependent Schrödinger equation. Statistical operator ρ , written as in (1.47), satisfies the so called Bloch equation:

$$\frac{\partial \rho}{\partial \beta} = -(H - \mu N)\rho \quad (1.48)$$

as is easily checked just by differentiation. There is direct correspondence between Schrödinger equation (1.1) and Bloch equation (1.48):

$$\psi \leftrightarrow \rho \quad H \leftrightarrow H - \mu N \quad it \leftrightarrow \beta \quad (1.49)$$

Thus, after the simple substitution of

$$H \rightarrow H - \mu N \quad it \rightarrow \tau \quad (1.50)$$

in the expressions of the previous section, we can obtain Matsubara Green's function formalism for \mathcal{G} of almost the same form as in the case of $T = 0$ for quantum mechanical G . Substitution $H \rightarrow H - \mu N$ leads only to the appropriate change of the single particle energy by μ :

$$H_0 - \mu N = \sum_{\mathbf{p}} (\varepsilon(\mathbf{p}) - \mu) a_{\mathbf{p}}^+ a_{\mathbf{p}} \quad (1.51)$$

Though Matsubara Green's functions \mathcal{G} depend on "imaginary time" τ ⁵, we may always return to the real time via substitution (in final expressions) $\tau \rightarrow it$, or, strictly speaking, via analytical continuation of Matsubara expressions from imaginary to real time axis.

Above we have already noted that the values of τ_1 and τ_2 in (1.45) are limited to the interval from 0 to β . Accordingly, to perform Fourier transformation over τ we have to introduce \mathcal{G} periodically continued on the interval from $-\infty$ to ∞ . Then we can write down the Fourier expansion as:

$$\mathcal{G}(\mathbf{p}\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau} \mathcal{G}(\mathbf{p}\omega_n) \quad (1.52)$$

where summation is over discrete (Matsubara) frequencies $\omega_n = \pi nT$. Then:

$$\mathcal{G}(\mathbf{p}\omega_n) = \frac{1}{2} \int_{-\beta}^{\beta} d\tau e^{i\omega_n\tau} \mathcal{G}(\mathbf{p}\tau) \quad (1.53)$$

"Time" difference $\tau = \tau_2 - \tau_1$ belongs to the interval $(-\beta, \beta)$, as both τ_1 and τ_2 vary on the interval $(0, \beta)$. The function $\mathcal{G}(\mathbf{p}\tau)$ periodically reproduces itself on intervals $(-\beta, \beta)$, $(\beta, 3\beta)$, $(3\beta, 5\beta)$, ..., $(-3\beta, -\beta)$, For the system

⁵The value τ was taken real, but Green's function \mathcal{G} can be obtained from G by a substitution $it \rightarrow \tau$, so that in thermodynamic formalism we are dealing with a transition to $t = -i\tau$, i.e. "imaginary time".

consisting of Fermions, the even values of n drop out from the series for $\mathcal{G}(\mathbf{p}\tau)$ due to “antiperiodic” boundary condition:

$$\mathcal{G}(\mathbf{p}, \tau) = -\mathcal{G}(\mathbf{p}, \tau + \beta) \quad \text{for } \tau < 0 \quad (1.54)$$

Validity of this expression is checked using the property of the trace: $SpAB = SpBA$. For $\tau' - \tau > 0$ we have:

$$\begin{aligned} \mathcal{G}(\mathbf{p}, \tau - \tau') &= \frac{i}{Z} Sp e^{-\beta(H - \mu N)} a_{\mathbf{p}}^+(\tau') a_{\mathbf{p}}(\tau) \\ &= \frac{i}{Z} Sp a_{\mathbf{p}}(\tau) e^{-\beta(H - \mu N)} a_{\mathbf{p}}^+(\tau') e \\ &= \frac{i}{Z} Sp e^{-\beta(H - \mu N)} e^{\beta(H - \mu N)} a_{\mathbf{p}}(\tau) e^{-\beta(H - \mu N)} a_{\mathbf{p}}^+(\tau') \\ &= \frac{i}{Z} Sp e^{-\beta(H - \mu N)} a_{\mathbf{p}}(\tau + \beta) a_{\mathbf{p}}^+(\tau') \end{aligned} \quad (1.55)$$

or

$$\mathcal{G}(\mathbf{p}, \tau - \tau') = -\mathcal{G}(\mathbf{p}, \tau - \tau' + \beta) \quad (1.56)$$

which for $\tau' = 0$ gives us (1.54). The minus sign appears here due to anticommutation of Fermi operators. Substituting (1.54) into (1.52) we see, that all contributions with even n are just zero. Thus for the Fermion case we are always dealing with the odd Matsubara frequencies:

$$\omega_n = \frac{(2n + 1)\pi}{\beta} = (2n + 1)\pi T \quad (1.57)$$

For Bosons, in a similar way, only contributions from even Matsubara frequencies

$$\omega_n = \frac{2n\pi}{\beta} = 2n\pi T \quad (1.58)$$

survive in the Fourier series for the Green’s function.

Returning to Eqs. (1.16), (1.17) and (1.18) for Green’s functions of the free particles at $T = 0$, we can easily write down the free-particle Matsubara Green’s function as:

$$\mathcal{G}_0(\mathbf{p}, \tau_2 - \tau_1) = -i\{\theta(\tau_2 - \tau_1)(1 - n(\mathbf{p})) - \theta(\tau_1 - \tau_2)n(\mathbf{p})\}e^{-(\varepsilon(\mathbf{p}) - \mu)(\tau_2 - \tau_1)} \quad (1.59)$$

where $n(\mathbf{p}) = [e^{\beta(\varepsilon(\mathbf{p}) - \mu)} + 1]^{-1}$ is the Fermi distribution for finite T . Thus, the step functions entering the definition of G_0 at $T = 0$ are smeared

by finite temperatures, leading to the simultaneous appearance of both particles and holes in a state with a given \mathbf{p} .

Substituting (1.59) into (1.53) we find⁶:

$$\mathcal{G}_0(\mathbf{p}\omega_n) = \frac{i}{i\omega_n - \varepsilon(\mathbf{p}) + \mu}, \quad \omega_n = (2n + 1)\pi T \quad (1.60)$$

With only the major change to discrete frequencies, Matsubara diagram technique at finite T is practically identical with quantum mechanical diagram technique at $T = 0$. The full Green's function is determined from Dyson equation:

$$\mathcal{G}(\mathbf{p}\omega_n) = \frac{i}{i\omega_n - \varepsilon(\mathbf{p}) + \mu - \Sigma(\mathbf{p}\omega_n)}, \quad \omega_n = (2n + 1)\pi T \quad (1.61)$$

Let us stress, however, that Matsubara Green's functions do not have the meaning of any kind of "transition amplitudes" (propagators) of the quantum (field) theory.

Calculating Matsubara Green's functions we can, in principle, find any thermodynamic characteristic of any many-particle system at equilibrium. Description of general non-equilibrium processes can be based on the more general formalism of Keldysh Green's functions [Lifshits E.M., Pitaevskii L.P. (1980)] and appropriate diagram technique. However, this formalism is outside the scope of our lectures.

⁶Here again we have an extra factor of i in comparison with standard notations of "AGD", which actually appeared in our Eq. (1.45).