

Chapter 2

Green's Functions at Zero Temperature

Men say that the Bodhisat Himself drew it with grains of rice upon dust, to teach His disciples the cause of things. Many ages have crystallised it into a most wonderful convention crowded with hundreds of little figures whose every line carries a meaning.

Rudyard Kipling. "Kim."

Abstract Green's functions as a tool for probing the response of a many-body system to an external perturbation. Similarity and difference from a one-particle propagator. Statistical ensembles. Definition of Green's functions at zero temperature. Analytical properties of Green's functions and their relation to quasiparticles. Perturbation theory and diagram techniques for Green's functions at zero temperature. "Dressing" of particles and interactions: Polarization operator and self energy. Many-particle Green's functions.

2.1 Green's Function of The Many-Body System: Definition and Properties

2.1.1 Definition of Green's Functions of the Many-Body System

When we discussed one-particle states in the second quantization representation, from the formally mathematical point of view *any* complete set of functions dependent on the coordinates (spin, etc.) of one particle would work. But from the point of view of physics it is not so: the set must be chosen in a "physically reasonable way." That is, since we virtually never can solve our equations exactly and not always can provide an "epsilon-delta"-style estimate of the approximations involved, the initial setup must be as close as possible to the solution that we are striving to reach.

For the one-particle state this means that it should be relatively stable, thus possessing some measurable characteristics and giving us a palatable zero-order approximation: the one of *independent quasiparticles*. (We have discussed this at some length in Chap. 1. Here we are going to elaborate that qualitative discussion and see how it fits the general formalism of perturbation theory developed so far.)

We have seen that the field operator satisfies the “Schrödinger equation”

$$i\hbar \frac{\partial}{\partial t} \psi(\xi, t) = (\mathcal{E}(\xi, t) + \mathcal{V}(\xi, t))\psi(\xi, t) + \int d\xi' \psi^\dagger(\xi', t) \mathcal{U}(\xi', \xi) \psi(\xi', t) \psi(\xi, t) + \dots \quad (2.1)$$

Here \mathcal{E} and \mathcal{V} are operators of kinetic energy and external potential; \mathcal{U} describes instantaneous particle–particle interactions, and so on. Evidently, if the basic set of one-particle functions is chosen correctly, the leading term in this equation will be the one-particle one; i.e.,

$$i\hbar \frac{\partial}{\partial t} \psi(\xi, t) \approx (\mathcal{E}(\xi, t) + \mathcal{V}(\xi, t))\psi(\xi, t). \quad (2.2)$$

This is a mathematical demonstration of the fact that we have a system of weakly interacting objects—“quasiparticles”—which can be approximately described by (2.2). Since the deviations from this description are small, the lifetimes of these objects are large enough to measure their characteristics in some way, and so they are reasonably well defined. And as often as not they are drastically different from the properties of free particles, already due to the presence of the \mathcal{V} -term in the above equation. Let us consider this point in more detail.

For example, when we investigate the properties of electrons in a metal, the reasonable first approximation is to take into account the periodic potential of the crystal lattice, neglecting for a while both electron–electron interactions and “freezing” the ions at their equilibrium positions. Even in this crude approximation the properties of these “quasielectrons” are very different from those of a QED electron, with its mass of 9.109×10^{-28} g and electric charge of -4.803×10^{-10} esu. Its mass is now, generally, anisotropic and may be significantly less or more; its charge may become positive; its momentum is no longer conserved due to the celebrated Umklapp processes; and there can exist several different species of electrons in our system! (See Fig. 2.1.)

On the other hand, when we are interested in the properties of the crystal lattice of the very metal, we quantize the motion of the ions, and come to the concept of *phonons*. These are quasiparticles, if there are any, because outside the lattice phonons simply don’t exist, while inside it they thrive. They even interact with electrons and each other—through terms like the third one in (2.1).

Of course, our ultimate goal is to take into account these other terms as well. *Then* we will have some other objects, governed by an equation like (2.2) without any extra interaction—and *they* will be the actual quasiparticles in our system.

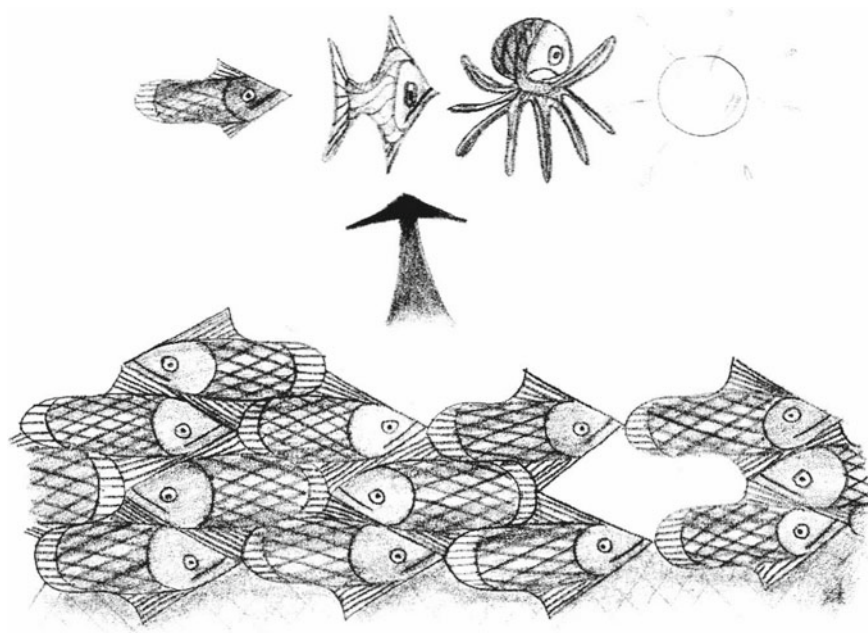


Fig. 2.1 Quasiparticles in the Fermi system

There is no contradiction here. In Chap. 1 we have seen how interactions “dress” a bare particle, making of it a quasiparticle; here we see it being made in two steps. The first step (a right choice of the basic set of one-particle states) is made *without* addressing any perturbation theory, usually based on symmetry considerations (or common physical sense), as when translation symmetry of the crystal lattice forces us to describe otherwise free electrons in terms of Bloch functions instead of simple plane waves, and we use the concept of phonons as a more adequate description of low-energy dynamics of the ions. Once chosen, this set of states (“basic quasiparticles,” if you wish) plays the very same role as the states of free particles in the absence of an external potential, and these two sets of states have a lot in common. For example, they live infinitely long (because by definition they have definite energy, $\mathcal{E}\phi_j = E_j\phi_j$). If—as is the case in most books—we are dealing with a “liquid” of interacting fermions on a uniform background, the most natural choice of “basic quasiparticles” is *real* particles.

Therefore, later on we will call them simply “particles”, while reserving the term “quasiparticles” (or “elementary excitations”) *par excellence* for the ones “dressed” due to interactions with other particles. (The assumption that the description of the Fermi liquid can be based on the picture of a weakly interacting gas of such quasifermions was in the foundation of Landau’s phenomenological theory.)

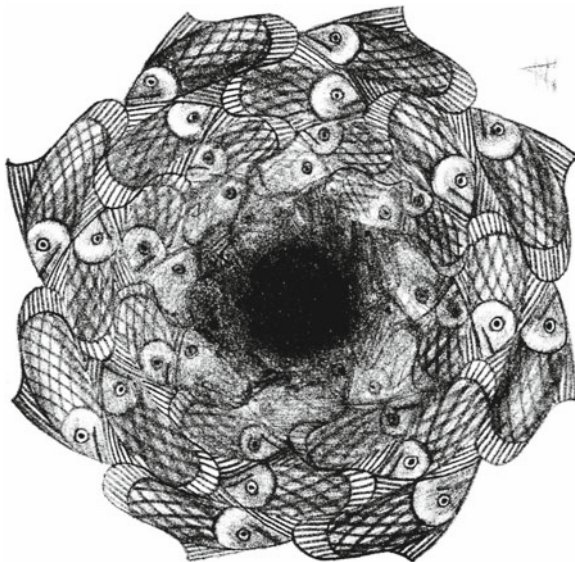


Fig. 2.2 Fermi surface and Fermi sphere

Now we can turn to the building of such a theory in the many-body case. We will begin with the case of single-component normal, uniform, and homogeneous Fermi and Bose system (the above-mentioned textbook case) at zero temperature.

This is the simplest possible *and* practically important case, since it does not involve superfluid (superconducting) condensate. (The discussion of the latter we postpone until Chap. 4.) In the Fermi case it applies to nonsuperconducting metals and semiconductors—if we forget for a while about the subtleties of band structures. Alkali metals are especially good examples (Fig. 2.2).

In the Bose case the example seems purely academic (since bosons must undergo Bose condensation at zero) until we recall that there is at least *one* practically important system of bosons that don't condense: phonons! (This is because the number of phonons is not conserved, but this is not important when we use the grand potential formalism.)

In Chap. 1 we introduced the one-particle propagator

$$K(x, t; x', t') = \langle x | S(t, t') | x' \rangle = \langle x t | x' t' \rangle$$

as a transmission amplitude of a particle between points (x', t') and (x, t) . A straightforward generalization of the former expression is a matrix element of the N -particle S -operator $\langle \Phi | S(t, t') | \Phi' \rangle$. Unfortunately, it is useless, since it involves transmission amplitude involving $N \approx 10^{23}$ particles. On the other hand, the one-particle propagator in the latter form suggests that we could look at two states with a single particle excited,

$$\begin{aligned} |x, t\rangle_{\text{state}} &\equiv \psi^\dagger(x, t)|\text{state}\rangle; \\ |x', t'\rangle_{\text{state}} &\equiv \psi^\dagger(x', t')|\text{state}\rangle \end{aligned}$$

(here the Heisenberg field operator $\psi^\dagger(x, t)$ creates a particle at a given point), and introduce Green's function as their overlap:

$$\text{Green's function} \rightsquigarrow \langle \text{state} | \psi(x, t) \psi^\dagger(x', t') | \text{state} \rangle.$$

Of course, we must average over the states of the many-body system on which our field operators act, in order to get rid of all other nonmacroscopic variables except the two coordinates and moments of time between which the quasiparticle travels. Such an averaging of an operator \mathcal{A} (both quantum and statistical) is achieved by taking its trace with the statistical operator (density matrix) of the system, $\hat{\rho}$,

$$\langle \mathcal{A} \rangle = \text{tr}(\hat{\rho} \mathcal{A}). \quad (2.3)$$

Now, the above formula indeed looks like a propagator, describing a process when we add to our system of N identical fermions one extra particle, let it propagate from (x', t') to (x, t) , and then take it away. It is a good probe of particle-particle interactions in the system. The other option would be *first* to take away the particle, look at how the resulting *hole* propagates, and then fill it, restoring the particle (Fig. 2.3).

Then the *one-particle causal Green's function*, describing both processes, can be defined by the expression

$$\begin{aligned} G_{\alpha\alpha'}(\mathbf{x}, t; \mathbf{x}', t') &= -i \left\langle \psi_\alpha(\mathbf{x}, t) \psi_{\alpha'}^\dagger(\mathbf{x}', t') \right\rangle \Theta(t - t') \mp i \left\langle \psi_{\alpha'}^\dagger(\mathbf{x}', t') \psi_\alpha(\mathbf{x}, t) \right\rangle \Theta(t' - t) \\ &\equiv -i \left\langle \mathcal{T} \psi_\alpha(\mathbf{x}, t) \psi_{\alpha'}^\dagger(\mathbf{x}', t') \right\rangle. \end{aligned} \quad (2.4)$$

Here we write spin indices explicitly. They can take two values (e.g., up and down) for fermions (and only one for phonons).¹

Averaging defined by (2.3) is a linear operation. Using this property, we can apply the time differentiation operator, $\partial/\partial t$, to $\mathcal{T} \psi_\alpha(\mathbf{x}, t) \psi_{\alpha'}^\dagger(\mathbf{x}', t')$, and average it to obtain

¹ It can be shown that no matter what the spin of real fermions, the (basic) quasiparticles will have spin 1/2 (though there will be *several* types of quasiparticles); see [4], §1).

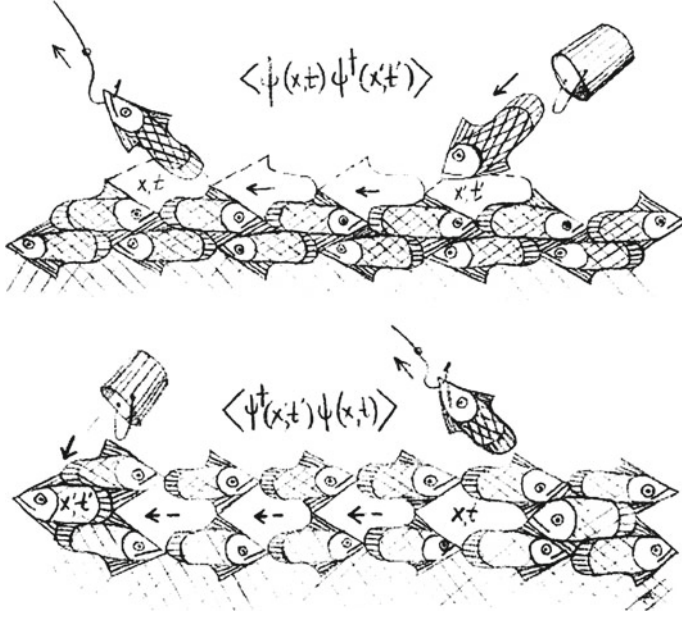


Fig. 2.3 Causal Green's function: the physical sense

$$i\hbar \frac{\partial}{\partial t_1} G_{\alpha\beta}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) \quad (2.5)$$

$$= \mathcal{E}(\mathbf{x}_1) G_{\alpha\beta}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) + \mathcal{V}(\mathbf{x}_1, t_1) G_{\alpha\beta}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) \\ - i \int d\mathbf{x}_3 U(\mathbf{x}_3, \mathbf{x}_1) \left\langle T \psi_\gamma^\dagger(\mathbf{x}_3, t_1) \psi_\gamma(\mathbf{x}_3, t_1) \psi_\alpha(\mathbf{x}_1, t_1) \psi_\beta^\dagger(\mathbf{x}_2, t_2) \right\rangle + \cdots \\ + \hbar \delta(\mathbf{x}_1 - \mathbf{x}_2) \delta(t_1 - t_2). \quad (2.6)$$

We see that the *many-body* Green's function defined above is not a Green's function in the mathematical sense. It is a solution to differential Eq.(2.6). This is not a closed equation for Green's function, since it contains averages of four and more field operators (two-particle, three-particle, etc. Green's functions). Thus (2.6) is only the first equation in the quantum analogue to the well known infinite *BBGKY chain* (Bogoliubov–Born–Green–Kirkwood–Yvon) in classical statistical mechanics. The latter consists of interlinked equations of motion for classical n -particle distribution functions (see e.g. in Chap. 3, [2]).

As in the classical case, breaking this chain leads to a *nonlinear* differential equation for Green's function, as distinct from the *linear* Eq. (1.25), which governs the one-particle propagator $K(x, t; x', t')$.

The averaging procedure in equilibrium can be performed most conveniently using either the *canonical* or *grand canonical* ensemble. Mathematically, the two reflect different choices of independent variables: (T, V, N : temperature, volume,

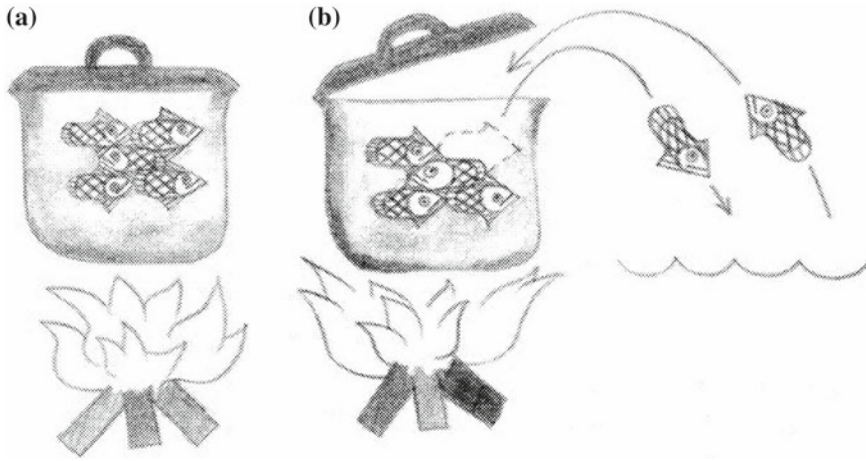


Fig. 2.4 Ensemble averaging. **a** Canonical ensemble; **b** grand canonical ensemble

number of particles) versus $(T, V, \mu; \text{temperature, volume, chemical potential})$. The physical difference is that in the former case the system can exchange only energy with its surroundings (thermostat), while in the latter the particles can leave and enter the system as well (Fig. 2.4), the average number of particles being fixed by the chemical potential, μ , as the temperature fixes the average kinetic energy of the particles in both cases.

The statistical operators are of Gibbs form,

$$\hat{\rho}_{CE} = e^{\beta(F - \mathcal{H})}, \quad (2.7)$$

or

$$\hat{\rho}_{GCE} = e^{\beta(\Omega - \mathcal{H}')}. \quad (2.8)$$

Here $\beta = 1/T$ (we put $k_B = 1$ to simplify the notation); $F = -(1/\beta) \times \ln \text{tr} e^{-\beta \mathcal{H}}$ is the free energy; $\mathcal{H}' = \mathcal{H} - \mu \mathcal{N}$, \mathcal{N} is the particle number operator; and the *grand potential* $\Omega = -(1/\beta) \ln \text{tr} e^{-\beta \mathcal{H}'} = -PV$. (The Lagrange term $-\mu \mathcal{N}$ evidently commutes with the rest of the Hamiltonian.) We can therefore introduce Heisenberg and interaction representations using \mathcal{H}' instead of \mathcal{H} and come to the same results, with the only difference being in corresponding eigenvalues of the Hamiltonian.

In the thermodynamic limit both approaches are equivalent. The situation may change when the size of the system under consideration becomes small enough, so that the fluctuations of the particle number cannot be ignored, and the two ensembles describe *physically* different systems (such as an isolated conducting grain vs. one connected to massive conductors by leads). At present, we will not deal with such a situation. Since the grand canonical ensemble is easier to work with, we will use it, and—to simplify notation—will henceforth omit primes in \mathcal{H}' and put $\hbar = 1$.

The Hamiltonian now has the complete set of eigenstates $|n\rangle$ with eigenvalues $E'_n = E_n - \mu N_n$, where N_n is the number of particles in state $|n\rangle$. The average of a time-ordered product of two field operators in Heisenberg representation can now be written as

$$\begin{aligned}
 & \left\langle \mathcal{T} \psi(t_1) \psi^\dagger(t_2) \right\rangle \\
 &= \text{tr}(e^{\beta(\Omega - \mathcal{H})} \mathcal{T} \psi(t_1) \psi^\dagger(t_2)) \\
 &= \sum_{n,m} \langle n | e^{\beta(\Omega - \mathcal{H})} | m \rangle \langle m | \mathcal{T} \psi(t_1) \psi^\dagger(t_2) | n \rangle \langle m | m \rangle^{-1} \langle n | n \rangle^{-1} \\
 &= \sum_n e^{\beta\Omega - \beta(E_n - \mu N_n)} \langle n | \mathcal{T} \psi(t_1) \psi^\dagger(t_2) | n \rangle \langle n | n \rangle^{-1} \\
 &= \sum_n e^{-\beta(E_n - \mu N_n)} \langle n | \mathcal{T} \psi(t_1) \psi^\dagger(t_2) | n \rangle \langle n | n \rangle^{-1} / \sum_n e^{-\beta(E_n - \mu N_n)}. \quad (2.9)
 \end{aligned}$$

(We have used the standard trick of inserting the complete set of states, and allow for the possibility that they are not normalized to unity.)

At zero temperature ($\beta \rightarrow \infty$) we are left with

$$G_{\alpha\beta}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = -i \frac{\langle 0 | \mathcal{T} \psi_\alpha(\mathbf{x}_1, t_1) \psi_\beta^\dagger(\mathbf{x}_2, t_2) | 0 \rangle}{\langle 0 | 0 \rangle}. \quad (2.10)$$

Here $|0\rangle$ is the exact *ground state* of the system in *Heisenberg representation*: it is time independent and includes all interaction effects.

In a homogeneous and isotropic system in a stationary state, Green's function can depend only on differences of coordinates and times:

$$G_{\alpha\beta}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = G_{\alpha\beta}(\mathbf{x}_1 - \mathbf{x}_2, t_1 - t_2). \quad (2.11)$$

If, moreover, the system is not magnetically ordered and is not placed in and external magnetic field, then spin dependence in (2.11) reduces to a unit matrix:

$$G_{\alpha\beta} = \delta_{\alpha\beta} G, \quad (2.12)$$

where $G = \frac{1}{2} \text{tr} G_{\alpha\beta}$ (otherwise there would be a special direction in space, the axis of spin quantization).

2.1.1.1 Unperturbed Green's Functions

It is straightforward now to calculate the unperturbed Green's functions, starting from the definition. For the fermions,

$$G^0(\mathbf{x}, t) = \frac{1}{i} \left\langle \mathcal{T} \psi(\mathbf{x}, t) \psi^\dagger(0, 0) \right\rangle_0. \quad (2.13)$$

Expanding the field operators in the basis of plane waves, $\psi(\mathbf{x}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\mathbf{x} - i(\epsilon_{\mathbf{k}} - \mu)t}$, and taking into account that at zero temperature in equilibrium the average $\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \rangle_0 = \delta_{\mathbf{k}, \mathbf{k}'} n_F(\epsilon_{\mathbf{k}}) = \delta_{\mathbf{k}, \mathbf{k}'} \theta(\mu - \epsilon_{\mathbf{k}})$, we find that

$$G^0(\mathbf{x}, t) = \frac{1}{iV} \sum_{\mathbf{k}} [\theta(t)(1 - \theta(\mu - \epsilon_{\mathbf{k}})) - \theta(-t)\theta(\mu - \epsilon_{\mathbf{k}})] e^{i\mathbf{k}\mathbf{x} - i(\epsilon_{\mathbf{k}} - \mu)t}. \quad (2.14)$$

The Fourier transform of this expression yields, finally,

$$\begin{aligned} G^0(\mathbf{p}, \omega) &= \frac{1}{\omega - (\epsilon_{\mathbf{p}} - \mu) + i0 \operatorname{sgn}(\epsilon_{\mathbf{p}} - \mu)} \\ &= \frac{1}{\omega - (\epsilon_{\mathbf{p}} - \mu) + i0 \operatorname{sgn} \omega}. \end{aligned} \quad (2.15)$$

The infinitesimal term in the denominator indicates in what half-plane of complex frequency the corresponding integrals will converge, exactly like what we had earlier for the retarded propagator. (For example, the integral $\int_0^\infty dt e^{i\omega t}$ due to the first term in (2.14) converges if $\Im \omega \rightarrow 0 +$.) The difference is that here we have the causal Green's function, which contains both $\theta(t)$ and $\theta(-t)$.

You are welcome to calculate the expression for the unperturbed phonon Green's function, defined as

$$D(\mathbf{x}, t; \mathbf{x}', t') = -i \langle 0 | \mathcal{T} \varphi(\mathbf{x}, t) \varphi(\mathbf{x}', t') | 0 \rangle, \quad (2.16)$$

where the phonon field operator is

$$\varphi(\mathbf{x}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \left(\frac{\omega_{\mathbf{k}}}{2} \right)^{1/2} \left\{ b_{\mathbf{k}} e^{i(\mathbf{k}\mathbf{x} - \omega_{\mathbf{k}}t)} + b_{\mathbf{k}}^\dagger e^{-i(\mathbf{k}\mathbf{x} - \omega_{\mathbf{k}}t)} \right\}, \quad (2.17)$$

and b, b^\dagger are the usual Bose operators. (Since the phonon field is ultimately a quantized sound wave, it should be Hermitian to yield in the classical limit a classical observable, the medium displacement.) You will see that

$$D^0(\mathbf{k}, \omega) = \frac{\omega_{\mathbf{k}}^2}{\omega^2 - \omega_{\mathbf{k}}^2 + i0}. \quad (2.18)$$

The unperturbed Green's function *is* the Green's function in the mathematical sense. For the fermions, e.g., it satisfies a linear equation,

$$\left(i\hbar \frac{\partial}{\partial t_1} - \mathcal{E}(\mathbf{x}_1) \right) G_{\alpha\beta}^0(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = \delta(\mathbf{x}_1 - \mathbf{x}_2) \delta(t_1 - t_2). \quad (2.19)$$

Symbolically this can be written as

$$(G^0)^{-1}(1)G^0(1, 2) = \mathcal{I}(1, 2),$$

where the operator $(G^0)^{-1}(1)$ in coordinate space is $(i\partial/\partial t_1 - \mathcal{E}(\nabla_{\mathbf{x}_1}))$, in momentum space $(\omega - \mathcal{E}(\mathbf{k}))$.

The derivation of the corresponding equation for $D^0(1, 2)$ is suggested as one of the problems to this chapter.

2.1.2 Analytic Properties of Green's Functions

When dealing with one-particle problems, we observed that some important properties of propagators could be obtained from general physical considerations, independently of the details of the system. This can be done in the many-body case as well. Specifically, we will derive the *Källen-Lehmann* representation for Green's functions in momentum space (as a function of (\mathbf{p}, ω)), which determines the analytic properties of Green's function in complex ω plane and leads to physically significant consequences.

Our only assumption here will be that our system is in a stationary and homogeneous state, or is space and time invariant. This means that (1) the full Hamiltonian \mathcal{H} is time independent and (2) the momentum operator \mathcal{P} commutes with \mathcal{H} (then the total momentum is by definition conserved); here

$$\mathcal{P} = \sum_{\alpha} \int d^3\mathbf{x} \psi_{\alpha}^{\dagger}(\mathbf{x})(-i\nabla)\psi_{\alpha}(\mathbf{x}). \quad (2.20)$$

It can be easily seen that for the simultaneous commutator,

$$[\psi_{\alpha}(\mathbf{x}, t), \mathcal{P}] = -i\nabla\psi_{\alpha}(\mathbf{x}, t) \quad (2.21)$$

for both Fermi and Bose field operators. (It is enough to substitute the definition of \mathcal{P} and use the canonical (anti)commutation relations.) Equation (2.21) is reminiscent of the Heisenberg equations of motion for a field operator (1.84), and they together imply

$$\begin{aligned} \psi_{\alpha}(\mathbf{x}, t) &= e^{-i(\mathcal{P}\mathbf{x} - \mathcal{H}t)}\psi_{\alpha}e^{i(\mathcal{P}\mathbf{x} - \mathcal{H}t)}, \\ \psi_{\alpha} &\equiv \psi_{\alpha}(\mathbf{0}, 0). \end{aligned} \quad (2.22)$$

In a more formal language, the Hamiltonian and the operator of total momentum are *generators of temporal and spatial shifts* respectively.

We can substitute the above expression into Green's function, (2.4), and then insert the unity operator constructed of the full set of common eigenstates of the two commuting operators \mathcal{H} , \mathcal{P} ,

$$\mathcal{I} = \sum_s |s\rangle\langle s|,$$

wherever it seems reasonable. The following calculations are tedious but straightforward.

$$\begin{aligned} \langle 0|\mathcal{T}\psi(x, t)\psi^\dagger(x', t')|0\rangle &= \theta(t-t') \sum_s \langle 0|\psi(x, t)|s\rangle\langle s|\psi^\dagger(x', t')|0\rangle \\ &\quad \mp \theta(t'-t) \sum_s \langle 0|\psi^\dagger(x', t')|s\rangle\langle s|\psi(x, t)|0\rangle \\ &= \theta(t-t') \sum_s \langle 0|e^{i(\mathcal{H}t-\mathcal{P}x)}\psi e^{-i(\mathcal{H}t-\mathcal{P}x)}|s\rangle\langle s|e^{i(\mathcal{H}t'-\mathcal{P}x')}\psi^\dagger e^{-i(\mathcal{H}t'-\mathcal{P}x')}|0\rangle \\ &\quad \mp \theta(t'-t) \sum_s \langle 0|e^{i(\mathcal{H}t'-\mathcal{P}x')}\psi^\dagger e^{-i(\mathcal{H}t'-\mathcal{P}x')}|s\rangle\langle s|e^{i(\mathcal{H}t-\mathcal{P}x)}\psi e^{-i(\mathcal{H}t-\mathcal{P}x)}|0\rangle \\ &= \theta(t-t') \sum_s e^{i(E_0-\mu N_0)t} \langle 0|\psi|s\rangle e^{-i((E_s-\mu N_s)t-P_sx)} \\ &\quad \times e^{i((E_s-\mu N_s)t'-P_sx')} \langle s|\psi^\dagger|0\rangle e^{-i(E_0-\mu N_0)t'} \\ &\quad \mp \theta(t'-t) \sum_s e^{i(E_0-\mu N_0)t'} \langle 0|\psi^\dagger|s\rangle e^{-i((E_s-\mu N_s)t'-P_sx')} \\ &\quad \times e^{i((E_s-\mu N_s)t-P_sx)} \langle s|\psi|0\rangle e^{-i(E_0-\mu N_0)t}. \end{aligned}$$

The momentum of the state $|0\rangle$ is zero. The energy exponents here contain some subtlety. Since the field operators create or annihilate particles one at a time, in the first part of the expression, which contains $\langle 0|\psi|s\rangle\langle s|\psi^\dagger|0\rangle \equiv |\langle 0|\psi|s\rangle|^2$ states $|s\rangle$ must contain one particle *more* than the state $|0\rangle$, say $N_s = N_0 + 1 \equiv N + 1$ (otherwise the annihilation operator has nothing to annihilate). On the other hand, in the second half of the expression, with $\langle 0|\psi^\dagger|s\rangle\langle s|\psi|0\rangle \equiv |\langle s|\psi|0\rangle|^2$ the states $|s\rangle$ contain $N - 1$ particles. Since, generally, the eigenvalues of the Hamiltonian depend on the number of particles both via the $-\mu N$ term and directly, we have in the exponents (showing explicitly the dependence of eigenenergies on the particle number)

$$\begin{aligned} &\exp[i(E_0(N) - \mu N)t - i((E_s(N+1) - \mu(N+1))t - P_sx)] \\ &\quad \times \exp[i((E_s(N+1) - \mu(N+1))t' - P_sx') - i(E_0(N) - \mu N)t'] \\ &= \exp[i[(E_0(N) - E_s(N+1) + \mu)(t-t') + P_s(x-x')]]; \\ &\quad \exp[i(E_0(N) - \mu N)t' - i((E_s(N-1) - \mu(N-1))t' - P_sx')] \\ &\quad \times \exp[i((E_s(N-1) - \mu(N-1))t - P_sx) - i(E_0(N) - \mu N)t] \\ &= \exp[i[(E_0(N) - E_s(N-1) - \mu)(t'-t) + P_s(x'-x)]]. \end{aligned}$$

As expected, everything depends on the differences of coordinates and times.

Denote the *excitation energies* by

$$\epsilon_s^{(+)} = E_s(N+1) - E_0(N) > \mu; \quad (2.23)$$

$$\epsilon_s^{(-)} = E_0(N) - E_s(N-1) < \mu. \quad (2.24)$$

Evidently, the former gives the energy change when a particle is added to the state $|s\rangle$; the latter, when the particle is removed from the state $|s\rangle$. (You can check the above inequalities, if you recall that at zero temperature for the ground-state energy (a thermodynamic observable!) $(\partial E_0/\partial N) = (\partial \Phi/\partial N)$, (Φ is thermodynamical potential) and that by definition $(\partial \Phi/\partial N) = \mu$.) For the phonons, $\mu = 0$.

Now we can sweep all the details of the system under the carpet by introducing

$$A_s = \left[\frac{1}{2} \right] \langle 0|0 \rangle^{-1} \left[\sum_{\alpha} \right] |\langle 0|\psi_{\alpha}|s \rangle|^2; \quad (2.25)$$

$$B_s = \left[\frac{1}{2} \right] \langle 0|0 \rangle^{-1} \left[\sum_{\alpha} \right] |\langle s|\psi_{\alpha}|0 \rangle|^2. \quad (2.26)$$

(The operations in the brackets are reserved for the spin degrees of freedom, α .) Those are some functions of index s only. Therefore, we can easily take the Fourier transform of Green's function, using the above results, and finally get the *Källén–Lehmann's representation*:

$$G(\mathbf{p}, \omega) = (2\pi)^3 \sum_s \left(\frac{A_s \delta(\mathbf{p} - \mathbf{P}_s)}{\omega - \epsilon_s^{(+)} + \mu + i0} \pm \frac{B_s \delta(\mathbf{p} + \mathbf{P}_s)}{\omega - \epsilon_s^{(-)} + \mu - i0} \right). \quad (2.27)$$

In this expression, delta functions of momenta arise from the exponential factors $\exp[i\mathbf{P}_s x]$; they indicate the values of momenta, corresponding to single-particle excitations (note that the second term in (2.27) clearly indicates the holes, with momenta $-\mathbf{P}_s$ and energies $\epsilon_s^{(-)}$). The frequency denominators contain the infinitesimal $\pm i0$, due to the presence of theta functions of time in the initial expression, exactly as when we calculated the unperturbed Green's functions. Of course, our present result is consistent with expressions (2.15, 2.18). Mathematically, the Källén–Lehmann representation tells us that Green's function of a finite system is a *meromorphic function* of the complex variable ω ; all its singularities are simple poles. Each pole corresponds to a definite excitation energy, $\epsilon_s^{(\pm)}$, and definite momentum of the system, $\pm \mathbf{P}_s$. The poles are infinitesimally shifted into the upper half-plane of ω when $\omega > 0$, and into the lower one when $\omega < 0$. Thus the causal Green's function is not analytic in either half-plane.

In the thermodynamic limit ($N, V \rightarrow \infty, N/V = \text{const}$) it is more convenient to use a different form of (2.27):

$$G(\mathbf{p}, \omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \left(\frac{\rho_A(\omega')}{\omega' - \omega - i0} + \frac{\rho_B(\omega')}{\omega' - \omega + i0} \right), \quad (2.28)$$

where

$$\rho_A(\mathbf{p}, \omega') = -\pi(2\pi)^3 \sum_s A_s \delta(\mathbf{p} - \mathbf{P}_s) \delta(\omega' - \epsilon_s^{(+)} + \mu); \quad (2.29)$$

$$\rho_B(\mathbf{p}, \omega') = \mp \pi(2\pi)^3 \sum_s B_s \delta(\mathbf{p} + \mathbf{P}_s) \delta(\omega' - \epsilon_s^{(-)} + \mu). \quad (2.30)$$

Indeed, in this limit we can no longer resolve the individual levels $\epsilon_s^{(\pm)}$. The densities $\rho_{A,B}(\mathbf{p}, \omega')$ become continuous functions, zero at negative (resp. positive) frequencies on the real axis; the latter becomes a *branch cut* in the complex ω plane.

The real and imaginary parts of Green's function (for *real* frequencies) can be easily obtained from (2.27), using the Weierstrass (or Sokhotsky—Weierstrass) formula

$$\frac{1}{x \pm i0} = \mathcal{P} \frac{1}{x} \mp i\pi \delta(x). \quad (2.31)$$

Here \mathcal{P} means the principal value. This is to be understood as a *generalized function*; that is, the above formula strictly speaking makes sense only under the integral, with an integrable function $F(x)$:

$$\int dx F(x) \frac{1}{x \pm i0} = \mathcal{P} \int dx \frac{F(x)}{x} \mp i\pi F(0).$$

The principal value integral $\mathcal{P} \int dx F(x)/x$ is defined as $\lim_{\epsilon \rightarrow 0} \left[\int^{-\epsilon} dx F(x)/x + \int_{\epsilon} dx F(x)/x \right]$. The other term arises from the integration over an infinitesimal semi-circle around the pole at $x = 0$. This formula is easy to prove using the technique of residues in the complex analysis.

Using this recipe, we find

$$\Re G(\mathbf{p}, \omega) = (2\pi)^3 \sum_s \mathbf{P} \left(\frac{A_s \delta(\mathbf{p} - \mathbf{P}_s)}{\omega - \epsilon_s^{(+)} + \mu} \pm \frac{B_s \delta(\mathbf{p} + \mathbf{P}_s)}{\omega - \epsilon_s^{(-)} + \mu} \right); \quad (2.32)$$

$$\Im G(\mathbf{p}, \omega) = (2\pi)^3 \pi \begin{cases} -\sum_s A_s \delta(\mathbf{p} - \mathbf{P}_s) \delta(\omega - \epsilon_s^{(+)} + \mu), & \omega > 0; \\ \pm \sum_s B_s \delta(\mathbf{p} + \mathbf{P}_s) \delta(\omega - \epsilon_s^{(-)} + \mu), & \omega < 0. \end{cases} \quad (2.33)$$

We thus obtain an important relation:

$$\begin{aligned} \text{sgn} \Im G(\mathbf{p}, \omega) &= -\text{sgn } \omega \text{ for Fermi systems;} \\ \text{sgn} \Im G(\mathbf{p}, \omega) &= -1 \text{ for Bose systems.} \end{aligned} \quad (2.34)$$

The difference reflects the fact that there is no Fermi surface in Bose systems (and thus “particles” and “holes” are the same).

The asymptotic behavior of $G(\omega)$ as $\omega \rightarrow \infty$ is very simple:

$$G(\omega) \sim 1/\omega. \quad (2.35)$$

To prove it, note that in this limit we can neglect all other terms in the denominators of (2.27), so that

$$G(\mathbf{p}, \omega) \sim \frac{1}{\omega} (2\pi)^3 \sum_s (A_s \delta(\mathbf{p} - \mathbf{P}_s) \pm B_s \delta(\mathbf{p} + \mathbf{P}_s)).$$

The sum can be evaluated by performing an inverse Fourier transform and making use of the canonical (anti)commutation relation between field operators in coordinate space:

$$\begin{aligned} (2\pi)^3 \sum_s (A_s \delta(\mathbf{p} - \mathbf{P}_s) \pm B_s \delta(\mathbf{p} + \mathbf{P}_s)) \\ &= \sum_s \int d^3(\mathbf{x} - \mathbf{x}') \left(A_s e^{i(\mathbf{p} - \mathbf{P}_s)(\mathbf{x} - \mathbf{x}')} \pm B_s e^{i(\mathbf{p} + \mathbf{P}_s)(\mathbf{x} - \mathbf{x}')} \right) \\ &= \sum_s \int d^3(\mathbf{x} - \mathbf{x}') \left[\frac{1}{2} \sum_\alpha \right] \left\{ |\langle 0 | \psi_\alpha(0) | s \rangle|^2 e^{i(\mathbf{p} - \mathbf{P}_s)(\mathbf{x} - \mathbf{x}')} \right. \\ &\quad \left. \pm |\langle s | \psi_\alpha(0) | 0 \rangle|^2 e^{i(\mathbf{p} + \mathbf{P}_s)(\mathbf{x} - \mathbf{x}')} \right\} \\ &= \int d^3(\mathbf{x} - \mathbf{x}') \left[\frac{1}{2} \sum_\alpha \right] e^{i\mathbf{p}(\mathbf{x} - \mathbf{x}')} \\ &\quad \times \langle 0 | \psi_\alpha(\mathbf{r}, t) \psi_\alpha^\dagger(\mathbf{r}', t) \pm \psi_\alpha^\dagger(\mathbf{r}', t) \psi_\alpha(\mathbf{r}, t) | 0 \rangle \\ &= 1. \end{aligned}$$

Poles of Green's Function and Quasiparticle Excitations

It is easy to see from the Källén–Lehmann representation that in the thermodynamic limit only those poles of $G(\omega)$ survive as distinct poles (and do not merge into the branch cut along the real axis) that correspond to the situation when all energy and momentum of the excited system can be ascribed to one object, a quasiparticle, with a definite dispersion law (i.e., energy-momentum correspondence). Otherwise, for any given energy there is a whole set of corresponding momenta, and the pole will be eliminated by the integration over them. Thus the quasiparticle dispersion law $\omega(\mathbf{p})$ is defined by the equation

$$\frac{1}{G(\mathbf{p}, \omega - \mu)} = 0. \quad (2.36)$$

2.1.3 Retarded and Advanced Green's Functions

We will define two more Green's functions: *retarded* and *advanced* ones, G^R and G^A .

$$G_{\alpha\beta}^R(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = -i \left\langle \psi_\alpha(\mathbf{x}_1, t_1) \psi_\beta^\dagger(\mathbf{x}_2, t_2) \pm \psi_\beta^\dagger(\mathbf{x}_2, t_2) \psi_\alpha(\mathbf{x}_1, t_1) \right\rangle \theta(t_1 - t_2); \quad (2.37)$$

$$G_{\alpha\beta}^A(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = +i \left\langle \psi_\alpha(\mathbf{x}_1, t_1) \psi_\beta^\dagger(\mathbf{x}_2, t_2) \pm \psi_\beta^\dagger(\mathbf{x}_2, t_2) \psi_\alpha(\mathbf{x}_1, t_1) \right\rangle \theta(t_2 - t_1). \quad (2.38)$$

The definition is chosen in such a way as to guarantee that (1) the retarded (advanced) Green's function is zero for all negative (positive) time differences $t - t'$, and (2) at $t = t'$ both have a $(-i\delta(x - x'))$ discontinuity, exactly as does the causal Green's function. The latter statement is easy to check by taking its time derivative and using the canonical relation

$$\begin{aligned} \lim_{t \rightarrow t'} \frac{\partial}{\partial t} G^{R(A)}(t - t') &= \mp i \langle 0 | \left[\psi_\alpha(\mathbf{x}, t), \psi_\beta^\dagger(\mathbf{x}', t') \right]_{\pm} | 0 \rangle \cdot (\pm \delta(t - t')) \\ &= -i \delta(\mathbf{x} - \mathbf{x}'). \end{aligned}$$

Again, in the uniform and stationary case, $G_{\alpha\beta}^{R(A)}(\mathbf{x}_1, t_1; \mathbf{x}_2, t_2) = G^{R(A)}(\mathbf{x}_1 - \mathbf{x}_2, t_1 - t_2) \delta_{\alpha\beta}$. Unperturbed retarded and advanced Green's functions, for example, can be easily found by direct calculation:

$$\begin{aligned} G^{0R,A}(\mathbf{p}, \omega) &= \frac{1}{\omega - (\epsilon_{\mathbf{p}} - \mu) \pm i0}; \\ D^{0R,A}(\mathbf{k}, \omega) &= \frac{\omega_{\mathbf{k}}}{2} \left(\frac{1}{\omega - \omega_{\mathbf{k}} \pm i0} - \frac{1}{\omega + \omega_{\mathbf{k}} \pm i0} \right) = \frac{\omega_{\mathbf{k}}^2}{\omega^2 - \omega_{\mathbf{k}}^2 + i0 \operatorname{sgn} \omega}. \end{aligned} \quad (2.39)$$

The Källén–Lehmann representation for $G^{R,A}$ can be obtained in the same way as for the causal Green's function. The result is as follows:

$$G^R(\mathbf{p}, \omega) = (2\pi)^3 \sum_s \left(\frac{A_s \delta(\mathbf{p} - \mathbf{P}_s)}{\omega - \epsilon_s^{(+)} + \mu + i0} \pm \frac{B_s \delta(\mathbf{p} + \mathbf{P}_s)}{\omega - \epsilon_s^{(-)} + \mu + i0} \right); \quad (2.40)$$

$$G^A(\mathbf{p}, \omega) = (2\pi)^3 \sum_s \left(\frac{A_s \delta(\mathbf{p} - \mathbf{P}_s)}{\omega - \epsilon_s^{(+)} + \mu - i0} \pm \frac{B_s \delta(\mathbf{p} + \mathbf{P}_s)}{\omega - \epsilon_s^{(-)} + \mu - i0} \right). \quad (2.41)$$

Taking real and imaginary parts of these expressions, we see that on the real axis

$$\begin{cases} \Re G^A(\mathbf{p}, \omega) = \Re G^A(\mathbf{p}, \omega) = \Re G(\mathbf{p}, \omega); \\ \Im G^R(\mathbf{p}, \omega) = \Im G(\mathbf{p}, \omega); & \omega > 0; \\ \Im G^A(\mathbf{p}, \omega) = \Im G(\mathbf{p}, \omega); & \omega < 0; \\ G_{\alpha\beta}^R(\mathbf{p}, \omega) = \left[G_{\beta\alpha}^A(\mathbf{p}, \omega) \right]^*. \end{cases} \quad (2.42)$$

On the other hand, the retarded (advanced) Green's function is clearly analytic in the upper (lower) ω -half-plane. This means that they are *analytic continuations* of the causal Green's function from the rays $\omega > 0$ ($\omega < 0$) respectively. Their asymptotic behavior is, of course, the same as that of the causal Green's function:

$$G^{R,A}(\omega) \sim 1/\omega, \quad |\omega| \rightarrow \infty.$$

In the thermodynamic limit, as in (2.28), we can write

$$G^{R,A}(\mathbf{p}, \omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\rho^{R,A}(\mathbf{p}, \omega')}{\omega' - \omega \pm i0}, \quad (2.43)$$

with *spectral density*

$$\begin{aligned} \rho^{R,A}(\mathbf{p}, \omega') &= -\pi(2\pi)^3 \sum_s (A_s \delta(\mathbf{p} - \mathbf{P}_s) \delta(\omega' - \epsilon_s^{(+)} + \mu) \\ &\quad \pm B_s \delta(\mathbf{p} + \mathbf{P}_s) \delta(\omega' - \epsilon_s^{(-)} + \mu)). \end{aligned} \quad (2.44)$$

Evidently,

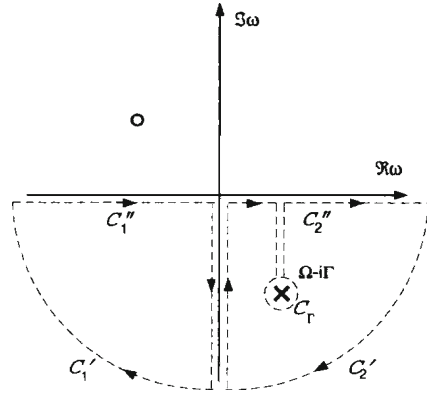
$$\rho^R(\mathbf{p}, \omega') = -\Im G^R(\mathbf{p}, \omega'). \quad (2.45)$$

From formula (2.44) it is clear that $\rho^R(\mathbf{p}, \omega')$ is proportional to the probability density of an elementary excitation with momentum \mathbf{p} having energy ω . In the non-interacting case, e.g., $-\Im G^{0,R} = \pi\delta(\omega - (\epsilon_{\mathbf{p}} - \mu))$, because in the absence of interactions, quasiparticles would indeed coincide with “basic” particles, with dispersion law $\epsilon_{\mathbf{p}}$.

2.1.3.1 Quasiparticle Excitations and Retarded and Advanced Green's Functions

We can now visualize the concept of a quasiparticle excitation and its relation to the existence of isolated poles of $G(\mathbf{p}, \omega)$. Suppose that there is such a pole at $\omega = \Omega - i\Gamma$, $\Gamma > 0$. (This corresponds to a particle added in the state \mathbf{p} .) To see the evolution of the excitation created by the operator $a_{\mathbf{p}}^{\dagger}$, calculate Green's function in the (\mathbf{p}, t) -representation:

Fig. 2.5 Contour integrations in the complex frequency plane. The poles of $G^R(\omega)$ are marked by crosses, those of $G^A(\omega)$ by circles



$$G(\mathbf{p}, t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} G(\mathbf{p}, \omega).$$

For negative t the integration contour can be closed in the upper half-plane, and since there are no singularities there, the integral is zero. For positive t the contour closes in the lower half-plane and will contain the pole. We cannot, though, simply calculate the residue, since the causal Green's function is not analytic in the lower half-plane. We must then replace it by its analytic continuations, $G^{R,A}$. In order to do this, we close the integration contour as shown in Fig. 2.5. For $\Re\omega < 0$ we can replace $G(\mathbf{p}, \omega)$ by $G^A(\mathbf{p}, \omega)$, and for $\Re\omega > 0$ by $G^R(\mathbf{p}, \omega)$. Now, the Cauchy theorem of complex analysis tells us that the integral we are interested in can be written as follows:

$$G(\mathbf{p}, t) = - \int_{C'_1 + C''_1} \frac{d\omega}{2\pi} e^{-i\omega t} G^A(\mathbf{p}, \omega) - \int_{C'_2 + C''_2 + C_r} \frac{d\omega}{2\pi} e^{-i\omega t} G^R(\mathbf{p}, \omega).$$

Watson's lemma, together with the $1/\omega$ asymptotics of Green's functions, ensures that the integrals over infinitely remote quarter circles C'_1 and C'_2 are zero. Therefore, we are left with two terms: the contribution from the pole, and the integral along the negative imaginary axis:

$$G(\mathbf{p}, t) = -iZ e^{-i\Omega t} e^{-\Gamma t} + \int_{-i\infty}^0 \frac{d\omega}{2\pi} e^{-i\omega t} [G^A(\mathbf{p}, \omega) - G^R(\mathbf{p}, \omega)], \quad (2.46)$$

where Z is the residue of $G^R(\omega)$ in the pole. The first term describes a free quasi-particle with finite lifetime $\sim 1/\Gamma$. The contribution from the integral is small, if only $\Omega t \gg 1$, $\Gamma t \ll 1$. (This means that the decay rate must be small enough, $\Gamma \ll \Omega$.) Indeed, invoking the Källén-Lehmann representation, we see that

$$\begin{aligned}
& \int_{-i\infty}^0 \frac{d\omega}{2\pi} e^{-i\omega t} \left[G^A(\mathbf{p}, \omega) - G^R(\mathbf{p}, \omega) \right] \\
& \approx \int_{-i\infty}^0 \frac{d\omega}{2\pi} e^{-i\omega t} \left[\frac{A}{\omega - \epsilon_p + \mu - i\Gamma} - \frac{A}{\omega - \epsilon_\rho + \mu + i\Gamma} \right] \\
& = -2i\Gamma A \int_{-i\infty}^0 \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{(\omega - \epsilon_p + \mu)^2 + \Gamma^2} \\
& \approx \frac{-\Gamma A}{\pi t} \frac{e^{-i\mu t}}{(\mu - \epsilon_\rho)^2} \ll Z e^{-i\Omega t} e^{-\Gamma t}
\end{aligned}$$

if $\Gamma \ll (\epsilon_\rho - \mu) = \Omega$.

2.1.3.2 Kramers-Kronig Relations

From the Källén–Lehmann representation for the retarded and advanced Green's functions (2.40, 2.41) follows a beautiful (and important) relation between the real and imaginary parts of those functions of *real* frequencies: the *Kramers–Kronig relation*

$$\Re G^{R,A}(\mathbf{p}, \omega) = \pm \mathbf{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\Im G^{R,A}(\mathbf{p}, \omega')}{\omega' - \omega}. \quad (2.47)$$

(This can be established directly by taking the imaginary and real parts of (2.40, 2.41). It can be shown that the reason why this relation holds is the *causality*, that is, the property of advanced and retarded Green's functions of *time* to be zero for $t > (<)t'$. The proof (which is quite straightforward) is like our calculation of the Fourier transform of the propagator in Chap. 1, where we established for the first time that the poles of $K(\omega)$ must be infinitesimally displaced from the real axis in order to provide for the $\theta(t)$ -like behavior of $K(t)$. Then, knowing that $G^{(R,A)}(\omega)$ is an analytic function in the corresponding half-plane, we can calculate the integral $\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\Im G^{R,A}(\mathbf{p}, \omega')}{\omega' - \omega}$ along the real axis, using the Cauchy theorem, and come to the above relations. In mathematics this relation is known as the Plemelj theorem [6].

2.1.4 Green's Function and Observables

The way of expressing observables (average values of quantum-mechanical operators) in terms of Green's function (once the latter is known) directly follows from its definition. (Since it contains only an average of two field operators, it is clear that only one-particle operators can be treated this way.)

For example, the particle density in the system (meaning real or “basic” particles) is by definition

$$n(\mathbf{r}) = \sum_{\alpha} \langle \psi_{\alpha}^{\dagger}(\mathbf{r}) \psi_{\alpha}(\mathbf{r}) \rangle \equiv \mp i \sum_{\alpha} G_{\alpha\alpha}(\mathbf{r}, t - 0; \mathbf{r}, t). \quad (2.48)$$

So, for a uniform system of spinful fermions we have

$$n = \frac{N}{V} = -2i G(\mathbf{r} = 0, t = -0) = 2\Im G(\mathbf{r} = 0, t = -0). \quad (2.49)$$

The relation between density and Green's function allows us, in turn, to express the thermodynamic properties of the system at $T = 0$ through its Green's function. Indeed, the grand potential of the system satisfies (see, e.g., [4])

$$d\Omega = -SdT - Nd\mu = -Nd\mu$$

at $T = 0$ (since the entropy $S(0) = 0$). This equation can thus be integrated (remembering that $\Omega(\mu = 0) = 0$):

$$\Omega = - \int_0^{\mu} d\mu N(\mu),$$

where we can substitute the expression for $N(\mu)$ from (2.48) or (2.49) (where Green's function is explicitly μ -dependent; see Problem 2.1).

A slightly more sophisticated example is presented by current, which in agreement with Sect. 1.4 is expressed through the field operators as

$$\mathbf{j}(\mathbf{r}) = \frac{ie}{2m} \sum_{\alpha} \langle (\nabla \psi_{\alpha}^{\dagger}(\mathbf{r})) \psi_{\alpha}(\mathbf{r}) - \psi_{\alpha}^{\dagger}(\mathbf{r}) (\nabla \psi_{\alpha}(\mathbf{r})) \rangle.$$

We can express the current through Green's function, using a “hair splitting” trick that allows us to separate the differentiation over two coinciding coordinates:

$$\begin{aligned} \mathbf{j}(\mathbf{r}) &= \frac{ie}{2m} \sum_{\alpha} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla_{\mathbf{r}'} - \nabla_{\mathbf{r}}) \langle \psi_{\alpha}^{\dagger}(\mathbf{r}') \psi_{\alpha}(\mathbf{r}) \rangle \\ &= \frac{ie}{2m} \sum_{\alpha} \lim_{t \rightarrow -0} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla_{\mathbf{r}'} - \nabla_{\mathbf{r}}) (\mp i G_{\alpha\alpha}(\mathbf{r}', t; \mathbf{r}, 0)). \end{aligned} \quad (2.50)$$

2.2 Perturbation Theory: Feynman Diagrams

The beautiful formulae of complex analysis and the physical insight we have achieved so far unfortunately do not provide more specific information about Green's functions of a realistic system—the one with interactions. On this level of generalization all Fermi systems look the same, and all Bose systems look the same (which is, of course,

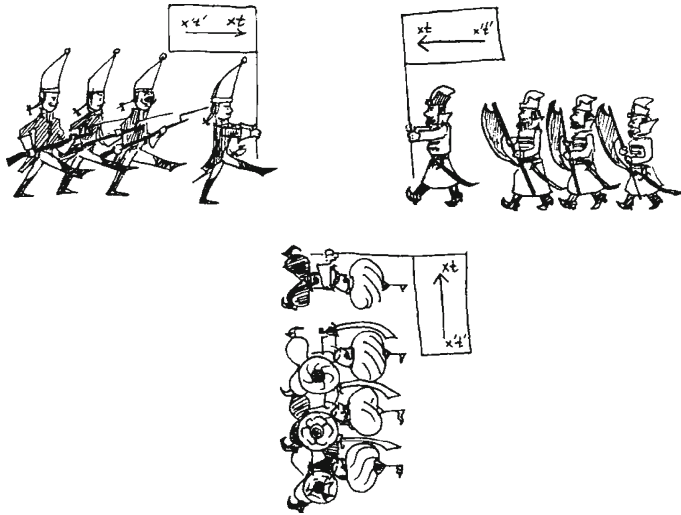


Fig. 2.6 Different ways of drawing Feynman diagrams

true, but not sufficient). On the other hand, we cannot look into the differences due to interactions, because, e.g., we have no way of determining the matrix elements of field operators in the Källén-Lehmann representation.

As always, we have to apply perturbation theory. The great achievement by Feynman was to build *the* perturbation theory formalism, in which the whole perturbation expansion, including its most cumbersome expressions, is reduced to a set of sometimes spectacular and always physically understandable graphs—*Feynman diagrams*.

As in medieval paintings, there is a strict set of rules for both drawing and reading those images (determined by the Hamiltonian of the system). This makes diagram techniques a highly symbolic form of art. (Of course, there are differences between various schools and books, as in Fig. 2.6.)

When calculating the Green's function of a system with interactions, we meet the usual obstacle of not knowing the wave function (state) of the system over which the average is to be taken. We don't know the ground state, $|0\rangle$. We don't know excited states. Moreover, *any* approximation we are going to make will be virtually *orthogonal* to the proper many-particle state. Luckily, the approximate *matrix elements* (like Green's function) can be quite accurate. The seeming paradox is just a reflection of the fact that while the wave function involves all N particle states, Green's function deals with only two one-particle states (initial and final). As Thouless has noted [7], if the one-particle state is approximated with a small mistake α , the projection of the corresponding many-particle state on the exact state will be of the order of $(1 - \alpha)^N \sim e^{-N\alpha} \rightarrow 0$ as $N \rightarrow \infty$ for my finite α . On the other hand, the average of a one-particle operator (like Green's function) will contain only a small mistake α !

Two conclusions can be drawn. (1) Green's functions provide a physically sensible method of approaching the many-body problem. (Something we could guess after a short glance cast at library shelves filled with numerous folios on the subject, to which we dare add a book of our own.) (2) The results are to be expressed in terms of averages over the unperturbed state of the system, rather than corrections to many-body wave functions. (In usual quantum mechanics both would be equivalent—*because* it is a one-body theory.)

2.2.1 Derivation of Feynman Rules. Wick's and Cancellation Theorems

In order to fulfill our program, let us turn to the interaction representation. We have seen before that this is a natural way to deal with perturbation theory. To avoid unnecessary subscripts, here we denote the field operators in the interaction representation by uppercase Greek letters. The connection between them and Heisenberg operators is given by

$$\psi(\mathbf{x}, t) = \mathcal{U}^\dagger(t) \psi_S(\mathbf{x}) \mathcal{U}(t) = \mathcal{U}^\dagger(t) e^{-i\mathcal{H}_0 t} \Psi(\mathbf{x}, t) e^{i\mathcal{H}_0 t} \mathcal{U}(t).$$

Inserting this into the definition of Green's function, we obtain

$$\begin{aligned} G_{\alpha\alpha'}(\mathbf{x}, t; \mathbf{x}', t') &= -i \left[\langle 0 | \mathcal{U}^\dagger(t) e^{-i\mathcal{H}_0 t} e^{i\mathcal{H}_0 t'} \mathcal{U}(t') | 0 \rangle \right]^{-1} \\ &\times \left\{ \langle 0 | \mathcal{U}^\dagger(t) e^{-i\mathcal{H}_0 t} \Psi_\alpha(\mathbf{x}, t) S_{(I)}(t, t') \Psi_{\alpha'}^\dagger(\mathbf{x}', t') e^{i\mathcal{H}_0 t'} \mathcal{U}(t') | 0 \rangle \theta(t - t') \right. \\ &\left. \pm \langle 0 | \mathcal{U}^\dagger(t') e^{-i\mathcal{H}_0 t'} \Psi_{\alpha'}^\dagger(\mathbf{x}', t') S_{(I)}(t', t) \Psi_\alpha(\mathbf{x}, t) e^{i\mathcal{H}_0 t} \mathcal{U}(t) | 0 \rangle \theta(t' - t) \right\}. \end{aligned} \quad (2.51)$$

Later on we suppress the (I) subscript in the S -matrix as well; we use it only in the interaction representation anyway; that is,

$$S(t, t') = \mathcal{T} e^{-i \int_{t'}^t dt \mathcal{W}(t)}, \quad t > t'.$$

Here $|0\rangle$ is a Heisenberg ground-state vector. Then $e^{i\mathcal{H}_0 t'} \mathcal{U}(t') |0\rangle = e^{i\mathcal{H}_0 t'} |0(t')\rangle_S = |0(t')\rangle_I$, i.e., the ground-state vector in interaction representation, and

$$|0(t')\rangle_I = S(t', t'') |0(t'')\rangle_I (t' > t'') = S(t', -\infty) |0(-\infty)\rangle_I, \quad (2.52)$$

because we can take the moment t'' to minus infinity.

We can repeat this argumentation for $\langle 0 | \mathcal{U}^\dagger(t) e^{-i\mathcal{H}_0 t}$ to get eventually

$$e^{i\mathcal{H}_0 t'} \mathcal{U}(t') |0\rangle = \mathcal{S}(t', -\infty) |0(-\infty)\rangle_I; \quad (2.53)$$

$$\langle 0 | \mathcal{U}^\dagger(t) e^{-i\mathcal{H}_0 t} = \langle 0(\infty) |_I \mathcal{S}(\infty, t). \quad (2.54)$$

Now we introduce a very important *adiabatic hypothesis*. First, let us assume that the perturbation was absent very long ago and was turned on in an infinitely slow way, say $\mathcal{W}(t \leq t_1) = \mathcal{W} \exp(\alpha(t - t_1))$, $\alpha \rightarrow 0+$. It will be turned off in some very distant future, say $\mathcal{W}(t \geq t_2) = \mathcal{W} \exp(-\alpha(t - t_2))$, $\alpha \rightarrow 0+$. Here $[t_1, t_2]$ is the time interval within which we investigate our system (and we don't care what happens later or previously: *après moi le déluge*).

Of course, physically it is rather easy to turn on and off the external potential, while we don't have such a free hand when the perturbation is due to particle—particle interaction. But nothing a priori prohibits such a property of the perturbation term in the Hamiltonian, and finally we take $\alpha = 0$ anyway. (A mathematically inclined reader may recognize that we are actually going to use so-called Abel regularization of conditionally convergent integrals, which appear a little later.)

Now, since at minus infinity there is no perturbation, we can write instead of $|0(-\infty)\rangle_I$ the *unperturbed ground state* vector $|\Phi_0\rangle$ (which is time independent, because $i\partial|\Phi_0(t \rightarrow -\infty)\rangle/\partial t = \mathcal{W} \exp(\alpha(t - t_1))|\Phi_0(t \rightarrow -\infty)\rangle \rightarrow 0$). It is convenient to choose a normalized state, $\langle \Phi_0 | \Phi_0 \rangle = 0$.

Now, it seems natural to think that since we had an unperturbed ground state at minus infinity, when there was no interaction, we should have the same state at plus infinity, when there will be no interaction. This is not true, though: it is known from usual quantum mechanics that the adiabatically slow perturbation can actually switch the system to a different state *with the same energy*. Our good luck is that the ground state of a quantum-mechanical system is always non-degenerate, and it is the ground state averages that we deal with! Therefore, the only difference between the states at minus and plus infinity may be a phase factor: $|0(+\infty)\rangle_I = (\exp(iL))|\Phi_0\rangle$, and this factor anyway cancels from the numerator and denominator of (2.51).

Thus we have derived the key formula

$$iG_{\alpha\alpha'}(x, t; x', t') = \frac{\langle \Phi_0 | \mathcal{T} \mathcal{S}(\infty, -\infty) \Psi_\alpha(x, t) \Psi_{\alpha'}^\dagger(x', t') | \Phi_0 \rangle}{\langle \Phi_0 | \mathcal{S}(\infty, -\infty) | \Phi_0 \rangle} \quad (2.55)$$

(we rearranged the terms under the sign of time ordering to gather all the parts of the \mathcal{S} -operator into $\mathcal{S}(\infty, -\infty) = \mathcal{T} \exp\{-i \int_{-\infty}^{\infty} dt \mathcal{W}(t)\}$). This formula is the basis for the perturbation theory: we have only to expand the exponent and obtain the series like the one we obtained for the one-particle propagator, containing terms

$$\langle \Phi_0 | \mathcal{T} \mathcal{W}(t_1) \mathcal{W}(t_2) \cdots \mathcal{W}(t_m) \Psi_\alpha(x, t) \Psi_{\alpha'}^\dagger(x', t') | \Phi_0 \rangle.$$

The difference is that (1) we need the matrix elements not between the coordinate (momentum) eigenstates, but between unperturbed ground state vectors of a many-body system, and (2) now we have the denominator $\langle \Phi_0 | \mathcal{S}(\infty, -\infty) | \Phi_0 \rangle$.

2.2.1.1 Wick's Theorem

This is *the* theorem of quantum field theory, because it makes all the formalism tick. After the exponent in the S -operator is expanded, we must calculate the matrix elements of the sort $\langle \Phi_0 | \mathcal{T} \phi_1 \phi_2 \cdots \phi_m | \Phi_0 \rangle$. Here $\phi_1, \phi_2, \dots, \phi_m$ are (Fermi or Bose) field operators in interaction representation, and it is Wick's theorem that allows us to do this.

For the sake of clarity, from now on we denote the set of variables (\mathbf{x}, t, α) by a single number or capital letter. For example:

$$\begin{aligned} \Psi_\alpha(x, t) &\rightsquigarrow \Psi_X; \\ \Psi_{\gamma_1}(\mathbf{x}_1, t_1) &\rightsquigarrow \Psi_1; \\ \sum_\alpha \int d^3\mathbf{x} \int dt &\rightsquigarrow \int dX; \\ \sum_{\gamma_1} \int d^3\mathbf{x}_1 \int dt_1 &\rightsquigarrow \int d1. \end{aligned}$$

Wick's theorem states that

The time-ordered product of field operators in interaction representation equals to the sum of their normal products with all possible contractions:

$$\begin{aligned} \mathcal{T} \phi_1 \phi_2 \cdots \phi_m \phi_{m+1} \phi_{m+2} \cdots \phi_n &= : \phi_1 \phi_2 \cdots \phi_m \phi_{m+1} \phi_{m+2} \cdots \phi_n : \\ &+ : \overbrace{\phi_1 \phi_2 \cdots \phi_m \phi_{m+1} \phi_{m+2} \cdots \phi_n} : \\ &+ : \overbrace{\phi_1 \phi_2 \cdots \phi_m \phi_{m+1} \phi_{m+2} \cdots \phi_n} : \\ &+ \cdots + : \phi_1 \underbrace{\phi_2 \cdots \phi_m}_{\phi_{m+1}} \overbrace{\phi_{m+2} \cdots \phi_n} : . \end{aligned} \quad (2.56)$$

Now some definitions.

The *normal ordering* of field operators, $:\phi_1 \phi_2 \cdots \phi_m:$, means that all “destruction” operators stay to the right of the “construction” ones. We label “destruction” those operators that give zero when acting on the unperturbed ground state (vacuum state); and the “construction” operators are their conjugates. In the Fermi case, e.g., the vacuum is the filled Fermi sphere, and therefore “destruction” operators are *annihilation* operators $a_{\mathbf{p}}$ with $p > p_F$, and *creation* operators $a_{\mathbf{p}}^\dagger$ with $p < p_F$. We can, if we wish, explicitly split the Fermionic field operator in two corresponding parts,

$$\begin{aligned} \psi_X &= \psi_X^{(-)} + \psi_X^{(+)} \\ &= \frac{1}{\sqrt{V}} \sum_{p > p_F} e^{i(\mathbf{p}\mathbf{x} - \epsilon_p t)} a_{\mathbf{p}} + \frac{1}{\sqrt{V}} \sum_{p < p_F} e^{i(\mathbf{p}\mathbf{x} - \epsilon_p t)} a_{\mathbf{p}}. \end{aligned} \quad (2.57)$$

The bosonic (e.g., phonon) field is already presented in this form,

$$\begin{aligned}\varphi_X &= \varphi_X^{(-)} + \varphi_X^{(+)} \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \left(\frac{\omega_{\mathbf{k}}}{2}\right)^{1/2} b_{\mathbf{k}} e^{i(\mathbf{k}\mathbf{x} - \omega_{\mathbf{k}}t)} + \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \left(\frac{\omega_{\mathbf{k}}}{2}\right)^{1/2} b_{\mathbf{k}}^{\dagger} e^{-i(\mathbf{k}\mathbf{x} - \omega_{\mathbf{k}}t)}. \quad (2.58)\end{aligned}$$

Since both time ordering and normal ordering are distributive, we can deal with the (+) and (-) parts separately, and therefore all the intermediate manipulations can be on the field operators ψ , φ themselves.

By definition, the normal product of any set of the field operators A , B , C , ... has zero ground-state average,

$$\langle \Phi_0 | : ABC \cdots : | \Phi_0 \rangle = 0. \quad (2.59)$$

The *contraction*, or *pairing*, of two operators, $\overbrace{\phi_m \phi_n}$, is the difference between their time- and normally ordered products

$$\overbrace{\phi_m \phi_n} = \mathcal{T} \phi_m \phi_n - : \phi_m \phi_n :. \quad (2.60)$$

If both operators here are of the same sort (both creation or both annihilation), the contraction is identically zero. Indeed, then the normal ordering does not affect their product, and

$$\begin{aligned}\overbrace{\phi_1 \phi_2} &= \theta(t_1 - t_2) \phi_1 \phi_2 \mp \theta(t_2 - t_1) \phi_2 \phi_1 - \phi_1 \phi_2 \\ &= (\theta(t_1 - t_2) + \theta(t_2 - t_1)) \phi_1 \phi_2 - \phi_1 \phi_2 \\ &= 0.\end{aligned}$$

On the other hand, a contraction of conjugate field operators is a *number*: taking into account that the operators are in interaction representation and their time dependence is trivial, we see that, for example,

$$\begin{aligned}\overbrace{\phi_1^{\dagger} \phi_2} &= \sum_k \sum_q \left(e^{i E_k t_1} \phi_k^{\dagger} \right) \left(e^{-i E_q t_2} \phi_q \right) \\ &= \sum_k \sum_q e^{i E_k t_1} e^{-i E_q t_2} \left(\theta(t_1 - t_2) \phi_k^{\dagger} \phi_q \mp \theta(t_2 - t_1) \phi_q \phi_k^{\dagger} - \phi_k^{\dagger} \phi_q \right) \\ &= \sum_k \sum_q e^{i E_k t_1} e^{-i E_q t_2} \left[(\theta(t_1 - t_2) + \theta(t_2 - t_1)) \phi_k^{\dagger} \phi_q - \phi_k^{\dagger} \phi_q + \theta(t_2 - t_1) \delta_{kq} \right],\end{aligned}$$

and all the operator terms cancel. This is an important fact, that the contraction of Fermi/Bose field operators is a usual number, because then we can write

$$\begin{aligned}
\overbrace{\phi_1 \phi_2} &= \langle \Phi_0 | \overbrace{\phi_1 \phi_2} | \Phi_0 \rangle \\
&= \langle \Phi_0 | \mathcal{T} \phi_1 \phi_2 | \Phi_0 \rangle - \langle \Phi_0 | : \phi_1 \phi_2 : | \Phi_0 \rangle \\
&= \langle \Phi_0 | \mathcal{T} \phi_1 \phi_2 | \Phi_0 \rangle = iG^0(12).
\end{aligned} \tag{2.61}$$

Contraction of Fermi/Bose operators is actually an *unperturbed* Green's function, which we know how to find! Look how lucky we are: *if* the commutation relations for our field operators contained an operator instead of a delta function (as they do for spin operators), we would have no use for Wick's theorem when calculating the averages of many-operator products. This is why there is no really handy diagrammatic approach to the corresponding problems.

But with bosons and fermions we can use the theorem to deal with the average $\langle \Phi_o | \phi(1) \cdots \phi(N) | \Phi_o \rangle$. Note that we can extract all the contractions from under the symbol of normal ordering. (We have only to commute the paired operators with their neighbors in order to bring them together, and then simply calculate the contraction (a number) and take it outside. This operation will give us at most a factor of $(-1)^P$, the parity of the permutation of Fermi operators that we did on our way.) Therefore only the contribution due to the sum of all possible *fully contracted* terms survives (the other terms contain some normally ordered operators and thus have zero vacuum average): evidently, only terms with an even number of operators can be fully contracted. This sum is actually a sum of products of unperturbed Green's functions, corresponding to all possible ways of picking pairs of conjugate field operators from the general crowd, taken with corresponding parity factors. Each of these terms can be presented by a distinctive Feynman diagram, of which the rules for drawing, reading, and calculating we are going to establish.

But before doing so, let us check that Wick's theorem is plausible. (The proof involves some tiresome algebra and can be found, e.g., in [2].) Following [4], we will make instead a simpler argument valid not for the operators themselves, but for their matrix elements (a so-called *weak* statement), and only in the thermodynamic limit. On the other hand, it is valid for averages over an arbitrary state of the system, not only its ground state.

The argument goes as follows. Write an Another example: average in Fourier components $\langle X | \phi_1 \phi_2 \cdots | X \rangle = \Omega^{-1/2} \sum_{k_1} \Omega^{-1/2} \sum_{k_2} \cdots e^{ik_1 x_1 - iE_1 t_1} e^{ik_2 x_2 - iE_2 t_2} \cdots \langle X | c_{k_1} c_{k_2} \cdots | X \rangle$. Ω is the volume of the system. In this expression there must be an even number of operators: $N/2$ creation operators and $N/2$ annihilation operators, with the same values of k (otherwise the matrix element is zero). There can be no more than $N/2$ *different* values of k . If indeed they are all different, we have, e.g.,

$$\begin{aligned}
&\Omega^{-N/2} \sum_{k_1} \sum_{k_2} \cdots e^{ik_1(x_1 - x'_1) - iE_1(t_1 - t'_1)} \cdots \langle X | c_{k_1}^+ c_{k_1} | X \rangle \\
&\quad \times \langle X | c_{k_2}^+ c_{k_2} | X \rangle \cdots \langle X | c_{k_{N/2}}^+ c_{k_{N/2}} | X \rangle (-1)^P
\end{aligned}$$

(we could here insert $|X\rangle\langle X|$ instead of the complete expression for the unit operator, $\sum_s |s\rangle\langle s|$, because the rest of it does not contribute anything.) The above expression

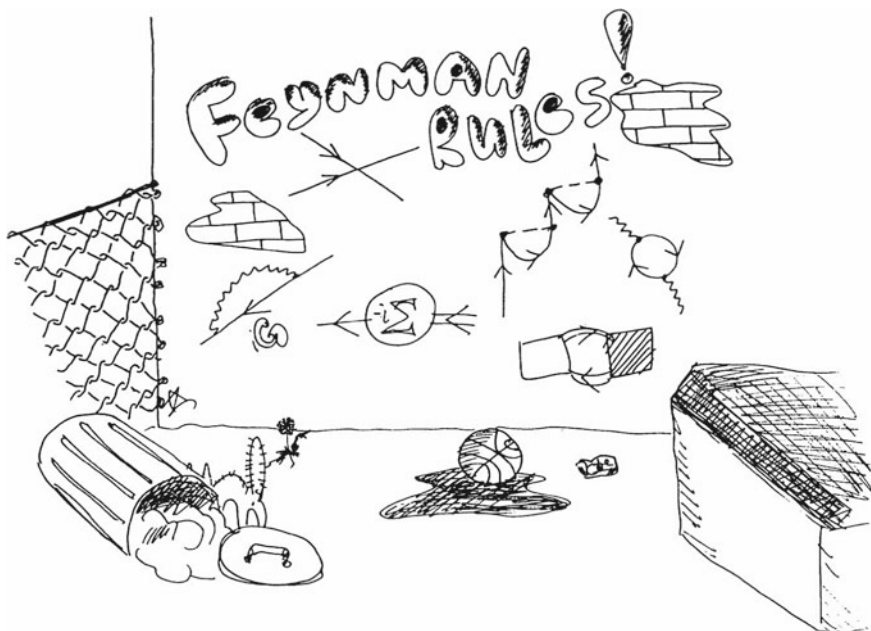


Fig. 2.7 The art of physics

is actually the fully contracted term of Wick's theorem. In the thermodynamic limit, $\Omega \rightarrow \infty$, it stays finite, because every power of Ω in the normalization term is compensated by the summation over k (both are proportional to the number of particles in the system).

On the other hand, there are other terms in the expression for $\langle X | \phi_1 \phi_2 \cdots | X \rangle$, but they contain $N/2 - 1$, $N/2 - 2$, etc. different values of k , and thus independent summations. Because of that, some powers of volume in the denominator will not be canceled by summations, and all these terms vanish, which concludes our reasoning (Fig. 2.7).

Now the path is straightforward. (1) Expand the time-ordered exponent in the expression for Green's function; (2) Take all averages over the ground state, using Wick's theorem, thus factoring all terms in products of unperturbed Green's functions (with appropriate integrations); (3) Represent these terms by graphs—Feynman diagrams. After the correspondence between those graphs and the analytic terms in the expansion series is established, it is much simpler to work with the diagrams, which give much clearer understanding of the structure of the expressions involved.

The rules of drawing and reading Feynman diagrams in some detail, of course, depend on the interaction. What is even worse, they depend on tastes and preferences of the author whose book or chapter you are reading (Fig. 2.6); there are at least three popular schools. Here we will take one of those approaches, where time flows from right to left and so it is also from right to left that the lines symbolizing Green's

functions are drawn. This has at least the advantage, that the order of letters labeling the diagram is the same as that in the analytic formulas, where later moments stand to the left.

For illustration, we derive the rules for the simple case of scalar electron—electron interaction, which by definition involves only one sort of particles (electrons) interacting via instantaneous spin-independent potential:

$$\begin{aligned} \mathcal{W}(t) = & \frac{1}{2} \sum_{\alpha_1} \sum_{\alpha_2} \int d^3 \mathbf{x}_1 \int d^3 \mathbf{x}_2 \Psi_{\alpha_1}^\dagger(\mathbf{x}_1, t) \Psi_{\alpha_2}^\dagger(\mathbf{x}_2, t) U(\mathbf{x}_1 - \mathbf{x}_2) \\ & \times \Psi_{\alpha_2}(\mathbf{x}_2, t) \Psi_{\alpha_1}(\mathbf{x}_1, t). \end{aligned}$$

For convenience we introduce

$$U(1-2) \equiv U(\mathbf{x}_1 - \mathbf{x}_2) \delta(t_1 - t_2);$$

and now we will integrate over space and time coordinates indiscriminately, and the whole set (\mathbf{x}, t, α) (α is spin index) is written down as X .

Expanding the exponent in the general expression for $iG(X, X')$ up to the first order in interactions and substituting out scalar electron—electron interaction, we find

$$\begin{aligned} iG(XX') & \quad (2.62) \\ \approx & \frac{\langle \Phi_0 | \Psi_X \Psi_{X'}^\dagger | \Phi_0 \rangle + (-\frac{i}{\hbar}) \frac{1}{2} \int d1 \int d2 U(1-2) \langle \Phi_0 | \mathcal{T} \Psi_1^\dagger \Psi_2^\dagger \Psi_2 \Psi_1 \Psi_X \Psi_{X'}^\dagger | \Phi_0 \rangle}{1 + (-\frac{i}{\hbar}) \frac{1}{2} \int d1 \int d2 U(1-2) \langle \Phi_0 | \mathcal{T} \Psi_1^\dagger \Psi_2^\dagger \Psi_2 \Psi_1 | \Phi_0 \rangle}. \end{aligned}$$

This was step one. In step two, the average of the six operators in the numerator and that of the four operators in the denominator must be evaluated using Wick's theorem.

The expression $\langle \Phi_0 | \mathcal{T} \Psi_1^\dagger \Psi_2^\dagger \Psi_2 \Psi_1 \Psi_X \Psi_{X'}^\dagger | \Phi_0 \rangle$ can be fully contracted in six different ways. For example, $\langle \Phi_0 | \mathcal{T} \underbrace{\Psi_1^\dagger \Psi_2^\dagger \Psi_2 \Psi_1}_{\text{contracted}} \underbrace{\Psi_X \Psi_{X'}^\dagger}_{\text{contracted}} | \Phi_0 \rangle = n^0(1) n^0(2) iG^0(X, X')$. Here $n^0(1) = \langle \Psi_1^\dagger \Psi_1 \rangle_0$ is simply unperturbed electronic density in the system. As you see, in this term the “probe” particle (traveling from X' to X) is decoupled—disconnected—from the rest of the system, that is, does not interact with it.

Another example:

$$\langle \Phi_0 | \mathcal{T} \underbrace{\Psi_1^\dagger \Psi_2^\dagger \Psi_2 \Psi_1}_{\text{contracted}} \underbrace{\Psi_X \Psi_{X'}^\dagger}_{\text{contracted}} | \Phi_0 \rangle = -iG^0(1, 2) iG^0(2, 1) iG^0(X, X')$$

also produces a disconnected term, with minus sign, because in order to put together the field operators to form corresponding pairings we had to change the places of an odd number of Fermi operators.

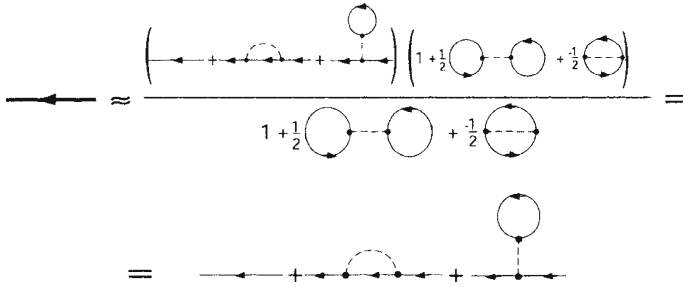


Fig. 2.8 Green's function to first order in scalar e-e interaction

Still another choice gives us at last a connected term, where the probe particle interacts with the system:

$$\langle \Phi_0 | \mathcal{T} \overbrace{\Psi_1^\dagger \Psi_2^\dagger \Psi_2} \overbrace{\Psi_1 \Psi_\chi} \Psi_{\chi'}^\dagger | \Psi_0 \rangle = iG^0(X, 2) iG^0(2, 1) iG^0(1, X').$$

All this is rather boring, but if we mark all the elements of the above expression—points where interaction occurs, unperturbed Green's functions, etc.—as suggested in Table 2.1, we can draw Green's function to first order in interaction as shown in Fig. 2.8. The resulting diagrams are like the ones we obtained earlier for the one-particle propagator. Once again, the probe particle interacts with the particles in the system, and propagates freely between those acts of scattering. But now the “background” particles interact with each other, and this is expressed in the structure of the graphs, which is now far richer.

You see that the first two terms in the numerator are indeed disconnected; they literally fall apart. On the other hand, the remaining four terms are connected, and they show that the probe particle is scattered (that is, interacts) with the other particles in the system.

By definition, the connected diagrams are the ones that do not contain parts disconnected from the external ends, that is, the coordinates of the “external” particle (in our case, external ends are X, X'). Only the external ends of the diagram carry significant coordinates (spins, etc.), the ones that actually appear as the arguments of the exact Green's function that we wish to calculate. All the rest are dummy labels, because there will be integrations (summations) over them. Of course, it does not matter how we denote a dummy variable, and all the diagrams that differ only by the mute labels are the same.

Here we see that connected terms contain integrations over the dummy variables 1 and 2. Therefore, of four connected terms there are only two that are different, and we can get rid of the factor one half before them.

Expanding the denominator, we find that

$$\langle \Phi_0 | \mathcal{S}(-\infty, \infty) | \Phi_0 \rangle = 1 + \frac{1}{2} \text{ (diagram)} + \frac{-1}{2} \text{ (diagram)} .$$

Within the same accuracy, we can factor the numerator (neglecting the higher-order terms in the interaction), and see that the denominator actually cancels the disconnected terms from the numerator!

This observation is actually a strict mathematical statement, and since the proof is very simple and general, let us prove.

2.2.1.2 Cancellation Theorem

All disconnected diagrams appearing in the perturbation series for the Green's function exactly cancel from its numerator and denominator. Therefore Green's function is expressed as a sum over all connected diagrams.

No need to specify the interaction term, \mathcal{W} . Let us consider the ν th order term in the numerator of Green's function:

$$\begin{aligned} & \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \delta_{m+n, \nu} (-i)^{m+n} \frac{1}{\nu!} \left(\frac{\nu!}{m!n!} \right) \int_{-\infty}^{\infty} dt_1 \cdots dt_m \langle \Phi_0 | \mathcal{T} \mathcal{W}(t_1) \cdots \mathcal{W}(t_m) \\ & \quad \times \Psi(X) \Psi^\dagger(X') | \Phi_0 \rangle_{\text{connected}} \\ & \quad \times \int_{-\infty}^{\infty} dt_{m+1} \cdots dt_\nu \langle \Phi_0 | \mathcal{T} \mathcal{W}(t_{m+1}) \cdots \mathcal{W}(t_{m+n}) | \Phi_0 \rangle. \end{aligned}$$

In this expression each term is explicitly presented as a product of a connected part (of m th order) and a disconnected part (of n th order), m and n , adding up to ν . We included here a combinatorial factor $(\frac{\nu!}{m!n!})$, which is the number of ways to distribute ν interaction operators $\mathcal{W}(t_i)$ in these two groups (connected and disconnected), consisting of m and n operators respectively. (Since interaction terms contain an even number of Fermi operators, no sign change occurs from such a redistribution.) This factor combines with the $\frac{1}{\nu!}$ (from the exponential series) and leaves us with $\frac{1}{m!} \frac{1}{n!}$.

Summation ν from 0 to ∞ simply eliminates the δ -symbol, and we have for a product of two series, of which the second, due to disconnected diagrams, is, after trivial relabeling of the integration variables,

Fig. 2.9 Example of topologically equivalent diagrams

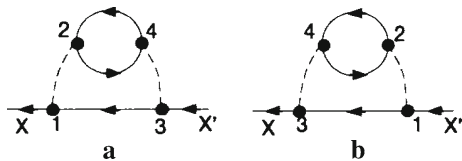


Table 2.1 Feynman rules for scalar electron-electron interaction

$\overline{X} \leftarrow X'$	$iG(XX') \equiv iG_{\alpha\alpha'}(\mathbf{x}; \mathbf{x}', t')$	Causal Green's function
$\overline{X} \leftarrow X'$	$iG^0(XX') \equiv iG^0(\mathbf{x} - \mathbf{x}', t - t')\delta_{\alpha\alpha'}$	Unperturbed causal Green's function
$1 \cdots 2$	$-iU(1-2) \equiv -iU(\mathbf{x}_1 - \mathbf{x}_2)\delta(t_1 - t_2) \times \delta(t_1 - t_2)$	Interaction potential
$1 \circlearrowleft$	$n^0(1) \equiv \langle \Phi_0 \Psi_1^\dagger \Psi_1 \Phi_0 \rangle$	Unperturbed electron density

The integration over all intermediate coordinates and times and summation over mute spin indices is implied

$$\begin{aligned}
 & \frac{1}{n!} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dt_1 \dots dt_n (-i)^n \langle \Phi_0 | \mathcal{T} \mathcal{W}(t_1) \dots \mathcal{W}(t_n) | \Phi_0 \rangle \\
 & = \langle \Phi_0 | \mathcal{T} e^{-i \int_{-\infty}^{\infty} dt \mathcal{W}(t)} | \Phi_0 \rangle,
 \end{aligned}$$

that is, the denominator of the expression for Green's function! This contribution cancels, which proves the theorem.

We see as well that in any connected term of m th order there will be exactly $m!$ identical contributions due to rearrangements of t_1, \dots, t_m in $\langle \Phi_0 | \mathcal{T} \mathcal{W}(t_1) \dots \mathcal{W}(t_m) \Psi(X) \Psi^\dagger(X') | \Phi_0 \rangle$ **connected**. This cancels the $\frac{1}{m!}$ factors and allows us to deal only with topologically different graphs. An example (Fig. 2.9): these two second order diagrams are the same diagram, because they differ only by labels of the interaction lines, $12 \leftrightarrow 34$. Returning to our specific form of the interaction, we will see that in our case there is also a 2^{-n} factor associated with diagram, due to the one half in the two-particle interaction term. This factor also cancels, this time because we don't distinguish between the ends of the interaction line, $1 \bullet \cdots \bullet 2$ being the same as $2 \bullet \cdots \bullet 1$. (As we said, only the labels of external ends matter. The rest are just dummy integration variables!) Then we finally come to

2.2.1.3 General Rules

1. Draw all topologically distinct connected Feynman diagrams,
2. Decode them according to Table 2.1,
3. Multiply every diagram by $(-1)^F$, where F is the number of closed loops with more than one vertex, consisting of fermionic lines. (“Bubbles” (n^0) do not count here.)

The origin of rule 3 is self-evident. When a fermionic loop is formed, we have to contract the Fermi operators like this: $\psi(1)\psi^\dagger(2)\psi(2)\psi(3)\cdots\psi(N)\psi^\dagger(1)$. Since in any Hamiltonian we have an arrangement $\psi^\dagger(1)\psi(1)$ etc., this means that the operator $\psi^\dagger(1)$ must have been dragged to the rightmost place through all the rest of the operators, that is, through an odd number of Fermi operators: its own conjugate, and no matter how many $\psi^\dagger\psi$ pairs. This yields the overall minus sign and explains the rule. The bubbles don’t count, because such a bubble corresponds to a $\psi^\dagger\psi$ pair, and no rearrangement is necessary.

If we now perform a Fourier transformation to the momentum representation, we will see that the same rules apply, but the decoding table is somewhat different (here we denote by P the set (\mathbf{p}, ω)), see Table 2.2. The energy and momentum conservation law in each vertex (which reduces the number of integrations in each vertex by one) has a simple origin. In coordinate representation, an intermediate integration in a vertex $Y = (\mathbf{y}, t_y)$ involves the expression $\int d^4Y G^0(.. - Y)G^0(Y - ..)U(Y - ..)$. (We take into account that the unperturbed Green’s function and interaction potential are spatially uniform.) Rewriting this in Fourier components, we obtain

$$\int \frac{d^4K}{(2\pi)^4} \int \frac{d^4K_1}{(2\pi)^4} \int \frac{d^4K_2}{(2\pi)^4} \int d^4Y e^{iK(..-Y)+iK_1(Y-..)+iK_2(Y-..)} \\ \times G^0(K)G^0(K_1)U(K_2).$$





The integral over Y can be taken immediately; it is a simple exponential integral yielding delta functions:

$$\int d^4Y e^{iY(-K+K_1+iK_2)} = \int dt_y e^{-it_y(-\omega+\omega_1-\omega_2)} \int d^3\mathbf{y} e^{i\mathbf{y}(-\mathbf{k}+\mathbf{k}_1+\mathbf{k}_2)} \\ = (2\pi)^4 \delta(-\omega+\omega_1-\omega_2) \delta(-\mathbf{k}+\mathbf{k}_1+\mathbf{k}_2).$$

Thus the energy (frequency) and momentum (wave vector) are conserved in each vertex. The physical reason for this is clear: each vertex of the diagram describes a scattering process. The Hamiltonian of our problem (which describes such scattering) is spatially uniform and time independent, which in agreement with general principles yields momentum and energy conservation.

Besides scalar electron–electron interaction, another important interaction in solid-state systems is electron–phonon interaction. We will not derive here the corresponding Hamiltonian in terms of electron and phonon field operators: this is rather

Table 2.2 Feynman rules for scalar electron–electron interaction (momentum representation)

	$iG(P) \equiv iG_{\alpha\alpha'}(\mathbf{p}, \omega)$	Causal Green's function
	$iG^0(P) \equiv iG^0(\mathbf{p}, \omega)\delta_{\alpha\alpha'}$	Unperturbed causal Green's function
	$-iU(Q) \equiv -iU(\mathbf{q})$	Fourier transform of the interaction potential
	$n^0(\mu)$	Unperturbed electron density

The integration over all intermediate momenta and frequencies ($dP/(2\pi)^4$) and summation over dummy spin indices is implied, taking into account energy (frequency)/momentum conservation in every vertex

a subject for a course in solid state physics. It is enough for us to note that the electron–phonon interaction is described by terms in the Hamiltonian proportional to $\psi^\dagger(X)\psi(X)\phi(X)$ (this expression is Hermitian, since the phonon operator ϕ (as we defined it) is real). It is clear then that only even-order terms in electron–phonon interaction enter the perturbation expansion, because otherwise there will be unpaired phonon operators, giving zero vacuum average. In the even-order terms, phonon operators pair to form unperturbed phonon Green's functions (propagators) $D^0(\mathbf{k}, \omega)$. The definition of the vertex and of the phonon propagator depends on convention; we give here for your convenience the rules used in two basic monographs on the subject. The following discussion will not actually depend on such details, but each time you perform or follow specific calculations, it pays to check all the conventions beforehand.

2.2.2 Operations with Diagrams. Self Energy. Dyson's Equation

One of reasons why Green's function are so widely used is that the corresponding diagrams have a very convenient property: *The value of any Feynman diagram for Green's function can be found as the composition of expressions corresponding to its parts, independently of the structure of the diagram as a whole.*

This means that any part of the diagram (subdiagram) can be calculated separately once and for all and then inserted into an arbitrary diagram containing such a part. (This is not so, e.g., in the case of diagram expansion for the grand potential.)

What does this mean? Let us look at two different diagrams shown in Fig. 2.10, of second and sixth order respectively. The expressions for them are easily written, and we underline the terms that correspond to the marked parts of the diagrams:

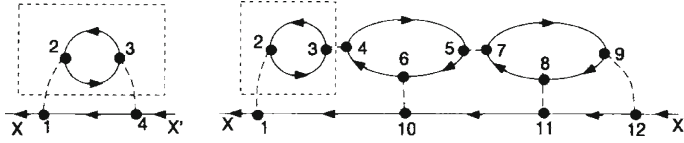







Fig. 2.10 Two diagrams

Table 2.3 Feynman rules for electron-phonon interaction (momentum representation)




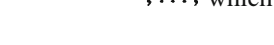
	$iD(K) \equiv iD(\mathbf{k}, \omega)$	Exact phonon propagator
[1] 	$iD^0(K) \equiv iD^0(\mathbf{k}, \omega) = i \frac{\omega_k^2}{\omega^2 - \omega_k^2 + i0}$	Unperturbed phonon propagator
	$-ig$	Electron-phonon coupling constant
[3] 	$iD^0(K) \equiv iD^0(\mathbf{k}, \omega) = i \frac{2\omega_k}{\omega^2 - \omega_k^2 + i0}$	Unperturbed phonon propagator
	$-i M_{\mathbf{k}} $	Electron-phonon matrix element

$$\begin{aligned}
 & \int d1d2d3d4[iG^0(X1)(-1)iG^0(23)iG^0(32) \\
 & \quad \times iG^0(14)iG(4X')(-iU(12))(-iU(34))]; \\
 & \int d1d2d3d4d5d6d7d8d9d10d11d12[iG^0(X1)(-1)iG^0(23)iG^0(32) \\
 & \quad \times iG^0(54)iG^0(46)iG^0(65)(-1)iG^0(97)iG^0(78)iG^0(89) \\
 & \quad \times (-1)iG^0(1, 10)iG^0(10, 11)iG^0(11, 12)iG^0(12, X') \\
 & \quad \times (-iU(12))(-iU(34))(-iU(57))(-iU(6, 10))(-iU(8, 11)) \\
 & \quad (-iU(9, 12))].
 \end{aligned}$$

The final expression is simply constructed of elementary blocks like

$$\begin{aligned}
 & \text{Diagram: a loop with vertices 2 and 3, connected by a dashed line from vertex 1 to vertex 4.} \\
 & = -iG^0(23)iG^0(32).
 \end{aligned}$$

This is very different from the diagrammatic series for the grand potential, Ω , where a factor $1/n$ in each n th-order diagram prohibits such *partial summation* of diagram series (Table. 2.3).

The idea of this summation is simple and mathematically shaky. Suppose we have a diagram, for example, . In the infinite series for Green's function there is an infinite subset of diagrams like , , , ..., which include all possible corrections to the inner line. Due to

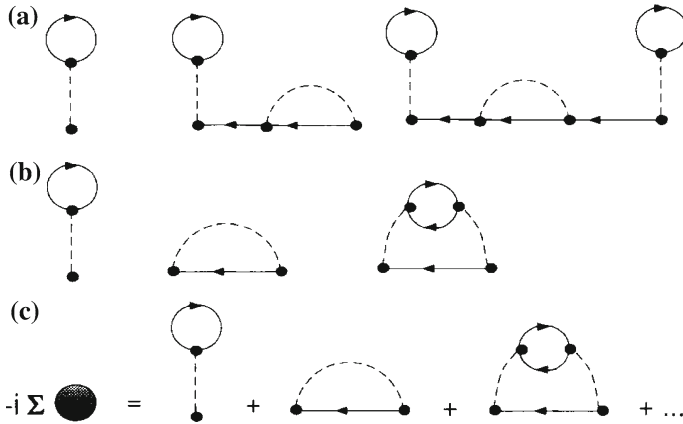



Fig. 2.11 Self energy diagrams: **a** self energy parts, **b** irreducible self energy parts, **c** proper self energy

the fact that there is no explicit dependence of the expression on the order of the diagram, we can forget about everything that lies beyond these interaction points and concentrate on the inside of the graph. The corrections here should transform the thin line (unperturbed Green's function, G^0) into a solid line (exact Green's function, G) in

the same way, as the whole series gives the exact Green's function G : ! We have partially summed the diagram series for Green's function!

This is not yet a victory, though. First, the summation of this sort still gives us an equation: a self-consistent equation for the exact Green's function, usually a nonlinear integral or integro-differential one. To solve it would be really tough! Second, there is absolutely no guarantee that this equation is correct. Indeed, we know from mathematics that only for a very restricted class of convergent series (*absolutely* convergent) the sum is independent of the order of the terms. What we have done here is to redistribute the terms of the perturbation series, about which we even do not know (and usually cannot know) whether it converges at all! The justification here comes from the results: if they are wrong, then something is wrong in our way of partial summation (evidently, there are many, and each is approximate, since some classes of diagrams are neglected). Or maybe something funny occurs to the system, and this is already useful information. We will meet such a case later, when discussing application of the theory to superconductivity. In most cases the results are right if the partial summation is made taking into account the physics of the problem. Usually we can show, with physical if not mathematical rigor, that a certain class of diagrams is more important than the others, and therefore the result of its summation reflects essential properties of the system.

To approach such partial summations systematically, let us make some definitions.

The *self energy part* is called any part of the diagram connected to the rest of it only by two particle lines (Fig. 2.11).

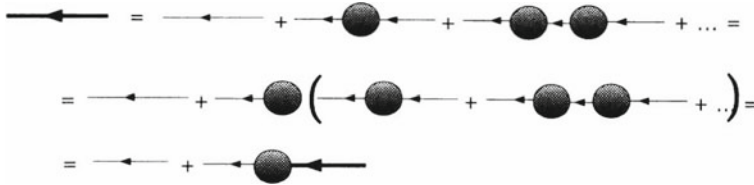


Fig. 2.12 Dyson's equation

The *irreducible*, or *proper*, *self energy part* is the one that cannot be separated by breaking one particle line, like the one in Fig. 2.11b.

Finally, the *proper self energy*, or *self energy par excellence*, or *mass operator*, is called the sum of all possible irreducible self energy parts and is denoted by $\Sigma_{\alpha\alpha'}(X, X')$. The name is given for historical field-theoretical reasons, and its meaning will become clear a little later.

It is convenient to include a $(-i)$ factor into the definition (Fig. 2.11). Then the series for Green's function can be read and drawn as follows (Fig. 2.12):

$$iG = iG^0 + iG^0\Sigma G^0 + iG^0\Sigma G^0\Sigma G^0 + \dots \quad (2.63)$$

Here the terms in the infinite series are redistributed in such a way as to make it a simple series (a geometric progression!) over the powers of self energy and unperturbed Green's function only. (Of course, all necessary integrations and matrix multiplications with respect to spin indices are implied, so that this is an *operator* series.)

Separating the iG^0 factor, we obtain the celebrated *Dyson's equation* (see Fig. 2.12), which is exactly of the self-consistent form we anticipated:

$$G(X, X') = G^0(X, X') + \int dX'' \int dX''' G^0(X, X'') \Sigma(X'', X''') G(X''', X'). \quad (2.64)$$

(Of course, we could take iG^0 from the other side, and get $G(P) = G^0 + G(P)\Sigma(P)G^0(P)$.) In a homogeneous stationary and nonmagnetic system (the last condition means that G and Σ are diagonal with respect to spin indices) we can make a Fourier transformation, reducing the above equation to $G(P) = G^0 + G^0(P)\Sigma(P)G(P)$. Then we see that

$$G(\mathbf{p}, \omega) = \left[(G^0(\mathbf{p}, \omega))^{-1} - \Sigma(\mathbf{p}, \omega) \right]^{-1} = \frac{1}{\omega - \epsilon(\mathbf{p}) + \mu - \Sigma(\mathbf{p}, \omega)}. \quad (2.65)$$

Symbolically this can be written as

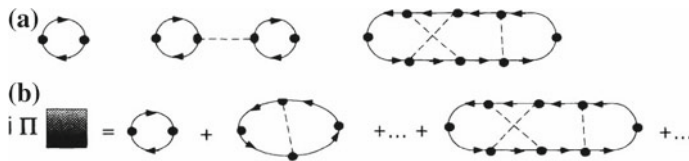


Fig. 2.13 Interaction renormalization: **a** polarization insertions, **b** polarization operator

$$G = \left[i \frac{\partial}{\partial t} - \varepsilon - \hat{\Sigma} \right]^{-1}. \quad (2.66)$$

The latter equation holds even if G and Σ are nondiagonal (e.g., in the nonhomogeneous case), understanding $[\dots]^{-1}$ as an inverse operator.

An important feature of (2.65) is that if we substitute there some finite-order approximation for the self energy, the resulting approximation for G will be equivalent to calculating an *infinite* subseries of the perturbation series, and this gives a much better result than the simple-minded calculation of the initial series term by term.

This is a natural consequence of a self-consistent approach. Another, less pleasant, one is that any approximate self energy is to be checked, lest it violates the general analytic properties of Green's function (which follow from the general causality principle and should not be toyed with). Returning to the simple case (2.65) and recalling the Källén–Lehmann representation, we see that necessarily

$$\begin{cases} \Im \Sigma(\mathbf{p}, \omega) \geq 0, & \omega < 0, \\ \Im \Sigma(\mathbf{p}, \omega) \leq 0, & \omega > 0. \end{cases} \quad (2.67)$$

We see as well that $\Im \Sigma$ is the inverse lifetime of the elementary excitation, while $\Re \Sigma$ defines the change of dispersion law due to interaction. (In quantum field theory this leads to the change of the particle mass, which is why Σ is also called the mass operator.)

2.2.3 Renormalization of the Interaction. Polarization Operator

Following the same approach, we can consider the insertions into the interaction line as well, like those shown in Fig. 2.13.

The *polarization insertion* is called the part of the diagram that is connected to the rest of it only by two interaction lines. The *irreducible polarization insertion* is one that cannot be separated by breaking of a single interaction line. Finally, the *polarization operator* is the sum of all irreducible polarization insertions, Π , and is a direct analogue to the self energy.

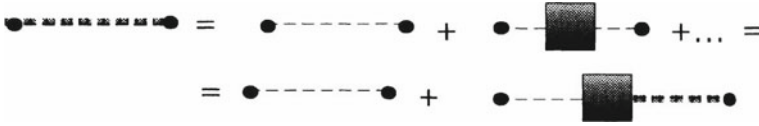


Fig. 2.14 Equation for the polarization operator

Since there is a $(-i)$ factor in the definition of the interaction line, it is convenient to introduce an (i) factor into the polarization operator. The analogue to Dyson's equation is readily obtained and reads (see Fig. 2.14)

$$U_{\text{eff}}(P) = U(P) + U(P)\Pi(P)U_{\text{eff}}(P). \quad (2.68)$$

Then we find the *generalized dielectric function*, $\kappa(\mathbf{p}, \omega)$:

$$U_{\text{eff}}(\mathbf{p}, \omega) \equiv \frac{U(\mathbf{p}, \omega)}{\kappa(\mathbf{p}, \omega)} = \frac{U(\mathbf{p}, \omega)}{1 - U(\mathbf{p}, \omega)\Pi(\mathbf{p}, \omega)}, \quad (2.69)$$

which describes the effect of the polarization of the medium on particle–particle interaction. A good example of such an effect is the following.

2.2.3.1 Screening of Coulomb Interaction

The Thomas–Fermi result concerning the screening of the Coulomb potential by the charged Fermi gas can be reproduced if we use the random phase approximation (RPA), which here means taking the lowest-order term in the polarization operator:

$$i\Pi_0(\mathbf{p}, \omega) = \begin{array}{c} \text{p} + \mathbf{q}, \omega + \zeta \\ \circ \quad \circ \\ \text{q}, \zeta \end{array} = 2 \int \frac{d^3\mathbf{q}d\zeta}{(2\pi)^4} G^0(\mathbf{p} + \mathbf{q}, \omega + \zeta) G^0(\mathbf{q}, \zeta). \quad (2.70)$$

The calculations give the following result for the static screening:

$$\Re\Pi_0(\mathbf{p}, 0) = -\frac{mp_F}{2\pi^2} \left(1 + \frac{p_F^2 - p^2/4}{p_F p} \ln \left| \frac{p_F + p/2}{p_F - p/2} \right| \right); \quad (2.71)$$

$$\Im\Pi_0(\mathbf{p}, 0) = 0. \quad (2.72)$$

For the long-range screening ($p \ll p_F$),

$$\Pi_0 \approx -2\mathcal{N}(\mu),$$

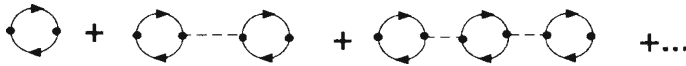
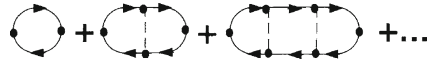


Fig. 2.15 Random phase approximation

Fig. 2.16 Ladder approximation



where $\mathcal{N}(\mu) \equiv \frac{m p_F}{2\pi^2}$ is the density of states on the Fermi surface. Thus the Fourier transform of the interaction is

$$U_{\text{eff}}(q) \approx \frac{4\pi e^2/q^2}{1 + 2\mathcal{N}(\mu)4\pi e^2/q^2} = \frac{4\pi e^2}{q^2 + 8\pi e^2\mathcal{N}(\mu)}. \quad (2.73)$$

The quantity

$$q_{TF}^2 = 8\pi e^2\mathcal{N}(\mu)$$

is the squared Thomas–Fermi wave vector, and the potential indeed takes the Yukawa form:

$$U_{\text{eff}}(r) = \frac{e^2}{r} \exp(-q_{TF}r). \quad (2.74)$$

Thus, the presence of other charged particles leads to screening of initial long-range Coulomb interactions, and limits it to a finite Thomas–Fermi radius. How this happens is graphically clear from the simplest polarization diagram. The interaction creates a *virtual* electron–hole pair. (Virtual, of course, because the energy–momentum relation for every internal line of a diagram is violated: we integrate over *all* energies and *all* momenta *independently*! For a real particle, $E = \frac{p^2}{2m}$ or something like this.) The approximation we used included only independent events of such virtual electron–hole creation: because the energy and momentum along the interaction line are conserved, the quantum-mechanical phase of the electron–hole pair is immediately lost and does not affect the next virtual pair. This is the reason it is called RPA, random phase approximation (Fig. 2.15). As we discussed in the very beginning of the book, this kind of approach works well if there is a large number of particles within the interaction radius: then indeed it is much more probable to interact with two different particles consecutively than with the same one twice. In the opposite case, when the density of particles is low, RPA naturally fails, while the *ladder approximation* is relevant: Here a virtual pair (quasiparticle–quasihole) interacts repeatedly before disappearing (Fig. 2.16). This is again reasonable, because when density is low, it is improbable to find some other quasiparticle close at hand to interact with.

Unfortunately, on our path to the Thomas–Fermi screening, Eq. (2.74), from the random phase approximation, Eqs. (2.71), (2.72), we made one simplification too

many when replaced the static polarization $\Pi_0(\mathbf{p}, 0)$ with its value at $p = 0$. The logarithmic term in (2.71) is non-analytical at $p = p_F$, and—as it turns out—it produces instead of the exponential screening (2.74) a qualitatively different potential, which far away from the charge behaves as

$$U_{\text{eff}}(r) \propto \frac{e^2}{r^3} \cos(2p_F r).$$

Not only it does not fall off exponentially, but it also demonstrates *Friedel oscillations*. Both effects are due to the sharp step of the Fermi distribution function at $T = 0$, which produced the non-analytical term in (2.71) in the first place (see Appendix A). At finite temperature the step is smeared, and the above expression is multiplied by an exponentially decaying factor, thus reverting to the Yukawa-type screening with Friedel oscillations superimposed.

2.2.4 Many-Particle Green's Functions. Bethe–Salpeter Equations. Vertex Function

We have seen that Green's functions give a convenient apparatus for a description of many-body systems. So far we have used a *one-particle* Green's function, dealing with a single quasiparticle excitation, though against the many-body background. They don't apply, e.g., to the case of the bound state of *two* such excitations. Indeed, in a Fermi system such a state would be a boson, while the one-particle Green's function describes a fermion.

This problem can be easily solved. Nobody limits us to consideration of averages $\langle \psi \psi^\dagger \rangle$ only. The “Schrödinger equation” for $G(X, X')$ included terms $\langle \psi \psi \psi^\dagger \psi^\dagger \rangle$. Therefore it is natural to introduce n -particle Green's functions. (As usual, there is no common convention here, so when reading a chapter be careful what definition is actually used.)

The n -particle (or $2n$ -point) Green's function (Fig. 2.17) is defined as follows:

$$\begin{aligned} G_{(n)\alpha_1\alpha_2\ldots\alpha_n,\alpha'_1\alpha'_2\ldots\alpha'_n}(\mathbf{x}_1t_1, \mathbf{x}_2t_2, \ldots, \mathbf{x}_nt_n; \mathbf{x}'_1t'_1, \mathbf{x}'_2t'_2, \ldots, \mathbf{x}'_nt'_n) \\ \equiv G_{(n)}(12\cdots n; 1'2'\cdots n') \\ = \frac{1}{(i)^n} \langle T \psi(1)\psi(2)\cdots\psi(n)\psi^\dagger(n')\cdots\psi^\dagger(2')\psi^\dagger(1') \rangle \end{aligned} \quad (2.75)$$

The rules of drawing and decoding Feynman diagrams stay intact and can be easily derived from the expansion of the S -operator in the average $\langle T \cdots \psi^\dagger \psi \rangle$. There is only one additional rule.

The diagram is multiplied by $(-1)^S$, where S is the parity of the permutation of the fermion lines' ends $(1'2'\cdots n') \leftrightarrow (12\cdots n)$ (see Fig. 2.18).

Fig. 2.17 Many-particle Green's function (This convenient “stretched skin” graphics are introduced in [5]; dots mark the outgoing ends)

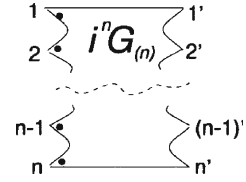
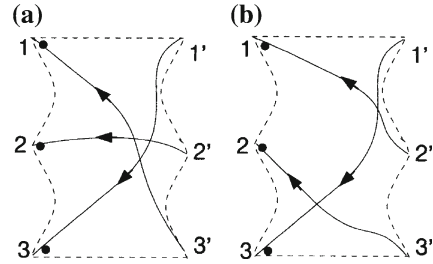


Fig. 2.18 Sign rule for a many-particle Green's function: **a** $(1, 2, 3) \Leftrightarrow (3', 2', 1')$, sign +1, **b** $(1, 2, 3) \Leftrightarrow (2', 3', 1')$, sign -1



The origin of this rule is easy to see applying Wick's theorem to the lowest order expression for the two-particle Green's function:

$$\begin{aligned}
 G_{(2)}(12, 1'2') &\equiv (-i)^2 \langle T \psi_1 \psi_2 \psi_2^\dagger \psi_1^\dagger \rangle & (2.76) \\
 &\approx (-i) \langle T \psi_1 \psi_1^\dagger \rangle_0 (-i) \langle T \psi_2 \psi_2^\dagger \rangle_0 \mp (-i) \langle T \psi_1 \psi_2^\dagger \rangle_0 (-i) \langle T \psi_2 \psi_1^\dagger \rangle_0 \\
 &= G^0(11') G^0(22') \mp G^0(12') G^0(21').
 \end{aligned}$$

The cancellation theorem removes only the diagrams with loose parts disconnected from the *external ends*. This means that not every diagram looking disconnected is actually disconnected! For example, the diagrams corresponding to (2.76) (see the two diagrams in Fig. 2.19) are not disconnected and are not canceled. As a matter of fact they provide a Hartree–Fock approximation for the two-particle Green's function (direct and exchange terms, as is evident from their structure).

The two-particle Green's function is most widely used and therefore has its own letter, K :

$$K(12; 1'2') = -\langle T \psi(1) \psi(2) \psi^\dagger(2') \psi^\dagger(1') \rangle. \quad (2.77)$$

Its diagram expansion to the second order is given in Fig. 2.19.

The importance of the two-particle Green's function is that (1) it determines the scattering amplitude of quasiparticles, that is, their interactions, and thus (2) its poles define the dispersion law of two-particle excitations (e.g., bosonic excitations in a normal Fermi system—say zero sound), as well as appearance of boundstate of two quasiparticles—and therefore the superconducting transition point.

We can define the *irreducible* two-particle Green's function by separating all “seemingly disconnected” diagrams (Fig. 2.20). The first two of this set give the

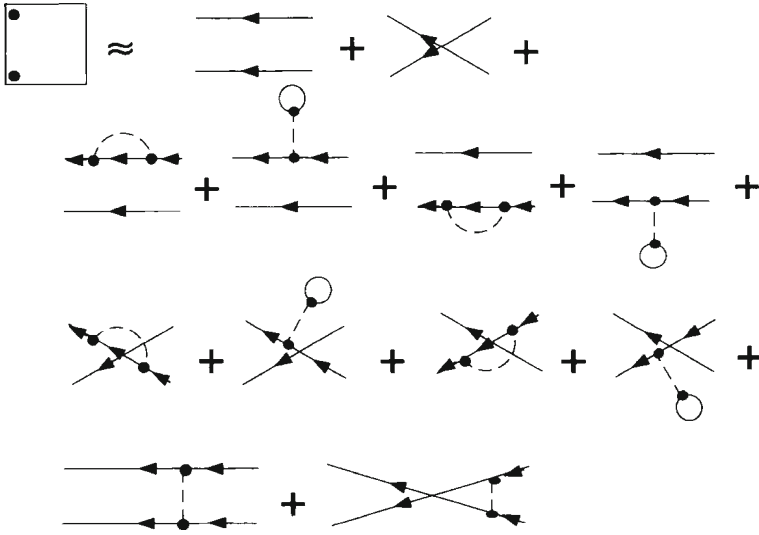


Fig. 2.19 Second-order expansion of the two-particle Green's function

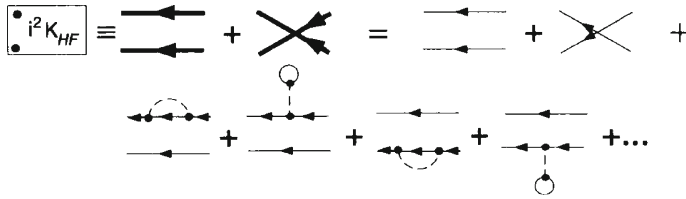


Fig. 2.20 Generalized Hartree-Fock approximation for the two-particle Green's function

self-consistent Hartree-Fock approximation for the two-particle Green's function (self-consistent, because it contains *exact* one-particle Green's functions):

$$G(11')G(22') \mp G(12')G(21') = G^0(11')G^0(22') \mp G^0(12')G^0(21') + \dots \quad (2.78)$$

The rest is the *irreducible two-particle Green's function* and is expressed through the *vertex function* Γ (Fig. 2.21):

$$\begin{aligned} \tilde{K}(12; 1'2') &= K(12; 1'2') - [G(11')G(22') \mp G(12')G(21')] \\ &= \int d3 \int d3' \int d4 \int d4' G(13)G(24)i\Gamma(33'; 44')G(3'1')G(4'2'). \end{aligned} \quad (2.79)$$

The poles of the two-particle Green's function define *two-particle excitations* of the system in the same fashion as the poles of the one-particle Green's function defined quasiparticles. Examples are such excitations in the Fermi systems as zero sound and plasmons. Evidently, the relevant poles of the two-particle Green's func-

$$\begin{array}{c} 1 \\ \bullet \\ \boxed{i^2 \tilde{K}} \\ \bullet \\ 2 \end{array} \begin{array}{c} 1' \\ \bullet \\ \boxed{\phantom{i^2 \tilde{K}}} \\ \bullet \\ 2' \end{array} \equiv \begin{array}{c} \bullet \\ \boxed{i^2 K} \\ \bullet \end{array} - \begin{array}{c} \bullet \\ \boxed{i^2 K_{HF}} \\ \bullet \end{array} = \begin{array}{c} 1 \quad 3 \quad 3' \quad 1' \\ \leftarrow \quad \rightarrow \quad \leftarrow \quad \rightarrow \\ \boxed{-i\Gamma} \\ \leftarrow \quad \rightarrow \quad \leftarrow \quad \rightarrow \\ 2 \quad 4 \quad 4' \quad 2' \end{array}$$

Fig. 2.21 Irreducible part of the two-particle Green's function and the vertex function

tion appear only in the vertex function: the “tails” are one-particle Green's functions and as such don't bring anything new. Therefore, we concentrate on the vertex function.

The discourse is simpler in momentum representation, if we are (as usual) dealing with a stationary, spatially uniform system. Evidently, only three sets of variables of four are independent (because a uniform shift of coordinates or times should not change anything). We choose the following set of independent combinations:

$$X_1 - X'_1, X_2 - X'_2, X'_1 - X_2. \quad (2.80)$$

Here and later on $X = \mathbf{x}, t$; $P = \mathbf{p}, \omega$; and the “scalar product” $PX = \mathbf{p} \cdot \mathbf{x} - \omega t$.

Then the two-particle Green's function in momentum space is defined as

$$\begin{aligned} & \int dX_1 \int dX_{1'} \int dX_2 \int dX_{2'} e^{-i(P_1 X_1 + P_2 X_2 - P_{1'} X_{1'} - P_{2'} X_{2'})} K(X_1, X_2; X'_1, X'_2) \\ &= (2\pi)^4 \delta(P_1 + P_2 - P_{1'} - P_{2'}) K(P_1, P_2; P_{1'}, P_1 + P_2 - P_{1'}). \end{aligned} \quad (2.81)$$

The Fourier transformation for any function of these four sets of variables is defined by

$$\begin{aligned} & K(P_1, P_2; P_{1'}, P_1 + P_2 - P_{1'}) \\ &= \int d(X_1 - X'_1) \int d(X_2 - X'_2) \int d(X_{1'} - X'_2) \\ & \quad \times e^{-iP_1(X_1 - X'_2) - iP_2(X_2 - X'_2) + iP'_{1'}(X'_{1'} - X_2)} K(X_1, X_2; X'_1, X'_2); \\ & K(X_1, X_2; X'_1, X'_2) \\ &= \int \frac{dP_1}{(2\pi)^4} \int \frac{dP_2}{(2\pi)^4} \int \frac{dP'_{1'}}{(2\pi)^4} \\ & \quad e^{iP_1(X_1 - X'_{2'}) + iP_2(X_2 - X'_{2'}) - iP'_{1'}(X'_{1'} - X'_2)} K(P_1, P_2; P_{1'}, P_1 + P_2 - P_{1'}). \end{aligned}$$

Then Eq. (2.79) can be rewritten as

$$\begin{aligned} \tilde{K}(P_1, P_2; P_{1'}, P_1 + P_2 - P_{1'}) &= G(P_1)G(P_2) \\ & \quad \times i\Gamma(P_1, P_2; P_{1'}, P_1 + P_2 - P_{1'}) \\ & \quad G(P'_{1'})G(P_1 + P_2 - P_{1'}). \end{aligned} \quad (2.82)$$

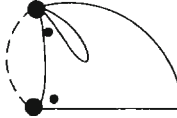
Now we are ready to derive (for scalar electron–electron interaction, our standard guinea pig) an important general relation between the vertex function and self energy. That such a relation should exist is reasonable, since both Σ and Γ have in common, besides being uppercase Greek letters, that they result from summation of all somehow irreducible diagrams. First, we present a very graphic proof, which will be then supported by more rigorous calculation (which, on the other hand, is only a translation of graphs into equations).

We start from writing down the equation of motion for the one-particle Green's function, in position space. As we observed much earlier, such an equation will contain the two-particle Green's function:



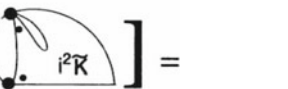
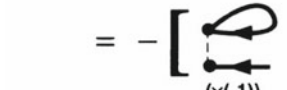


$$\left(i \frac{\partial}{\partial t} + \frac{1}{2m} \nabla_{\mathbf{x}}^2 + \mu\right) G_{\alpha\alpha'}(X, X') = \delta_{\alpha\alpha'} \delta(X - X') - i \int d^4 Y U(X - Y) K_{\alpha\gamma, \alpha'\gamma}(X, Y; X', Y) \quad (2.83)$$

(we have made use of the definition: $\langle T \Psi_{\gamma}^{\dagger}(Y) \Psi_{\gamma}(Y) \Psi_{\alpha}(X) \Psi_{\alpha}^{\dagger}(X') \rangle \equiv K_{\alpha\gamma, \alpha'\gamma}(X, Y; X', Y)$). Since $G = G^0 + G^0 \Sigma G$, the relation in question is indeed here, and we have only to extract it.

Graphically, it is simple: the equation can be symbolically written as $[iG^0]^{-1} iG = \mathcal{I} - (-iU)(i^2 K)$, that is,

$$[\leftarrow]^{-1} \leftarrow = I - \text{diagram}$$


Then we do a series of transformations:

$$\begin{aligned} [\leftarrow]^{-1} \leftarrow &= [\leftarrow]^{-1} [\leftarrow + \text{diagram}] = I + \text{diagram} \\ \text{diagram} &= - \text{diagram} = - [\text{diagram} + \text{diagram}] = \\ &= - [\text{diagram} - \text{diagram} + \text{diagram}] \end{aligned}$$







The result is shown in Fig. 2.22. Notice that we used the specific for ($n > 2$)-particle Green's function sign convention in order to determine the signs of the first two terms on the right-hand side of Fig. 2.22: if “decoded” following the one-particle rules, they would lack a (-1) -factor due to the exchange of tails of the two-particle diagram.

Fig. 2.22 Relation between the self energy and vertex function



In analytical form, this equation (sometimes called Dyson's equation, but less often than *the* Dyson equation we encountered earlier) reads

$$\begin{aligned} \Sigma(P)\delta_{\alpha\beta} = & U(0)n(\mu)\delta_{\alpha\beta} + i\delta_{\alpha\beta} \int \frac{dP_1}{(2\pi)^4} U(P - P_1)G(P_1) \\ & + \int \frac{dP_1}{(2\pi)^4} \int \frac{dP_2}{(2\pi)^4} G(P_1)G(P_2) \\ & \times \Gamma_{\alpha\gamma,\beta\gamma}(P_1, P_2; P, P_1 + P_2 - P)G(P_1 + P_2 - P)U(P - P_1). \end{aligned} \quad (2.84)$$

Now let us derive it without graphs, or rather write down each step instead of drawing it. Again, assume a uniform, stationary, and isotropic system. Then, in momentum space, (2.83) looks like

$$\left[(G^0(P))^{-1}G(P) - 1 \right] \delta_{\alpha\alpha'} = -i \int \frac{dP_1 dP_2}{(2\pi)^8} K_{\alpha\gamma,\alpha'\gamma}(P_1, P_2; P, P_1 + P_2 - P)U(P - P_1).$$

(Here $(G^0(P))^{-1} \equiv \left(\omega - \frac{p^2}{2m} + \mu \right)$ is a function, not an operator, and simply equals $1/G^0(P)$.) Now substitute in this equation the definition (2.79) and divide by $G(P)$. After this messy operation we obtain

$$\begin{aligned} [1/G^0(P) - 1/G(P)]\delta_{\alpha\alpha'} = & -i\delta_{\alpha\alpha'}U(0) \int \frac{dP_2}{(2\pi)^4} G(P_2) \\ & \pm i\delta_{\alpha\alpha'} \int \frac{dP_1}{(2\pi)^4} U(P - P_1)G(P_1) \\ & + \int \frac{dP_1 dP_2}{(2\pi)^8} \Gamma_{\alpha\gamma,\gamma\alpha'}(P_1, P_2; P, P_1 + P_2 - P) \\ & \times G(P_1)G(P_2)G(P_1 + P_2 - P)U(P - P_1). \end{aligned}$$

Since by virtue of the Dyson equation $1/G^0(P) - 1/G(P) = \Sigma(P)$, then we eventually recover Eq. (2.84). See how much easier it was with the diagrams? By the way, the graphs immediately show the physical sense of this relation. The first two terms in (2.84) give the self-consistent Hartree–Fock approximation with initial (bare) potential: they take into account the interaction of the test particle with the medium, and with itself (exchange term). The rest must contain the effects of renormalization of the interaction, and indeed, the third graph can be understood as containing the *renormalized interaction vertex* (Fig. 2.23). As you see, it contains, in particular, all the polarization insertions in the interaction line. This is the reason we had a bare potential line in Fig. 2.22 and Eq. (2.84): otherwise certain diagrams would be included

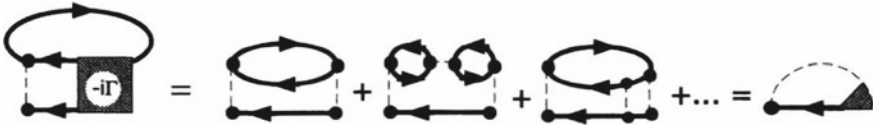


Fig. 2.23 Vertex function and renormalized interaction

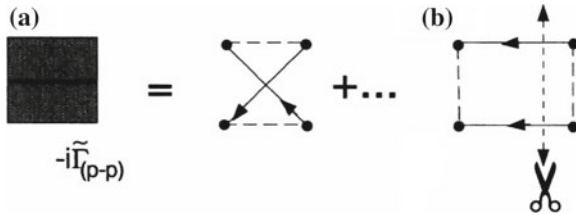


Fig. 2.24 Particle–particle irreducible vertex function



Fig. 2.25 Particle–particle irreducible vertex function and two–particle Green's function

twice. In all operations with diagrams we must pay special attention to avoiding the double count.

2.2.4.1 The Bethe–Salpeter Equation

Earlier we introduced the irreducible self energy as a sum of all diagrams that cannot be separated by severing one fermion line. Let us generalize this and introduce the *particle–particle irreducible* vertex function, $\tilde{\Gamma}_{(PP)}$, which includes all diagrams that cannot be separated by severing *two* fermion lines between in- and outgoing ends. (In Fig. 2.24 diagram (a) is particle–particle irreducible, but diagram (b) is not.)

Then the diagram series for the particle–particle irreducible vertex part (or the particle–particle irreducible two–particle Green's function, if drop the external tails) can be drawn as in Fig. 2.25.

For the vertex function we thus obtain the *Bethe–Salpeter equation*, which is a direct analogue of the Dyson equation for the one-particle Green's function² (Fig. 2.26):

² Of course, this equation can as well be written for the two–particle Green's function itself, instead of the vertex function.

Fig. 2.26 Bethe-Salpeter equation (*particle-particle channel*)

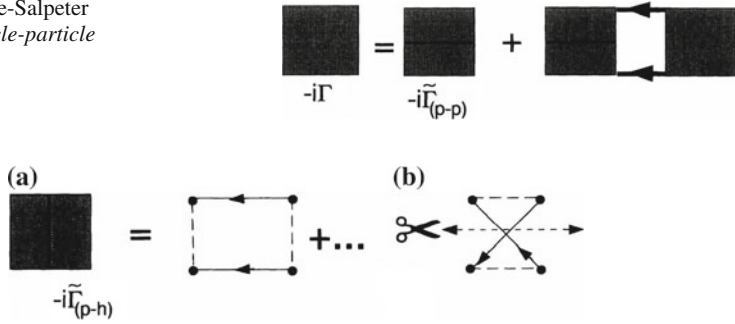


Fig. 2.27 Particle-hole irreducible vertex function

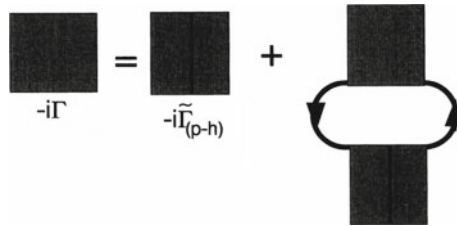


Fig. 2.28 Bethe-Salpeter equation (*particle-hole channel*)

$$\Gamma(12; 1'2') = \tilde{\Gamma}_{(PP)}(12; 1'2') + i \int d3 \int d3' \int d4 \int d4' \tilde{\Gamma}_{(PP)}(12; 3'4') G(33') G(44') \Gamma(3'4'; 1'2'). \quad (2.85)$$

Two-particle functions allow for more possibilities: there are more loose ends in a diagram! Thus, we have a different *particle-hole irreducible* vertex, $\tilde{\Gamma}_{(PH)}$, (Fig. 2.27, where diagram (b) is now (particle-hole) irreducible, while diagram (a) is not). This yields another version of the Bethe-Salpeter equation (Fig. 2.28):

$$\Gamma(12; 1'2') = \tilde{\Gamma}_{(PH)}(12; 1'2') + i \int d3 \int d3' \int d4 \int d4' \tilde{\Gamma}_{(PH)}(42; 4'2') G(43) G(3'4') \Gamma(13; 1'3'). \quad (2.86)$$

Of course, both versions are equivalent mathematically, but not physically. Since there is little hope that either can be solved exactly, some approximations are in order, and we should choose, as usual, the version that is better as a starting point. The latter one, e.g., proves to be useful for investigation of the processes with small momentum transfer between quasiparticles, but this is beyond the scope of this book.

2.3 Problems

• Problem 1

starting from the expression for the grand potential, $\Omega = -PV$,

$$\Omega = \int_0^\mu d\mu (2iV) \lim_{t \rightarrow -0} \int \frac{d\mathbf{p} d\omega}{(2\pi)^4} e^{-i\omega t} G(\mathbf{p}, \omega),$$

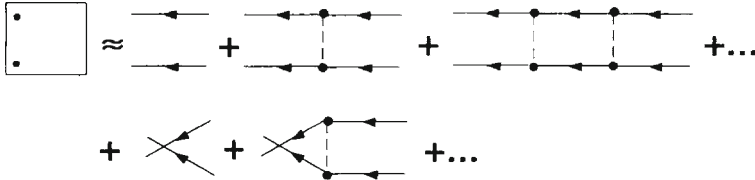
find the pressure of the ideal Fermi gas at zero temperature

$$\left(G(\mathbf{p}, \omega) = G^0(\mathbf{p}, \omega) = \frac{1}{\omega - (\epsilon_{\mathbf{p}} - \mu) + i0 \operatorname{sgn} \omega} \right).$$

Compare to the classical expression $P = nk_B T$ and find the “effective pressure temperature.” How is it related to the “effective energy temperature” $T_F = \mu/k_B$?

• Problem 2

Reduce the *ladder approximation* series for the two-particle Green’s function to an integral equation:



• Problem 3

Calculate the lowest order diagram for the polarization operator:



and reproduce the results of Eqs. (2.71), (2.72).

• Problem 4

Starting from the definition (2.16), derive the equation of motion for the unperturbed phonon propagator.

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