We shall not actually apply this formalism to the calculation of classical quasi particles—this would take us too far afield. Instead we go on directly to the quantum case.

Exercises

2.1 Write the diagram series for the propagator $P(\mathbf{r}_2,\mathbf{r}_1)$ assuming that the scattering at both the monkey and the lion are large, while all other interactions are small. Include all terms through second order, plus a couple of third-order terms. How many diagrams are there in nth order?
2.2 Translate the first few terms of Ex. 2.1 into functions.
2.3 Evaluate the above propagator by partial summation assuming that all $P_0(\mathbf{r}_i,\mathbf{r}_j)=c$.
2.4 Assuming all free propagators $=c$, generalize the above results to include scattering from all animals.

Chapter 3

Quantum Quasi Particles and the Quantum Pinball Propagator

3.1 The quantum mechanical propagator

In this chapter we are going to solve the simplest existing example of a quantum field theoretical problem. We call it the 'quantum pinball game' since it is the precise quantum analogue of the classical pinball machine just discussed, and in fact gives rise to a diagrammatic series having exactly the same form as (2.25). It is a sub-trivial problem, one which can be solved in a microsecond by elementary quantum mechanics. It takes a little longer to do by diagrams, but like its classical cousin in Fig. 2.3 has the great merit of illustrating all the basic principles without immersing the reader in a morass of mathematics. At the end of the chapter, the diagram method is applied to a non-trivial problem, i.e., finding the energy and lifetime of an electron propagating through a set of randomly distributed scattering centres (e.g., impurity atoms in a metal).

The fundamental difference between the classical propagator, P, and the quantum propagator, G, is that P is a probability, whereas G is a probability *amplitude*, with corresponding probability given by $|G|^2\,(=G^*G)$. Thus in the classical case, the total probability for propagation from point 1 to point 2 is just the sum of the probabilities for each propagation process taken separately:

$$P(2,1)_{\text{classical}} = P(\text{process I}) + P(\text{process II}) + \cdots.$$

But in the quantum case, the total probability *amplitude* is the sum of the probability *amplitudes* for each process taken separately

$$G(2,1) = G(\text{process I}) + G(\text{process II}) + \cdots$$

so that the corresponding probability is given by

$$P(2,1)_{\text{quantum}} = G^*G = \underbrace{|G(\text{I})|^2}_{P(\text{I})} + \underbrace{|G(\text{II})|^2}_{P(\text{II})} + \underbrace{G(\text{I})^*\,G(\text{II}) + G(\text{II})^*\,G(\text{I})}_{\text{interference terms}} + \cdots.$$

Because of the characteristic 'interference terms', the quantum probability is not just the sum of the probabilities for the individual processes, in contrast to the classical case.

A familiar example of this is the decay of an atom, molecule, or nucleus from a state i to a state f by means of photon emission. Suppose the atom can either decay directly: $i \to f$, or via the intermediate state m: $i \to m \to f$. Then we have (call A the probability amplitude):

$$\begin{aligned} P(i \to f) &= A^* A = |A(i \to f) + A(i \to m \to f)|^2 \\ &= |A(i \to f)|^2 + |A(i \to m \to f)|^2 + A^*(i \to f)\, A(i \to m \to f) \\ &\quad + A^*(i \to m \to f)\, A\,(i \to f), \end{aligned}$$

which shows the interference between processes $i \to f$ and $i \to m \to f$. (See also Feynman (1965), pp. 19, 20.)

Let us begin by defining the quantum propagator in general, then show what it looks like in the case of free particles and quasi particles. The quantum analogue of the classical propagator is (assuming that the Hamiltonian is time-independent, so that the propagator depends only on time differences):

$$\begin{aligned} iG(\mathbf{r}_2, \mathbf{r}_1, t_2 - t_1)_{t_2 > t_1} &= iG^+(\mathbf{r}_2, \mathbf{r}_1, t_2 - t_1) \\ &= \text{probability amplitude that if at time } t_1 \text{ we add a particle at point } \mathbf{r}_1 \text{ to the interacting system in its ground state, then at time } t_2 \text{ the system will be in its ground state with an added particle at } \mathbf{r}_2. \end{aligned} \tag{3.1}$$

The i factor is purely for decoration (a matter of convention) and the $+$ superscript denotes $t_2 > t_1$. (The precise meaning of the word 'add' here is discussed in detail in §9.2.) The probability corresponding to the amplitude (3.1) is

$$P(\mathbf{r}_2, \mathbf{r}_1, t_2 - t_1) = G^+(\mathbf{r}_2, \mathbf{r}_1, t_2 - t_1)^* G^+(\mathbf{r}_2, \mathbf{r}_1, t_2 - t_1).$$

Note that it is not necessarily the 'same' particle which is observed at t_2, since this has no meaning in the systems of identical particles with which we shall generally deal. Note also that a more precise way of saying that the particle is 'at point $\mathbf{r}_1$' is to say that it is 'in the position eigenstate $\delta(\mathbf{r} - \mathbf{r}_1)$'.

The quantity G^+ defined in (3.1) is called a 'retarded' propagator (or Green's function). By definition, it is equal to zero for $t_2 \leqslant t_1$. There is also an 'advanced' propagator, G^-, which is finite for $t_2 \leqslant t_1$; this will be discussed in chapter 4. (See appendix L for other types of retarded and advanced propagators.)

It is actually more convenient to work with an equivalent definition of G in terms of arbitrary single-particle eigenstates, $\phi_k(\mathbf{r})$, instead of position eigenstates. Then we have

$$\begin{aligned} iG^+(k_2, k_1, t_2 - t_1)_{t_2 > t_1} &= \text{probability amplitude that if at time } t_1 \text{ we add a particle in } \phi_{k_1}(\mathbf{r}) \text{ to the interacting system in its ground state, then at time } t_2 \text{ the system will be in its ground state with an added particle in } \phi_{k_2}(\mathbf{r}). \end{aligned} \tag{3.2}$$

For $t_2 \leqslant t_1$, G^+ is defined so that:

$$iG^+(k_2, k_1, t_2 - t_1)_{t_2 < t_1} = 0. \tag{3.3}$$

A convenient choice for $\phi_k(\mathbf{r})$ is the eigenstates of the unperturbed single particle Hamiltonian H_t in Appendix (𝒜.2), which we will call H_0:

$$H_0 = \frac{p^2}{2m} + U(\mathbf{r}) = -\frac{1}{2m}\nabla_r^2 + U(\mathbf{r}) \quad (\hbar \text{ set } = 1)$$

with

$$H_0 \phi_k(\mathbf{r}) = \epsilon_k \phi_k(\mathbf{r}). \tag{3.4}$$

If $U(\mathbf{r}) = 0$, then this is just the free particle case:

$$H_0 = -\frac{\nabla_r^2}{2m}, \quad \phi_k(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad \epsilon_k = \frac{k^2}{2m} \tag{3.5}$$

where Ω = normalization volume. We shall usually set $\hbar = 1$. Spin has been neglected for simplicity.

(Note regarding notation: In (3.4), the subscript k (or k_1, or k_2, etc.) stands for all the quantum numbers necessary to designate an *arbitrary* energy eigenstate. The *particular* eigenstates will be labelled with p-subscripts thus: $\phi_{p_1}(\mathbf{r}), \phi_{p_2}(\mathbf{r}), \phi_{p_3}(\mathbf{r}), \ldots$, or, for short $\phi_1(\mathbf{r}), \phi_2(\mathbf{r}), \ldots$ (the arrangement is roughly in order of increasing energy). In the special case where $U(\mathbf{r}) = 0$, k is a wave-vector and will be written $\mathbf{k}$ (or $\mathbf{k}, \sigma$ if spin is included).)

Definition (3.2) describes 'propagation' of a particle from state $\phi_{k_1}(\mathbf{r})$ to $\phi_{k_2}(\mathbf{r})$. Note that if $k_1 = k_2$, the particle propagates in time only.

Let us first get the free propagator G_0^+ (no perturbing interaction). Suppose at time t_1 the wave function of the free particle is $\phi_{k_1}(\mathbf{r})$. Then we have:

$$\psi(\mathbf{r}, t_1) = \phi_{k_1}(\mathbf{r}). \tag{3.6}$$

At later time t_2, by the time-dependent Schrödinger equation, we find that the wave function has become

$$\psi(\mathbf{r}, t_2) = \phi_{k_1}(\mathbf{r})\, e^{-i\epsilon_{k_1}(t_2 - t_1)} \tag{3.7}$$

where ϵ_{k_1} is the single particle energy of (3.4). The probability amplitude for the particle being in state ϕ_{k_2} at time t_2 is then just the component of $\psi(\mathbf{r}, t_2)$ along ϕ_{k_2} or:

$$\int d^3\mathbf{r}\psi(\mathbf{r}, t_2)\,\phi^*_{k_2}(\mathbf{r}) = e^{-i\epsilon_{k_1}(t_2-t_1)} \underbrace{\int d^3\mathbf{r}\phi_{k_1}(\mathbf{r})\,\phi^*_{k_2}(\mathbf{r})}_{\delta_{k_2 k_1}}, \tag{3.8}$$

whence, by definition of G^+:

$$\begin{aligned} G_0^+(k_2, k_1, t_2-t_1) &= -i\theta_{t_2-t_1} e^{-i\epsilon_{k_1}(t_2-t_1)}\,\delta_{k_2 k_1} \\ &= \delta_{k_2 k_1}\, G_0^+(k_1, t_2-t_1) \end{aligned} \tag{3.9}$$

where

$$G_0^+(k, t_2-t_1) = \begin{cases} -i\,\theta_{t_2-t_1} e^{-i\epsilon_k(t_2-t_1)}, & \text{for } t_2 \neq t_1 \\ 0, \quad \text{for } t_2 = t_1 \end{cases} \tag{3.10}$$

and

$$\theta_{t_2-t_1}\begin{cases} = 1, & \text{if } t_2 > t_1 \\ = 0, & \text{if } t_2 < t_1. \end{cases} \tag{3.11}$$

The $\theta_{t_2-t_1}$ factor is put in to take care of the fact that by definition (3.3), $G^+=0$ for $t_2<t_1$. Note also that $G_0^+=0$ for $t_2=t_1$, by (3.3). (See (9.2), (9.4), end of appendix F.) Note that for fermions, all levels up to ϵ_F (=Fermi energy—see §4.2) are filled, so we can only propagate a particle with $\epsilon_{k_1} > \epsilon_F$.

Just as with the classical pinball propagator, it is convenient to work with the Fourier transform of (3.10) (ω=frequency or 'energy parameter'):

$$\begin{aligned} G_0^+(k, \omega) &= -i\int_{-\infty}^{+\infty} d(t_2-t_1)\,\theta_{t_2-t_1}\, e^{i\omega(t_2-t_1)}\, e^{-i\epsilon_k(t_2-t_1)} \\ &= (-1)\frac{e^{i(\omega-\epsilon_k)(t_2-t_1)}}{\omega-\epsilon_k}\bigg|_0^\infty = \frac{1}{\omega-\epsilon_k} - \frac{e^{i(\omega-\epsilon_k)\,\infty}}{\omega-\epsilon_k}. \end{aligned} \tag{3.12}$$

Because of the exponential oscillating at ∞, this function is not well defined. In order to get around this difficulty, we have to slightly modify the expression for the free propagator. This is done by multiplying the propagator by the factor $\exp(-\delta(t_2-t_1))$, where δ is a positive infinitesimal such that $\delta\times\infty=\infty$. Then (3.10) becomes:

$$G_0^+(k, t_2-t_1) = -i\theta_{t_2-t_1}\, e^{-i(\epsilon_k - i\delta)(t_2-t_1)}. \tag{3.12'}$$

For any finite (t_2-t_1), we have $\delta\times(t_2-t_1)=0$, so this is just (3.10). But for infinite (t_2-t_1), $\delta\times(t_2-t_1)=\infty$ so $G_0^+=0$. When (3.12') is placed in (3.12), we find

$$G_0^+(k, \omega) = \frac{1}{\omega-\epsilon_k+i\delta} - \frac{e^{i(\omega-\epsilon_k+i\delta)\infty}}{\omega-\epsilon_k+i\delta} = \frac{1}{\omega-\epsilon_k+i\delta}. \tag{3.13}$$

In Appendix I, it is shown that the inverse transform, i.e., the Fourier transform of (3.13), yields exactly (3.12').

The above modification of G_0^+ has no physical significance since t_2-t_1 is always finite in any experiment. However, it is mathematically very convenient, because it allows us to work with well-defined integrals.

Note: The usual way of introducing the modified free propagator employs the integral representation of the step function:

$$\theta_{t_2-t_1} = -\int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi i}\,\frac{e^{-i\omega'(t_2-t_1)}}{\omega'+i\delta}. \tag{3.13'}$$

This is not precisely a true step function but rather a modified step function, which can be seen by evaluating it using exactly the same technique as in appendix I. This yields

$$\theta_{t_2-t_1} = \begin{cases} e^{-\delta(t_2-t_1)}, & \text{for } (t_2-t_1) > 0 \\ 0, & \text{for } (t_2-t_1) < 0 \end{cases} \tag{3.13''}$$

which is just (3.11), except when $(t_2-t_1)\to\infty$, where it goes to zero. Inserting (3.13'') in (3.10) yields just (3.12'). Alternatively, we can place (3.13') in (3.12), integrate over t_2-t_1 first (which gives $2\pi\delta(\omega'-\omega+\epsilon_k)$, then over ω' and immediately obtain (3.13).

In this transformed version, (3.13) it is seen that the free propagator possesses poles at (i.e., infinitesimally close to) $\omega=\epsilon_k$, i.e., at the energy of the added particle in state ϕ_k. This turns out to be quite general, and in fact it may be shown that (see appendix H):

> The poles of $G^+(k, l; \omega)$, the Fourier transform of the single-particle propagator, occur at values of ω equal to the excited state energies of the interacting $(N+1)$-particle system minus the ground energy of the interacting N-particle system. (3.14)

This property accounts for the extraordinary utility of the propagator in many-body theory.

Now consider the propagator in the presence of interaction. Analogous to the classical case in chapter 2, quantum quasi particles act like free particles except that they have a new energy ϵ_k' instead of ϵ_k, and a lifetime τ_k. Therefore we expect that if the added particle behaves as a quasi particle, the single-particle propagator will have the same form as the free propagator except for the replacement of ϵ_k by ϵ_k' and the inclusion of an exponential decay factor with time constant τ_k. One more thing: In a Fermi system, because of the Pauli principle, each state can hold at most one particle. Therefore, if state k is already partially (or fully) occupied, the probability amplitude that we can

add an extra particle in state k will be less than 1. Hence we have to multiply by a factor $Z_k \leqslant 1$. This gives us:

$$G^+_{\substack{quasi\\particle}}(k, t_2-t_1) = -iZ_k e^{-i\epsilon_k'(t_2-t_1)} e^{-(t_2-t_1)/\tau_k}. \tag{3.15}$$

This has the Fourier transform

$$G^+_{\substack{quasi\\particle}}(k, \omega) = \frac{Z_k}{\omega - \epsilon_k' + i\tau_k^{-1}}. \tag{3.16}$$

For these expressions to be sensible, it is evident that the lifetime of the quasi particles must be long, so that the width of the energy levels, τ_k^{-1} (see appendix $\mathscr{A}$ after ($\mathscr{A}$.43)) is much less than the values of the energies themselves, i.e.:

$$\tau_k^{-1} \ll \epsilon_k'. \tag{3.17}$$

(A more exact condition on τ_k is given in (8.21).)

Thus, if G^+ is calculated, and it is found that it has the above form, then the system is describable in terms of the simple quasi particle picture. Such systems are rewarded with the name 'normal'. On the other hand, even if the system turns out to be of the less co-operative 'abnormal' variety where (3.16) does not hold (like for example the one-particle system of (4.39), or the superconducting system of chapter 15), we can still get the excited state energies by means of (3.14).

It is still possible (in the case of normal systems) to interpret the poles of the quasi particle propagator (3.16) as yielding the excited state energies of the system (as in (3.14)), if the energy is regarded as being complex, with ϵ_k' being its real, and $i\tau_k^{-1}$ its (small) imaginary part:

$$\omega_{\text{pole}} = \epsilon_k' - i\tau_k^{-1}. \tag{3.18}$$

Such complex energies are the same sort of thing we meet in the case of an atom in an excited state, ϕ_n, with energy ϵ_n. In the absence of interaction with other atoms or with radiation, the wave function is

$$\psi_n(t) = \phi_n e^{-i\epsilon_n t}. \tag{3.18'}$$

If weak interactions are turned on, the energy shifts to ϵ_n' and the atom starts to decay out of state ϕ_n. Thus, the approximate wave function may be written

$$\psi_n'(t) \approx \phi_n e^{-i\epsilon_n' t} e^{-t/\tau_n} = \phi_n e^{-i(\epsilon_n' - i\tau_n^{-1})t} \tag{3.18''}$$

which has just the form of (3.18'), but with a complex energy $\epsilon_n' - i\tau_n^{-1}$ replacing the real energy ϵ_n. (See note after (3.70) and also after appendix (H.10).)

3.2 The quantum pinball game

In order to illustrate the principles involved, we will now find the propagator for a simple system consisting of one particle in an external momentum-conserving potential, which turns out to be the exact quantum analogue of the classical pinball game. Of course, in a one-particle system, we cannot have quasi particles in the 'real particle plus cloud of other particles' sense. However, as mentioned in connection with conduction electrons in §0.2, we may rather loosely regard the particle as being clothed by the external potential itself.

The quantum pinball game consists of a single free particle subjected simultaneously to two perturbing potentials V_M, V_L, which are the analogues of two different animal scatterers in the classical pinball game. The unperturbed Hamiltonian, wave functions, and energies are given by (3.5). We take as the perturbation the 'velocity dependent' potential

$$V(\mathbf{p}) = V_M + V_L = Mp^2 + Lp^4 = -M\nabla_r^2 + L\nabla_r^4 \tag{3.19}$$

where M, L, are real constants, and it is assumed that $M \gg L$.

This odd-looking potential, which has been chosen because of its great mathematical simplicity, may have a traumatic effect on some readers. It is certainly not the sort of potential one meets on the street—those are mostly of the familiar $V(\mathbf{r})$ form. Nevertheless it is quite easy to construct perturbations of the form (3.19) artificially. For example, the Hamiltonian for the centre of mass motion of a free hydrogen atom is $H = p^2/(m+m_e)$ where m = proton mass and m_e = electron mass. This may be broken up into

$$H = \frac{p^2}{2m} - \frac{m_e}{(m_e+m)m}p^2, \qquad \frac{m+m_e-m_e}{2m(m+m_e)}$$

and the second term treated as if it were a 'perturbing potential'. In a similar fashion, a p^4 term can come as a relativistic correction when we expand the relativistic Hamiltonian:

$$H = (m_0^2c^4 + p^2c^2)^{\frac{1}{2}} \approx m_0c^2 + \frac{p^2}{2m_0} - \frac{p^4}{8m_0^3c^2}.$$

In fact, if we regard this as the relativistic Hamiltonian for the centre of mass motion of a free hydrogen atom, with $m_0 = m + m_e$, then we can write

$$H \approx (m+m_e)c^2 + \frac{p^2}{2m} - \frac{m_e}{(m_e+m)m}p^2 - \frac{p^4}{8(m+m_e)^3c^2},$$

which has just the form (3.19), except for the unimportant constant term. Examples of real velocity-dependent potentials arise in the case of an electron in a magnetic field ($V \propto \mathbf{A}\cdot\mathbf{p}$), and in nuclear physics.

The problem, then, is to find the energy of the free particle when it is perturbed by $V(\mathbf{p})$.

Let us first look at the conventional solution of the problem. Since $M \gg L$, we may at first neglect the L term and have $V(\mathbf{p}) \approx Mp^2$ so

$$H \approx \frac{p^2}{2m} + Mp^2. \tag{3.20}$$

Because the perturbation has the same form as the unperturbed $H_0 = p^2/2m$, the perturbed wave functions are just the old ϕ_k's of (3.5) and the new energy is

$$\epsilon_k' = \left(\frac{1}{2m} + M\right)k^2. \tag{3.21}$$

For purposes of comparison with appendix (*A*.21), this result may be obtained by means of the trivial 'canonical transformation'

$$H = \underbrace{\frac{p^2}{2m}}_{H_0} + \underbrace{Mp^2}_{H_1} \to H' = \underbrace{\left(\frac{1}{2m} + M\right)p^2}_{H_0'} + \underbrace{0}_{H_1'}. \tag{3.22}$$

Thus, H_0' may be regarded as describing a sort of rudimentary 'quasi particle' having a modified energy dispersion law given by (3.21). (In this simple example, the 'fictitious bodies' of (*A*.21) and the quasi particles of (*A*.43) are the same thing.)

Consider next the effect of adding the L term. This also has the same eigenfunctions as H_0 and we find:

$$L\nabla^4 \phi_k = Lk^4 \phi_k \tag{3.23}$$

from which it follows that the total energy of the particle is

$$\epsilon_k'' = \left(\frac{1}{2m} + M\right)k^2 + Lk^4. \tag{3.24}$$

Let us now solve the same trivial problem with the aid of the single-particle propagator and see how we can get the above energies, ϵ_k', ϵ_k'', as 'quasi particle' energies from the poles of the propagator. This requires that we first obtain the perturbation series for the propagator analogous to the series (2.21) for the classical animal game case. We will get this series by the same sort of physically intuitive argument used in the classical case. (The rigorous mathematical way of getting the perturbation series is outlined in §3.4.)

According to the instructions in the definition of the propagator, at time t_1 a particle is introduced into the (in this case, initially empty) system in state

$\phi_{k_1}(\mathbf{r}) = \Omega^{-\frac{1}{2}} \exp(i\mathbf{k}_1 \cdot \mathbf{r})$, and propagates through the system, being scattered zero, one or more times by the external potentials:

$$V_M = Mp^2 \quad \text{or} \quad V_L = Lp^4. \tag{3.25}$$

By definition (3.2) the propagator $iG^+(\mathbf{k}_2, \mathbf{k}_1, t_2 - t_1)$ is just the probability amplitude that the particle will be in the state $\phi_{k_2}(\mathbf{r}) = \Omega^{-\frac{1}{2}} \exp(i\mathbf{k}_2 \cdot \mathbf{r})$ at time t_2. Analogous to the animal case, this amplitude iG^+ is just the sum of the probability amplitudes for all the different ways the particle can go through the system, beginning in state ϕ_{k_1} and winding up in state ϕ_{k_2}.

For example, the simplest way the particle can propagate through the system is freely, without interaction. The probability amplitude for this is just the free propagator $i\delta_{k_1 k_2} G_0^+(\mathbf{k}_1, t_2 - t_1)$ as in (3.9), (3.10). Another way is to enter in ϕ_{k_1} at time t_1, be scattered into state ϕ_{k_2} at time t_M by the potential V_M, then continue freely in ϕ_{k_2} until time t_2. (It may seem peculiar to say that the particle is scattered by the potential V_M at time t_M, or to say that the particle is scattered several times by the potential, when the potential is actually there the whole time. However, this is just a result of the fact that what we are doing in such a perturbation expansion is to decompose the total propagator into primitive components, each component being an instantaneous scattering by the potential. At the end we integrate over all times as shown in (3.28), and sum over all sequences of scattering processes as in (3.30), thus 'putting the propagator back together again'.) The amplitude for this second way will be, by analogy with the classical pinball case, the product of the amplitudes for the independent processes it is composed of. (That these processes are independent can be seen from the fact that a particle which has been scattered into state ϕ_k from state ϕ_l cannot be distinguished from one scattered into ϕ_k from another state $\phi_{l'}$. That is, the particle now in ϕ_k has no 'memory' of how it got there, just as in the classical pinball case.)

The first of these independent processes, free propagation from t_1 to t_M in state ϕ_{k_1}, has amplitude $iG_0^+(k_1, t_M - t_1)$, according to (3.10). The amplitude for the second process, i.e., scattering from ϕ_{k_1} to ϕ_{k_2} by V_M at time t_M, can be obtained from ordinary time-dependent perturbation theory as follows: Let c_l be the probability amplitude that at time t_0 a system is in state ϕ_l. Then at later time, t, the time rate of change of any particular c_l, say c_p, under the influence of perturbation V, is given by:

$$\dot{c}_p(t) = -i \sum_l V_{pl} c_l e^{i(\epsilon_p - \epsilon_l)(t - t_0)} \tag{3.26}$$

where V_{pl} is the matrix element of V between states ϕ_p, ϕ_l (see, for example, Dicke (1960), Eq. 14–57, with $\hbar = 1$). In the process under consideration, at time $t_0 = t_M$, the system is definitely in state ϕ_{k_1}, so $c_l = \delta_{lk_1}$. The perturbation $V = V_M$. Hence the probability amplitude per unit time that the system under-

goes a transition from ϕ_{k_1} to $\phi_p=\phi_{k_2}$, at time t_M (i.e., t here is also equal to t_M) is

$$\dot{c}_{k_2}(t=t_M) = -iV_{M_{k_2k_1}} = -i\int d^3\mathbf{r}\,\phi^*_{k_2}(\mathbf{r})V_M\phi_{k_1}(\mathbf{r}) =$$

$$= +iM\int d^3\mathbf{r}\,\phi^*_{k_2}\nabla^2\phi_{k_1} = -iMk_1^2\delta_{k_2k_1}. \qquad (3.27)$$

The $\delta_{k_1k_2}$ shows that the process here conserves momentum so that the particle still has the same momentum after scattering. The amplitude for the last process is $iG_0^+(\mathbf{k}_2, t_2-t_M)$. Hence the total amplitude is the product

$$\left[\begin{matrix}\textit{Probability}\\ \textit{Amplitude}\end{matrix}\right]_{t_1\to t_M\to t_2} = i\int_{-\infty}^{+\infty} dt_M G_0^+(\mathbf{k}_1, t_M-t_1)\,V_{M_{k_1k_1}}G_0^+(\mathbf{k}_2, t_2-t_M). \qquad (3.28)$$

We have integrated over t_M since the collision with V_M could have occurred at any intermediate time $t_1<t_M<t_2$. Note that the θ-function in G_0^+ (see (3.10)) automatically restricts the region of integration to $t_1<t_M<t_2$.

Similarly, there can be an interaction with V_L described by the matrix element

$$-iV_{L_{k_2k_1}} = -iLk_1^4\delta_{k_2k_1} \qquad (3.29)$$

which also conserves momentum. There are also second- and higher-order processes in which the particle collides with V_M and V_L any number of times. This gives us the series expansion for the propagator (set $\mathbf{k}_1=\mathbf{k}_2=\mathbf{k}$ because of conservation of momentum here), after cancelling the i's:

$$G^+(\mathbf{k}, t_2-t_1) = G_0^+(\mathbf{k}, t_2-t_1) + \int_{-\infty}^{+\infty} dt_M G_0^+(\mathbf{k}, t_M-t_1)\,V_{M_{kk}}G_0^+(\mathbf{k}, t_2-t_M)$$

$$+\int_{-\infty}^{+\infty} dt_L G_0^+(\mathbf{k}, t_L-t_1)\,V_{L_{kk}}G_0^+(\mathbf{k}, t_2-t_L)+$$

$$+\int dt_M dt'_M\cdots+\int dt_M dt_L\cdots+\cdots+$$

$$+\int dt_M dt'_M dt''_M\cdots+\cdots. \qquad (3.30)$$

Just as in the classical pinball case, the integrals in the above series may be eliminated by taking the Fourier transform. This yields, analogous to (2.24):

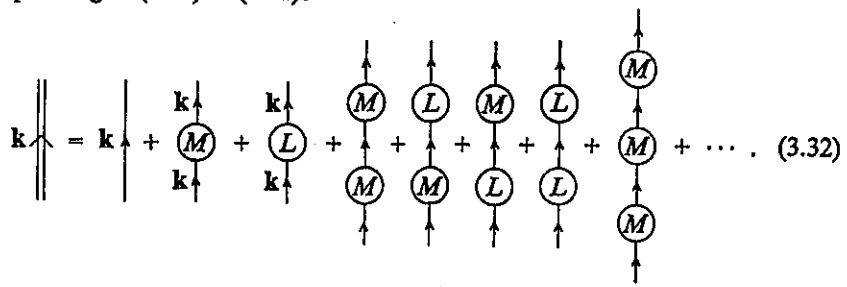
$$G^+(\mathbf{k},\omega) = G_0^+(\mathbf{k},\omega)+[G_0^+(\mathbf{k},\omega)]^2V_{M_{kk}}+[G_0^+(\mathbf{k},\omega)]^2V_{L_{kk}}+$$
$$+[G_0^+]^3V_{M_{kk}}^2+2[G_0^+]^3V_{M_{kk}}V_{L_{kk}}+[G_0^+]^3V_{L_{kk}}^2+$$
$$+[G_0^+]^4V_M^3+\cdots. \qquad (3.31)$$

We now pull the same trick used in the classical case and make a dictionary to translate the above series into diagrams. The primitive diagrams are in Table 3.1. Compare this with Table 2.2, which is in $(\mathbf{r},t)$-space, and Table 2.3 in $(\mathbf{r},\omega)$-space. (Equations (3.30), (3.31) could also be written out in $(\mathbf{r},t)$- and $(\mathbf{r},\omega)$-space but in the present case this would not be very useful.)

Table 3.1 *Diagram dictionary for quantum pinball propagator*

$(\mathbf{k},t)$-space		$(\mathbf{k},\omega)$-space	
Word	Diagram	Word	Diagram
$iG^+(\mathbf{k}_2,\mathbf{k}_1,t_2-t_1)$	$\mathbf{k}_2\,t_2$ / $\mathbf{k}_1\,t_1$	$iG^+(\mathbf{k}_2,\mathbf{k}_1,\omega)$	ω: $\mathbf{k}_2$ / $\mathbf{k}_1$
$iG_0^+(\mathbf{k},t_2-t_1)$ $=\theta_{t_2-t_1}e^{-i\epsilon_k(t_2-t_1)}$	$\mathbf{k}$: t_2 / t_1	$iG_0^+(\mathbf{k},\omega)=\dfrac{i}{\omega-\epsilon_k+i\delta}$	$\mathbf{k},\omega$
$-iV_{A_{ml}}$	m / A / l	$-iV_{A_{ml}}$	m / A / l

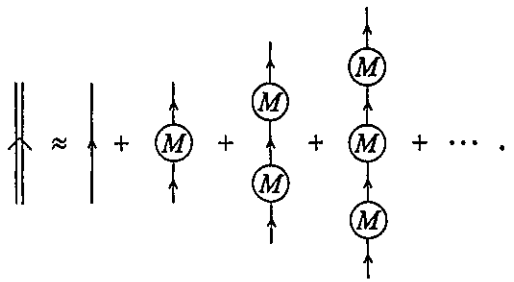
With this dictionary it is easy to write out the series of diagrams corresponding to (3.30) or (3.31):



(3.32)

where the lines may be labelled with t's to give (3.30) or ω's for (3.31). This is evidently the sum of all possible different diagrams for this case.

Now, since we assumed that $M \gg L$, all interactions with V_L may be neglected, and the above series may be approximated by

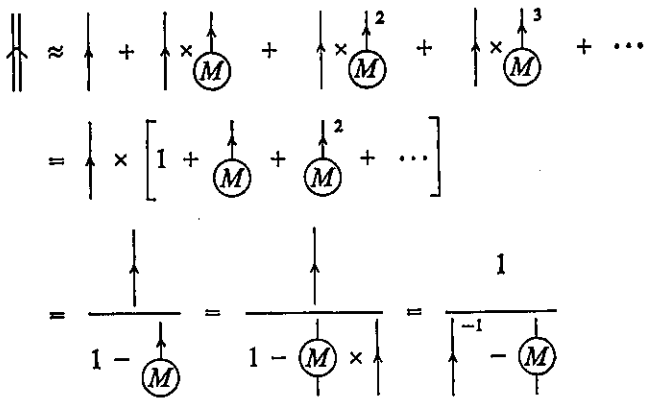


(3.33)

This is the precise analogue of the partial sum over all monkey diagrams in (2.17). And, as in the monkey case, the summation is easy, since once again it is just a geometric series. Translating (3.33) into words with the aid of Table 3.1 (use $(\mathbf{k},\omega)$-space), cancelling i's and dropping $(\mathbf{k},\omega)$'s for brevity yields

$$\begin{aligned} G^+(\mathbf{k},\omega) &\approx G_0^+ + (G_0^+)^2 V_{M\mathbf{k}\mathbf{k}} + (G_0^+)^3 V_{M\mathbf{k}\mathbf{k}}^2 + \cdots \\ &= G_0^+ [1 + G_0^+ V_{M\mathbf{k}\mathbf{k}} + (G_0^+)^2 V_{M\mathbf{k}\mathbf{k}}^2 + \cdots] \\ &= \frac{G_0^+}{1 - G_0^+ V_{M\mathbf{k}\mathbf{k}}} = \frac{1}{(G_0^+)^{-1} - V_{M\mathbf{k}\mathbf{k}}}, \quad \text{for } |G_0^+ V_{M\mathbf{k}\mathbf{k}}| < 1. \end{aligned} \tag{3.34}$$

This same result may be obtained conveniently in a way which saves a lot of writing by manipulating the diagrams themselves; this is legitimate because in $(\mathbf{k},\omega)$-space each diagram part stands for a factor. Thus (3.34) may be re-written:



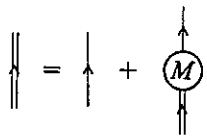
(3.35)

which may be then translated into

$$G^+(\mathbf{k},\omega) \approx \frac{1}{(G_0^+)^{-1} - V_{M\mathbf{k}\mathbf{k}}} \tag{3.36}$$

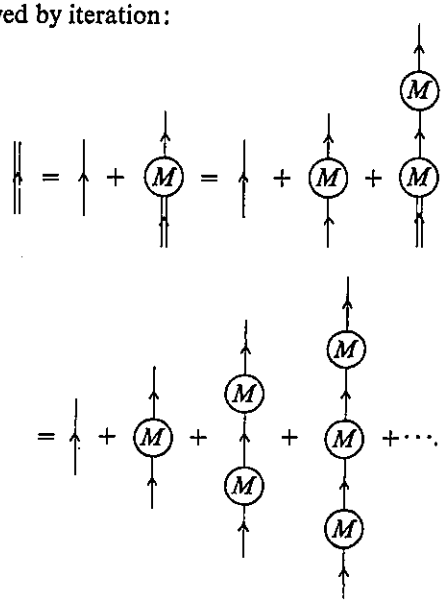
i.e., just the result (3.34). (Note: the little 'stumps' of line connected to (M) have no value in themselves. They just show where the propagator lines are to be attached!)

(Observe that (3.35) may be written in a very useful alternative form, i.e.

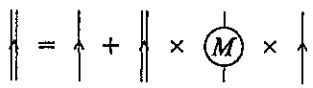


(3.36′)

This may be proved by iteration:



In $(\mathbf{k},\omega)$-space, (3.36′) may be factored into



which may be solved algebraically to yield (3.35). However, (3.36′) has the advantage of being more general than (3.35) since it may also be used when the diagrams do not factor. For example in $(\mathbf{k},t)$-space, it yields an integral equation instead of an algebraic one. (See exercise 3.8).)

Finally, we substitute for G_0^+ and for V_M and obtain:

$$G^+(\mathbf{k},\omega) = \frac{1}{\omega-\epsilon_k+i\delta-V_{M_{kk}}} = \frac{1}{\omega-(\epsilon_k+Mk^2)+i\delta}. \tag{3.37}$$

Comparing this with the quasi particle propagator (3.16), we find

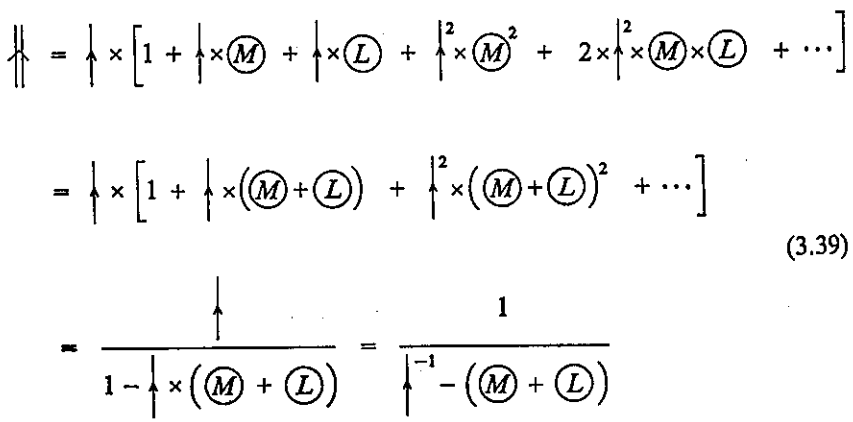
$$\epsilon_k' = \epsilon_k+Mk^2 = \left(\frac{1}{2m}+M\right)k^2$$

$$\tau_k = \frac{1}{\delta} = \infty. \tag{3.38}$$

That is, the interaction with V_M has 'clothed' the particle, turning it from a 'bare' into a 'quasi' particle, having modified energy dispersion law given by ϵ_k' in (3.38) and infinite lifetime. And comparison with (3.21) shows this to be precisely the same result obtained by direct solution of the Schrödinger equation!

On second thought, when we realize that it has taken us three pages to do by diagrams what we did directly in three lines, there appears to be little cause for celebration. We seem to have built an elephant cannon to shoot a horse-fly. Of course this is not true. The quantum pinball game is intended only as a transparent example to introduce the general principles. The big many-body game will come later. Furthermore, at the end of this chapter, in §3.5, we apply the method to a non-trivial one-particle problem: finding the energy and lifetime of an electron in an impure metal.

In this simple example, it is actually possible to do much better than just the partial sum (3.33). We can in fact sum over all the diagrams of (3.32) as follows:



(3.39)

or, translating:

$$G^+(\mathbf{k},\omega) = \frac{1}{(G_0^+)^{-1}-(V_{M_{kk}}+V_{L_{kk}})} = \frac{1}{\omega-\left(\frac{k^2}{2m}+Mk^2+Lk^4\right)+i\delta} \tag{3.40}$$

which gives

$$\epsilon_k'' = \frac{k^2}{2m}+Mk^2+Lk^4 \tag{3.41}$$

in agreement with (3.24). This shows that we could just as well have taken $V=V_M+V_L$ together from the start and represented them by a single diagram,  . The potential was broken up into two parts just to make the parallel with the classical pinball game more obvious.

3.3 Disappearance of disagreeable divergences

It is important to note a weakness in the above method. The geometric series in (3.34) converges only for $|G_0^+ V_{M_{kk}}| < 1$, which means that

$$\left|\frac{Mk^2}{\omega-\epsilon_k+i\delta}\right| < 1 \quad \text{or} \quad \begin{matrix}\omega > \epsilon_k+Mk^2 \\ \omega < \epsilon_k-Mk^2.\end{matrix} \tag{3.42}$$

But to get (3.38) we set $\omega=\epsilon_k+Mk^2$, which is just where the series begins to diverge! This is a typical example of the sort of divergence which plagues the diagram method. The usual household remedy is to assume that the propagator is still valid for ω in the region of divergence. Or, in more fancy language, one assumes that the partial sum result for the propagator may be 'analytically continued' into the divergent region. This might be called 'the Hypothesis of the Disappearance of Disagreeable Divergences'.

In many cases one can justify this by using a different method to get the propagator. We can do just this in the present case. All that is necessary is to take for the unperturbed Hamiltonian of (3.4)

$$H_0' = \frac{p^2}{2m}+Mp^2 \tag{3.43}$$

instead of just the $p^2/2m$ in (3.5). The free propagator for this new H_0' is, by exactly the same argument leading to (3.13) just

$$G_0^{+\prime}(\mathbf{k},\omega) = \frac{1}{\omega-\left(\frac{k^2}{2m}+Mk^2\right)+i\delta} \tag{3.44}$$

which is precisely the result in (3.37). This shows that the propagator (3.37) is good for all ω.

Another indication that such divergences are largely spurious (Kurki-Suonio (1965)) is that if we do the partial sum in t-space instead of ω-space, the divergence does not occur, at least not in this simple case. Thus, using (3.30) and Table 3.1 and summing just over terms containing the V_M interaction, we find:

$$\begin{aligned} G^+(\mathbf{k}, t_2-t_1) &= -ie^{-i\epsilon_k(t_2-t_1)}\Big[1+(-iV_{M_{kk}})\int_{t_1}^{t_2} dt_M + \\ &\quad +(-iV_{M_{kk}})^2\int_{t_1}^{t_2} dt'_M\int_{t_1}^{t_M'} dt_M+\cdots\Big] \\ &= -ie^{-i\epsilon_k(t_2-t_1)}\Big[1+(-iV_{M_{kk}})(t_2-t_1)+\frac{1}{2!}(-iV_{M_{kk}})^2(t_2-t_1)^2+ \\ &\quad +\frac{1}{3!}(-iV_{M_{kk}})^3(t_2-t_1)^3+\cdots\Big] \\ &= -ie^{-i\epsilon_k(t_2-t_1)}\,[e^{-iV_{M_{kk}}(t_2-t_1)}] \end{aligned} \tag{3.45}$$

which is just the Fourier transform of (3.37) and converges for all values of $-iV_{M_{kk}}(t_2-t_1)$.

3.4 Where the diagram expansion of the propagator really comes from

The results in this chapter were obtained by analogy with the classical pinball case. Since such intuitive arguments may seem like voodoo to some readers, we will now show in a rough way how the diagram expansion of G^+ in this single-particle case can be gotten from the Schrödinger equation. (The derivation for the many-body case is in the Appendices.)

The first thing to realize is that G_0^+ and G^+ are actually Green's functions. Recall that if we have a differential equation of the form

$$L\psi(\mathbf{x},t) = f(\mathbf{x},t), \tag{3.46}$$

where L is a linear differential operator which does not depend explicitly on x or t, then the Green's function, G, associated with this equation is the solution of

$$LG(\mathbf{x}-\mathbf{x}', t-t') = \delta(\mathbf{x}-\mathbf{x}')\,\delta(t-t'). \tag{3.47}$$

Now the unperturbed Schrödinger equation may be written

$$\left(+\frac{\nabla^2}{2m}+i\frac{\partial}{\partial t}\right)\psi(\mathbf{x},t) = 0. \tag{3.48}$$

This has the form (3.46) (with $f(x,t)=0$), so that the associated Green's function obeys

$$\left(+\frac{\nabla^2}{2m}+i\frac{\partial}{\partial t}\right)G(\mathbf{x}-\mathbf{x}', t-t') = \delta(\mathbf{x}-\mathbf{x}')(t-t'). \tag{3.49}$$

Fourier transforming G, we have

$$G(\mathbf{x}-\mathbf{x}', t-t') = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} G(\mathbf{k}, t-t'). \tag{3.50}$$

Setting this into (3.49) yields

$$\left(-\frac{k^2}{2m}+i\frac{\partial}{\partial t}\right)G(\mathbf{k}, t-t') = \delta(t-t'). \tag{3.51}$$

If we now use for G the free propagator in (3.10):

$$G = G_0^+(\mathbf{k}, t-t') = -i\theta_{t-t'}\,e^{-i\epsilon_k(t-t')} \tag{3.52}$$

and use the fact that

$$\frac{d\theta_x}{dx} = \delta(x), \quad f(x)\,\delta(x) = f(0)\,\delta(x), \tag{3.53}$$

we find that (3.51) is satisfied, showing that G_0^+ is indeed a Green's function.

In a similar way, the Schrödinger equation with a perturbing potential of form $V(\nabla)$ (as in (3.19)),

$$\left[+\frac{\nabla^2}{2m}+i\frac{\partial}{\partial t}-V(\nabla)\right]\psi(\mathbf{x},t) = 0, \tag{3.54}$$

has the associated Green's function equation (in k-space):

$$\left[-\frac{k^2}{2m}+i\frac{\partial}{\partial t}-V(\mathbf{k})\right]G^+(\mathbf{k}, t-t') = \delta(t-t'), \tag{3.55}$$

where $V(\mathbf{k})$ is the Fourier transform of $V(\nabla)$. The solution to this may be written as an integral equation

$$G^+(\mathbf{k}, t-t') = G_0^+(\mathbf{k}, t-t')+\int_{-\infty}^{+\infty} dt''\,G_0^+(\mathbf{k}, t-t'')\,V(\mathbf{k})\,G^+(\mathbf{k}, t''-t'), \tag{3.56}$$

as can be seen by substituting (3.56) in (3.55) and using (3.51) with $G=G_0^+$. Finally, we obtain the perturbation expansion for G^+ in terms of G_0^+ by iterating (3.56):

$$\begin{aligned} G^+(\mathbf{k}, t-t') &= G_0^+(\mathbf{k}, t-t')+\int_{-\infty}^{+\infty} dt''\,G_0^+(\mathbf{k}, t-t'')\,V(\mathbf{k})\,G_0^+(\mathbf{k}, t''-t')+ \\ &\quad +\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dt''\,dt'''\,G_0^+\,VG_0^+\,VG_0^+ +\cdots \end{aligned} \tag{3.57}$$

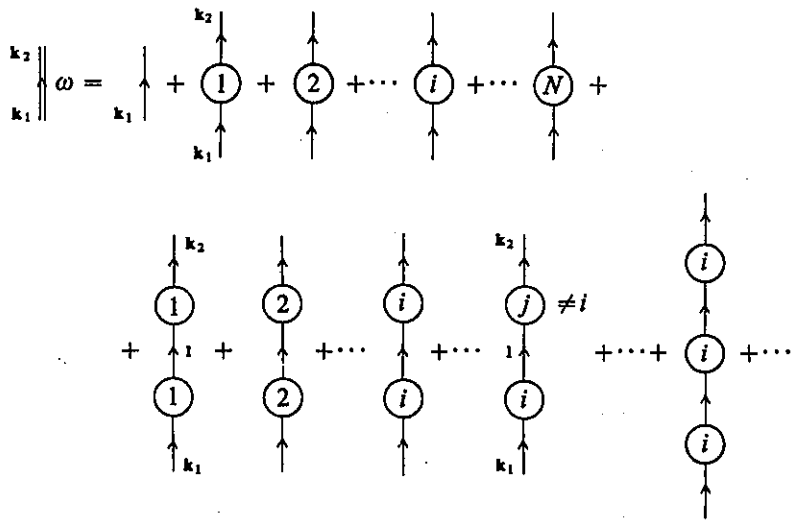
which is just the series (3.30). The translation into diagrams is accomplished immediately by using dictionary Table 3.1.

It may be remarked that the Green's function for the many-body case obeys an equation of type (3.47) but with L a non-linear operator.

3.5 [Energy and lifetime of an electron in an impure metal]

(This section can be skipped on first reading!)

We will now apply the propagator method to a more realistic problem, i.e., an electron in an impure metal. For simplicity, let us pretend that the regularly arranged lattice ions in the metal have been removed, so that all we have left is an electron interacting with a set of N randomly distributed impurity ions (see Fig. 0.13B), which we assume are identical, in a volume Ω. Then, as discussed in §1.3, the propagator will be given by (1.2) or (2.25) with the circles interpreted as scattering from the various ions:



(3.58)

where the $\mathbf{k}$'s denote momentum eigenstates of a free electron as in (3.5), and i denotes the impurity ion at position $\mathbf{R}_i$.

If the potential well for an impurity at the origin has the form $W(\mathbf{r})$, then an identical ion at point $\mathbf{R}_i$ will have the potential $W(\mathbf{r}-\mathbf{R}_i)$. Hence the matrix element for the transition $\mathbf{k} \to \mathbf{l}$ at ion i is given by

$$-iV_{lk}(\mathbf{R}_i) = \frac{-i}{\Omega}\int d^3\mathbf{r} e^{-i(\mathbf{l}-\mathbf{k})\cdot\mathbf{r}} W(\mathbf{r}-\mathbf{R}_i) = \frac{(-i)}{\Omega} e^{-i(\mathbf{l}-\mathbf{k})\cdot\mathbf{R}_i} W_{lk}$$

where

$$W_{lk} = \int d^3\mathbf{r}' e^{-i(\mathbf{l}-\mathbf{k})\cdot\mathbf{r}'} W(\mathbf{r}') \tag{3.59}$$

The series (3.58) may now be written out in terms of functions as follows (after eliminating the i's and suppressing ω's for brevity, and noting that it is necessary to sum over all values of the intermediate momentum, $\mathbf{l}$):

$$\begin{aligned} G^+(\mathbf{k}_2,\mathbf{k}_1) = {} & G_0^+(\mathbf{k}_1)\,\delta_{k_1k_2} + G_0^+(\mathbf{k}_2)\sum_{i=1}^{N} V_{k_2k_1}(\mathbf{R}_i)\,G_0^+(\mathbf{k}_1) + \\ & + G_0^+(\mathbf{k}_2)\left[\sum_{l}\sum_{i=1}^{N} V_{k_2l}(\mathbf{R}_i)\,G_0^+(\mathbf{l})\,V_{lk_1}(\mathbf{R}_i)\right] G_0^+(\mathbf{k}_1) + \\ & + G_0^+(\mathbf{k}_2)\left[\sum_{l}\sum_{j\neq l} V_{k_2l}(\mathbf{R}_j)\,G_0^+(\mathbf{l})\sum_{i=1}^{N} V_{lk_1}(\mathbf{R}_i)\right] G_0^+(\mathbf{k}_1) + \cdots. \end{aligned} \tag{3.60}$$

The above G^+ is for a particular set of $\mathbf{R}_i$'s, i.e., a particular arrangement of impurities in the system, and for each different set of $\mathbf{R}_i$'s, we will get a different value of G^+. Consider now an ensemble consisting of all possible arrangements of impurities. Suppose this ensemble is *random*, i.e., the coordinate for the ith impurity, $\mathbf{R}_i$, is equally likely to be found anywhere in the volume Ω. Let us imagine that we compute $\langle G^+\rangle$, the average value of G^+ for the ensemble. Clearly, for any specific arrangement, $G^+ \neq \langle G^+\rangle$. But, as is common in large systems (see Landau and Lifshitz (1959), pp. 5–8), in the limit $N \to \infty$ (with $N/\Omega =$ constant), the ratio of the mean square fluctuation $(\langle G^{+2}\rangle - \langle G^+\rangle^2)$ to $\langle G^+\rangle^2$ will go to zero, so that we can take $G^+ = \langle G^+\rangle$ for all but a negligible number of arrangements (see Kohn and Luttinger (1957), especially Appendix B). Hence our object here will be to calculate $\langle G^+\rangle$.

The average $\langle G^+\rangle$ is the sum of the average of each term in the perturbation expansion (3.60). For the second term on the right side of (3.60) we have, noting that free propagators may be factored out when averaging since they are independent of $\mathbf{R}_i$,

$$\left\langle G_0^+(\mathbf{k}_2)\,G_0^+(\mathbf{k}_1)\sum_{i=1}^{N} V_{k_2k_1}(\mathbf{R}_i)\right\rangle = G_0^+(\mathbf{k}_2)\,G_0^+(\mathbf{k}_1)\,\frac{W_{k_2k_1}}{\Omega}\left\langle\sum_{i=1}^{N} e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_i}\right\rangle \tag{3.61}$$

The last factor here may be written

$$\left\langle\sum_{i=1}^{N} e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_i}\right\rangle = \sum_{i=1}^{N}\langle e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_i}\rangle = N\langle e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_i}\rangle \tag{3.61'}$$

since each of the N terms is identical in form, so that we can just average over one of them and multiply by N. For a random ensemble, the probability of finding the ith impurity atom within volume $d^3\mathbf{R}_i$ surrounding the point $\mathbf{R}_i$ will be independent of $\mathbf{R}_i$ and equal to $d^3\mathbf{R}_i/\Omega$. Hence we have

$$\langle e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_i}\rangle = \frac{1}{\Omega}\int d^3\mathbf{R}_i\, e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{R}_i} = \frac{1}{\Omega}\times\Omega\delta_{k_2k_1}. \tag{3.62}$$

(Note: In a one-dimensional box of length L,

$$I \equiv \int_{-L/2}^{+L/2} dx \exp(-ikx) = 2k^{-1}\sin(kL/2).$$

Because of periodic boundary conditions, the wave function at $x=0$ equals that at $x=L$, i.e., $\exp(ikx)=\exp(ik(x+L))$. Hence $\exp(ikL)=1$, or $k=2\pi n/L$ (n=integer). Thus $I=L\delta_{k,0}$. Equation (3.62) is just the three-dimensional version of this, with $\Omega=L^3$. If k is continuous, the integral (3.62) yields $(2\pi)^3\delta(\mathbf{k}_2-\mathbf{k}_1)$, which is a Dirac δ-function.)

In the third term of (3.60), which represents two successive scatterings from the *same* impurity, we have, using the same method as above:

$$\sum_{\mathbf{l}} G_0^+(\mathbf{l})\Big\langle \sum_i V_{k_2 i}(\mathbf{R}_i)V_{i k_1}(\mathbf{R}_i)\Big\rangle = \sum_{\mathbf{l}} G_0^+(\mathbf{l})\frac{W_{k_2 l}W_{l k_1}}{\Omega^2}\Big\langle \sum_i e^{-i(\mathbf{k}_2-\mathbf{l}+\mathbf{l}-\mathbf{k}_1)\cdot\mathbf{R}_i}\Big\rangle$$

$$= \frac{N}{\Omega^2}\sum_{\mathbf{l}} G_0^+(\mathbf{l})\, W_{k_2 l}W_{l k_1}\delta_{k_2 k_1}. \tag{3.63}$$

It is convenient at this point to change from a sum over $\mathbf{l}$ to an integral by

$$\sum_{\mathbf{l}} \to \frac{\Omega}{(2\pi)^3}\int d^3\mathbf{l}. \tag{3.64}$$

This is legitimate in the case of a large (i.e., macroscopic) system, since the points $\mathbf{l}$ in $\mathbf{k}$-space are very close to each other. The factor $\Omega/(2\pi)^3$ is the density of points in $\mathbf{k}$-space. To see this, we note that in one dimension, $k=2\pi n/L$ (n=integer). (See just after (3.62).) Thus there are $L/2\pi$ points per unit length in $\mathbf{k}$-space in one dimension. In three dimensions we have $L^3/(2\pi)^3=\Omega/(2\pi)^3$ points per unit volume in $\mathbf{k}$-space. Using (3.64), (3.63) becomes

$$= \frac{N}{\Omega}\int \frac{d^3\mathbf{l}}{(2\pi)^3} G_0^+(\mathbf{l})\, W_{k_2 l}\, W_{l k_1}\delta_{k_2 k_1}. \tag{3.64'}$$

The fourth term of (3.60) (two successive scatterings from *different* impurities) contains the average

$$\sum_{\mathbf{l}} G_0^+(\mathbf{l})\Big\langle \sum_{i,j\neq i} V_{k_2 l}(\mathbf{R}_i)V_{l k_1}(\mathbf{R}_j)\Big\rangle$$

$$= \sum_{\mathbf{l}} G_0^+(\mathbf{l})\frac{W_{k_2 l}W_{l k_1}}{\Omega^2}\Big\langle \sum_{i,j\neq i} e^{-i(\mathbf{k}_2-\mathbf{l})\cdot\mathbf{R}_j}e^{-i(\mathbf{l}-\mathbf{k}_1)\cdot\mathbf{R}_i}\Big\rangle$$

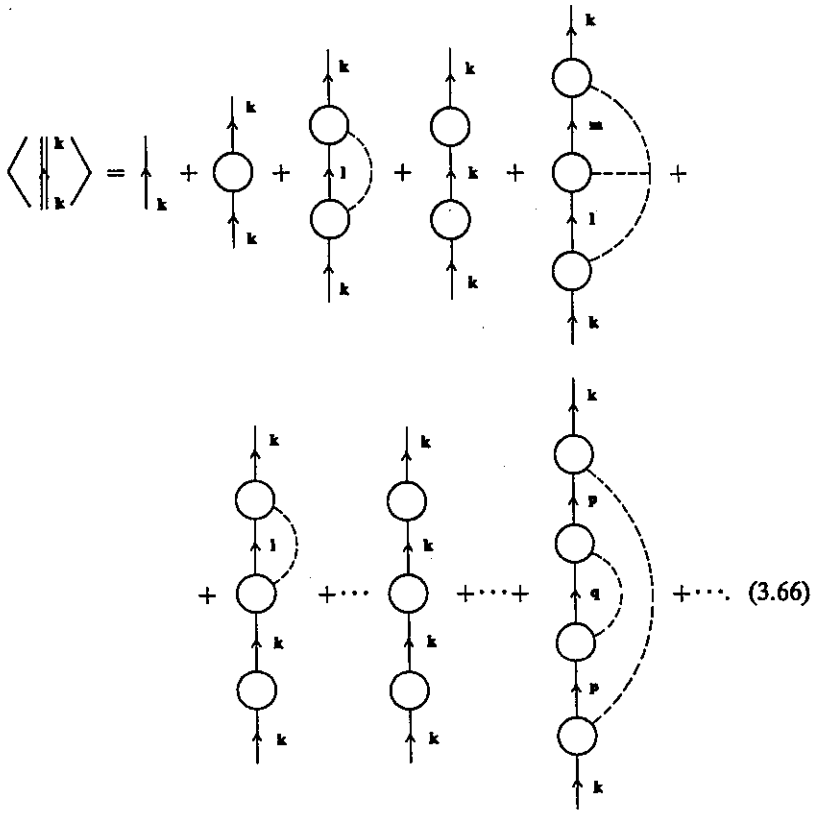
$$= \sum_{\mathbf{l}} G_0^+(\mathbf{l})\frac{W_{k_2 l}W_{l k_1}}{\Omega^2}N(N-1)\int\frac{d^3\mathbf{R}_j}{\Omega}\int\frac{d^3\mathbf{R}_i}{\Omega}e^{-i(\mathbf{k}_2-\mathbf{l})\cdot\mathbf{R}_j}e^{-i(\mathbf{l}-\mathbf{k}_1)\cdot\mathbf{R}_i}$$

$$\approx \left(\frac{N}{\Omega}\right)^2\sum_{\mathbf{l}} G_0^+(\mathbf{l})W_{k_2 l}W_{l k_1}\delta_{k_2 l}\delta_{l k_1}$$

$$= \left(\frac{N}{\Omega}\right)^2 G_0^+(\mathbf{k}_1)W_{k_1 k_1}^2\delta_{k_2 k_1} \tag{3.65}$$

Here we have used that for the random distribution, the probability that impurity i is in $d^3\mathbf{R}_i$, and j is simultaneously in $d^3\mathbf{R}_j$ is $(d^3\mathbf{R}_i/\Omega)(d^3\mathbf{R}_j/\Omega)$. Also, we have assumed $N\gg 1$. Averages of higher order terms are done in a similar way.

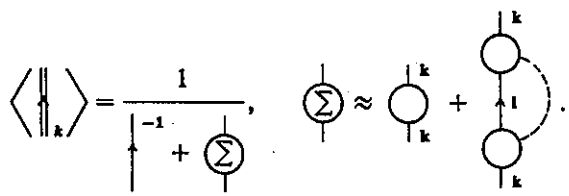
With the aid of these results, we can write out the series for the averaged propagator. It helps here to introduce a couple of new diagram conventions. First of all, since $V_{kl}(\mathbf{R}_i)$ does not occur any more we use just an empty circle, for the transition probability amplitude W_{kl}. Secondly, because each group of two or more successive scatterings at the same ion has an associated density factor N/Ω, we connect successive circles representing the same ion by dotted lines. (Note that a single scattering also has this factor associated with it.) Thus, taking the δ-functions into account, and letting $\mathbf{k}_1=\mathbf{k}=\mathbf{k}_2$, we have for the averaged propagator:



(3.66)

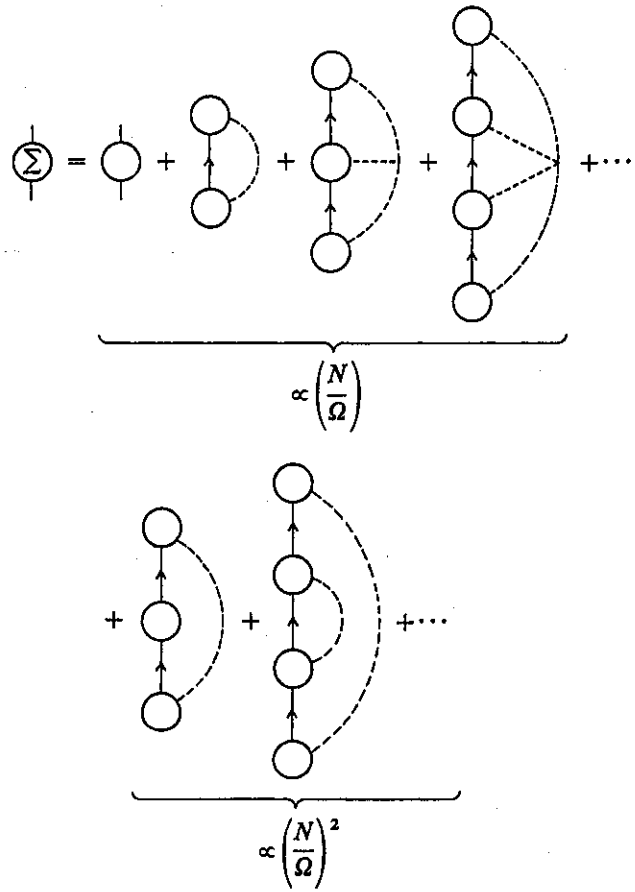
This may be translated with the dictionary in Table 3.2. Note that in this table, there is no factor Ω^{-1} in front of $\int d^3\mathbf{l}/(2\pi)^3$ because all Ω^{-1} factors are already included in the (N/Ω) factor in line 4 of the table. (See e.g. exercise 3.9).

Let us now evaluate (3.66) assuming the most important processes are single scattering, and double scattering by the same impurity. This means that diagrams containing more than two successive scatterings off the same ion (such as for example, the fifth diagram on the right of (3.66)) are neglected. The partial sum may easily be carried out and yields



(3.67)

(Note that the complete series for (Σ) is:



(3.67′)

For small (N/Ω), we only need to keep terms$\propto(N/\Omega)$, i.e., terms representing multiple scattering from a single impurity.) Translating (3.67) into functions

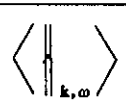
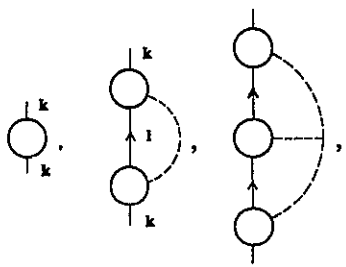
$$\langle G(\mathbf{k},\omega)\rangle = 1/[\omega - \epsilon_k + i\delta - \Sigma(\mathbf{k},\omega)] \tag{3.68}$$

where

$$\Sigma(\mathbf{k},\omega) = \frac{N}{\Omega} W_{kk} + \frac{N}{\Omega}\int \frac{d^3\mathbf{l}}{(2\pi)^3} \frac{|W_{kl}|^2}{\omega - \epsilon_l + i\delta} \tag{3.69}$$

and we have used Table 3.2.

Table 3.2 *Diagram dictionary for electron propagating through a system of randomly distributed impurity ions*

Diagram element	Factor
	$i\langle G^+(\mathbf{k},\omega)\rangle$
	$iG_0^+(\mathbf{k},\omega) = \dfrac{i}{\omega-\varepsilon_k+i\delta}$
	$-iW_{lk}$
	factor $\dfrac{N}{\Omega}$.
intermediate momentum, $\mathbf{l}$	$\displaystyle\int \frac{d^3\mathbf{l}}{(2\pi)^3}$

In order to find the new energy and lifetime of the electron, we need the complex pole of (3.68), i.e., the ω which is the solution of

$$\omega - \epsilon_k - \sum(\mathbf{k},\omega) + i\delta = 0. \tag{3.70}$$

(Note: If in (3.69) we use the original sum over $\mathbf{l}$, i.e., $\sum_l$ in (3.60) instead of $\int d^3\mathbf{l}$ (see (3.64)), we find that, as expected from (3.14), the pole equation (3.70) will have *real* solutions. This can be seen at once by plotting $\sum(\mathbf{k},\omega) = (N/\Omega)W_{kk} + (N/\Omega)\sum_l |W_{kl}|^2/(\omega-\epsilon_l+i\delta)$ and $y(\mathbf{k},\omega)=\omega-\epsilon_k$ vs. ω and noting that the poles occur at the intersection of $\sum(\mathbf{k},\omega)$ and $y(\mathbf{k},\omega)$. The *complex* solutions of (3.70) arise because we have gone from a sum to an integral. The physical meaning of this is discussed at the end of appendix H.) If W is small, so that $\sum$ is small, then the zeroth-order approximation to ω is $\omega=\epsilon_k$. The first-order approximation may be obtained by setting $\omega=\epsilon_k$ into $\sum(\mathbf{k},\omega)$ and

re-solving for ω, which gives

$$\omega = \epsilon_k + \sum(\mathbf{k},\epsilon_k) = \underbrace{\epsilon_k + \mathrm{Re}\sum(\mathbf{k},\epsilon_k)}_{\epsilon_k'} + i\underbrace{\mathrm{Im}\sum(\mathbf{k},\epsilon_k)}_{-\tau_k^{-1}}. \tag{3.71}$$

Hence we need to find the real and imaginary parts of $\sum(\mathbf{k},\epsilon_k)$.

To do this, we imagine δ is finite to start with, then take the limit $\delta\to 0$. Multiplying numerator and denominator of the integrand of $\sum$ in (3.69) by $\omega-\epsilon_l-i\delta$ we find for the real and imaginary parts of $\sum(\mathbf{k},\epsilon_k)$:

$$\begin{aligned}\mathrm{Re}\sum(\mathbf{k},\epsilon_k) &= \frac{N}{\Omega}W_{kk} + \lim_{\delta\to 0}\left(\frac{N}{\Omega}\right)\int\frac{d^3\mathbf{l}}{(2\pi)^3}\frac{|W_{lk}|^2(\epsilon_k-\epsilon_l)}{(\epsilon_k-\epsilon_l)^2+\delta^2}\\ &= \frac{N}{\Omega}W_{kk} + \left(\frac{N}{\Omega}\right)P\int\frac{d^3\mathbf{l}}{(2\pi)^3}\frac{|W_{lk}|^2}{(\epsilon_k-\epsilon_l)}\end{aligned} \tag{3.72}$$

$$\begin{aligned}\mathrm{Im}\sum(\mathbf{k},\epsilon_k) &= -\lim_{\delta\to 0}\left(\frac{N}{\Omega}\right)\int\frac{d^3\mathbf{l}}{(2\pi)^3}|W_{lk}|^2\frac{\delta}{(\epsilon_k-\epsilon_l)^2+\delta^2}\\ &= -\pi\left(\frac{N}{\Omega}\right)\int\frac{d^3\mathbf{l}}{(2\pi)^3}|W_{lk}|^2\,\delta(\epsilon_k-\epsilon_l).\end{aligned} \tag{3.73}$$

In (3.72), P stands for 'principal part'. (We will show why the limit in (3.72) is a principal part by illustrating with a simple case, the function $1/x$. Using the usual definition:

$$P\int_{-a}^{+b}\frac{dx}{x} = \lim_{\delta\to 0}\left\{\int_{-a}^{-\delta}\frac{dx}{x} + \int_{+\delta}^{+b}\frac{dx}{x}\right\} = \lim_{\delta\to 0}\{\ln(-\delta) - \ln(-a) + \ln b - \ln\delta\} = \ln b/a \tag{3.74}$$

Using the alternative definition in (3.72):

$$P\int_{-a}^{+b}\frac{dx}{x} = \lim_{\delta\to 0}\int_{-a}^{+b}dx\,\frac{x}{x^2+\delta^2} = \lim_{\delta\to 0}\tfrac{1}{2}\int_{-a}^{+b}\frac{d(x^2)}{x^2+\delta^2} = \lim_{\delta\to 0}\tfrac{1}{2}\ln(x^2+\delta^2)\Big|_{-a}^{b} = \ln b/a.) \tag{3.75}$$

In (3.73) we have used the 'squeezed Lorentzian' definition of the δ-function. The results (3.72, 3.73) are usually obtained with the aid of the so-called 'well-known theorem from complex function theory', (see, e.g., Dennery and Krzywicki (1967), p. 64),

$$\frac{1}{x+i\delta} = P\frac{1}{x} - i\pi\delta(x) \tag{3.76}$$

which is short for

$$\int \frac{dx\, f(x)}{x+i\delta} = P\int \frac{dx\, f(x)}{x} - i\pi \int dx\, f(x)\,\delta(x). \tag{3.76'}$$

This can be applied in the present case by noting that the integral in (3.69) may be written in the general form

$$\int d^3\mathbf{l}\, \frac{A(\mathbf{l},\ldots)}{B(\mathbf{l},\ldots)+i\delta} = \int d\phi \int d\theta \sin\theta \int dl\, l^2\, \frac{A(l,\theta,\phi,\ldots)}{B(l,\theta,\phi,\ldots)+i\delta}$$

where l, ϕ, θ are the polar coordinates of $\mathbf{l}$ and the dots ... refer to all the other variables. Only the $\mathbf{l}$-variable is relevant here. If we let $x=B(l)$ so $l=B^{-1}(x)$ then $\int dl$ may be written in terms of x, allowing (3.76') to be used. Transforming back to $\mathbf{l}$ again after this is done yields

$$\int d^3\mathbf{l}\, \frac{A(\mathbf{l},\ldots)}{B(\mathbf{l},\ldots)+i\delta} = P\int d^3\mathbf{l}\, \frac{A(\mathbf{l},\ldots)}{B(\mathbf{l},\ldots)} - i\pi \int d^3\mathbf{l} A(\mathbf{l},\ldots)\,\delta[B(\mathbf{l},\ldots)] \tag{3.76''}$$

Applying this to $\sum$ with $\omega=\epsilon_k$ gives just (3.72), (3.73).

Hence, placing (3.72, 3.73) in (3.71), we find for the electron energy and lifetime:

$$\epsilon_k' = \epsilon_k + \frac{N}{\Omega} W_{kk} + \left(\frac{N}{\Omega}\right) P\int \frac{d^3\mathbf{l}}{(2\pi)^3}\, \frac{|W_{lk}|^2}{\epsilon_k - \epsilon_l} \tag{3.77}$$

$$\tau_k^{-1} = \pi\left(\frac{N}{\Omega}\right)\int \frac{d^3\mathbf{l}}{(2\pi)^3} |W_{lk}|^2\, \delta(\epsilon_k - \epsilon_l) \tag{3.78}$$

Equation (3.77) is just the result obtained from second-order perturbation theory. Equation (3.78) is what comes out of applying the 'golden rule' for transition probabilities, i.e., τ_k^{-1} is just the transition probability/sec for the electron to jump from state $\mathbf{k}$ to $\mathbf{l}$, $|W_{lk}|^2$, integrated over all final states $\mathbf{l}$, subject to conservation of energy as expressed by the δ-function. (For a review of electrons in disordered systems see Leath (1970). The method above is applied to the case where the impurity distribution is not completely random but has 'short-range order' by Woolley and Mattuck (1972).)

Further Reading

Feynman (1965), chap. 1.
Bjorken (1964), §6.2.
Feynman (1962), p. 168, §2.

Exercises

3.1 Consider a one-dimensional system with an unperturbed Hamiltonian such that $U(x)$ in (3.4) is a square well of width a with infinitely high walls, i.e., $U(x)=0$ for $0<x<a$ and $U(x)=\infty$ for $x<0$, $x>a$. What are the eigenstates $\phi_n(x)$ and energies ϵ_n for this system? Write out the free propagator and its Fourier transform for this system.

3.2 The system in Ex. 3.1 is acted on by a hypothetical external perturbing potential $V(x)=B\times(p^2/2m+U(x))^3$, where $U(x)$ is defined in Ex. 3.1. Calculate the transition amplitude from single particle eigenstate $\phi_n(x)$ (calculated in Ex. 3.1) to $\phi_m(x)$ under the influence of the perturbation.

3.3 Write out the diagram series for the propagator of the system in Ex. 3.1, with the perturbation in Ex. 3.2 and evaluate it by summing to infinite order (assume the propagating particle is the only particle present).

3.4 What is the quasi particle energy dispersion law and lifetime in the above system?

3.5 Carry out the Fourier transform of the first-order terms in (3.30) and show that you get the corresponding terms in (3.31).

3.6 Use (3.53) to verify that G_0^+ satisfies the equation of the Green's function (3.51).

3.7 We have a random distribution of ions with a potential such that $W_{kl}=Wf_kf_l$, where $f_p=1$ for $|\mathbf{p}|<a$ and $f_p=0$ for $|\mathbf{p}|>a$. Show that the energy and reciprocal lifetime of an electron propagating in this sytem are

$$\epsilon_k' = \frac{k^2}{2m} + \left(\frac{N}{\Omega}\right)W + \left(\frac{N}{\Omega}\right)\frac{mW^2}{\pi^2}\left[-a + \frac{k}{2}\ln\left(\frac{a+k}{a-k}\right)\right] \quad \text{for } k<a$$

$$= \frac{k^2}{2m} \quad \text{for } k>a, \text{ where } k=|\mathbf{k}|$$

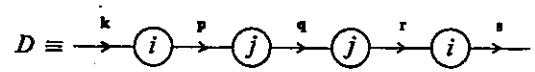
$$\tau_k^{-1} = \left(\frac{N}{\Omega}\right)\frac{mW^2 k}{2\pi} \quad \text{for } k<a$$

$$= 0 \quad \text{for } k>a$$

What is the effective mass in the limit $k \ll a$?

3.8 Write (3.36') with lines labelled in $(\mathbf{k},t)$-space. (Answer: see (10.15).) Translate into functions and show that you get an integral equation of form (3.56).

3.9 Consider the fourth-order diagram (drawn on its side to save space):



where $j \neq i$. Calculate its average value, using the same technique as, e.g., in (3.63) or (3.65). Show that this is the same result as you get from applying Table 3.2 to the last diagram in (3.66).

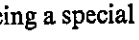
Chapter 4

Quasi Particles in Fermi Systems

4.1 Propagator method in many-body systems

We have thus far defined the quantum Green's function propagator for $t_2 > t_1$, shown what it looks like for free and quasi particles, and evaluated it by partial summation for the case of a single particle in an external potential. In this chapter, the technique will be generalized to many-body systems.

The starting point will be a system consisting of N non-interacting fermions in an external field. This is really a fake many-body system, since, as pointed out in chapter 0, if there are no mutual interactions between particles the problem is actually only a one-body problem. Nevertheless, such a 'trivial' system paves the way for the bona fide many-body case. First, it shows us how to describe Fermi systems very simply in terms of a few particles above the Fermi level, and a few removed particles, or '*holes*' below. Second, it allows us to introduce the language of the many-body problem, i.e., '*occupation number formalism*' or '*second quantization*'. We won't really start talking this language until the second half of the book, but it helps to learn some of the easier words in it now. Finally, it shows us how to extend the definition of the propagator to the case where $t_2 < t_1$. This is the time domain where we have the apparent paradox that the particle is observed in the system before it is put in! In this case, the Green's function turns out to describe the propagation of removed particles, or 'holes', which are represented diagrammatically by a downward-going arrow ↓.

As an illustration of a real many-body system, we will take a Fermi system with interaction between each pair of particles (no external potential). Examples of such systems are N electrons or nucleons in a macroscopic box. By introducing a special diagram:  for the two-body interaction, it is again possible to represent the propagator for this case as an infinite series of diagrams, which may be evaluated approximately by partial summation. Some of these partial sums are listed in Table 4.1.

The Hartree and Hartree–Fock are the crudest of the approximations and yield quasi particles with infinite lifetimes. The RPA yields the energy and lifetime of quasi particles in a high-density electron gas, while the ladder approximation is good for low-density systems like nuclear matter. Only the Hartree and Hartree–Fock will be discussed in detail in this chapter; the latter two are in chapter 10.

Table 4.1. *Some important partial sum approximations*

Types of diagrams summed over	Name of approximation
Bubbles	Hartree
Bubbles and open oysters	Hartree–Fock
Rings	Random phase approx. (RPA)
Ladders	Ladder approximation

4.2 Non-interacting Fermi system in external potential: particle–hole picture

Let us first talk about the particle–hole way of describing Fermi systems. Suppose we have a single particle in a potential $U(\mathbf{r})$, with energy eigenstates $\phi_k(\mathbf{r})$ ($\equiv \phi_{p_1}, \phi_{p_2}, \ldots$) and energies given by (3.4) (see note on notation after (3.5)!). The energy levels may be represented as in Fig. 4.1, where for simplicity the system is assumed non-degenerate.

The ground state of the single particle has energy ϵ_{p_1}. If we now put $N-1$ other particles into the system (with no mutual interaction), as for example when filling up atomic energy levels with electrons, we find that by the Pauli principle there can be no more than one particle in each state. The lowest energy for the whole system will occur when each state is filled in turn, starting from the bottom, as shown in Fig. 4.1(*a*) for the case $N=5$. The highest filled single-particle level is called the *Fermi level*, and has energy ϵ_F.

In the case where $U(\mathbf{r})=0$, the particles are free, and the k-subscript means momentum, or, more precisely, wavenumber. Then, in the ground state, the free particles fill a sphere in k-space having radius $k_F = \sqrt{(2m\epsilon_F)}$, where k_F is called the *Fermi momentum*. The filled sphere is called the *Fermi sea*. The surface of this sphere is the *Fermi surface*. If $U(\mathbf{r}) \neq 0$, then k is just a set of three indices (we are neglecting spin for simplicity) which in general can no longer be interpreted as momentum components. The Fermi surface is then no longer spherical and k_F becomes the vector $\mathbf{k}_F$. (Any reader unfamiliar with the above should see Raimes (1961), chap. 7.)

The various excited states of the system are formed by removing a particle from a state below the Fermi level and placing it in a state above, as shown for example in Fig. 4.1(*b*). The empty state, e.g., the state p_3 in Fig. 4.1(*b*), is called a 'hole'. This is just the hole defined in connection with Fig. 0.10, except that here it is in 'p'-space instead of real space.

To avoid the strain of drawing all the particles which were not transferred in forming the excited state, it is convenient to refer everything to the ground state, Fig. 4.1(*a*), and just record *changes* from the ground state. To draw this,

we remove the filled Fermi sea from the picture, yielding Figs. 4.1(*c*) and 4.1(*d*). This is called '*particle–hole* description'. Note that the Fermi sea is *physically* still present—it has only been removed from the *drawing* of the system.

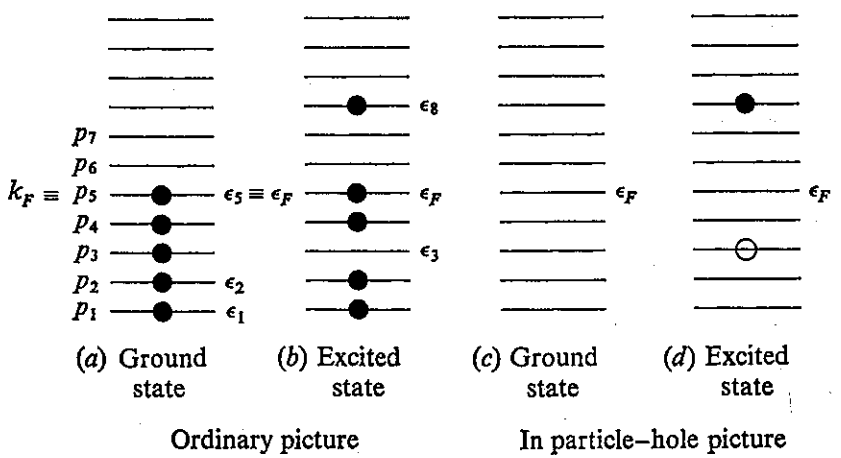


Fig. 4.1 *Non-interacting Fermi System*

Observe that the 'hole' in Fig. 4.1(*d*) is not the same as that in Fig. 4.1(*b*), since a Fermi sea particle has been removed from the empty state in p_3 in order to produce this new type of hole. That is, the hole in Fig. 4.1(*d*) is a 'minus particle' or 'anti-particle' rather than just an 'empty place'. Thus it is analogous to a 'positron' in Dirac's electron theory. This new type of hole can also be defined in position space instead of 'p'-space if we imagine that in Fig. 0.10, the undisturbed electron gas (coloured grey) is removed from the entire figure, *including* the empty places (coloured white) where the old holes are. Thus, each of the empty places will now be coloured 'minus grey' (evidently a job for the surrealist painter Salvador Dali!) which indicates the presence of an anti-particle.

Note that 'particles' in the new sense exist only above the Fermi surface. In cases where there is a possibility of confusion, we will distinguish between 'particle-hole' type particles and ordinary particles by writing the 'p' in italics, thus:

particle: particle in particle–hole sense. Exists only above Fermi surface.
particle: ordinary particle. Exists above and below Fermi surface. (4.1)

Since a hole in state ϕ_k is actually removal of a particle from the system, the hole represents energy ϵ_k removed. Hence the hole energy is negative and we have

$$\epsilon_k^{\text{hole}} = -\epsilon_k. \tag{4.2}$$

The shape of the hole wave function in space will be exactly the same as the shape of the wave function of the removed particle. This is analogous to removing a single piece from a completed jig-saw puzzle: the 'hole' thus created in the puzzle has exactly the same shape as the removed piece. Thus the time-dependent wave function for a hole in state ϕ_k is (see §7.5, just after (7.77) for rigorous proof):

$$\psi(t)^{\text{hole}} = \phi_k e^{-i(-\epsilon_k)t}, \quad \epsilon_k < \epsilon_F. \tag{4.3}$$

If we now associate the sign change in the $\epsilon_k t$ term with the t instead of the ϵ_k, the hole may be viewed as a particle moving backward in time. This should not be regarded as theoretical grounds for constructing a time machine, but simply as a convenient mode of description. It was originated by Feynman in his theory of positrons.

4.3 [[A primer of occupation number formalism (second quantization)]]

(This section can be skipped on first reading!)

Although we shall not make any essential use of it until after chapter 7, it is a good idea for orientational purposes to inject a few words here on the occupation number formalism or 'second quantization' as it is often called. This formalism is a sort of 'census-taking' notation which is extremely convenient for keeping track of what is going on in a many-particle system. The details are in chapter 7.

The total wave function for the ground and excited states of a system of non-interacting particles is, (see appendix (𝒜.3)), the product of single-particle wave functions. However, because we are dealing with identical fermions, this product must be antisymmetrized and the proper wave function is the Slater determinant

$$\Phi_{k_1,\ldots,k_N}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \frac{1}{\sqrt{(N!)}}\begin{vmatrix} \phi_{k_1}(\mathbf{r}_1)\ldots\phi_{k_1}(\mathbf{r}_N) \\ \vdots \quad\quad \vdots \\ \phi_{k_N}(\mathbf{r}_1)\ldots\phi_{k_N}(\mathbf{r}_N) \end{vmatrix} \tag{4.4}$$

where the ϕ_k's are the single-particle states of (3.4). If the particles are allowed to interact with each other, or with an external perturbing potential, then the exact wave functions of the system are no longer (4.4) but a linear combination of Φ's thus:

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \sum_{k_1,\ldots,k_N} A_{k_1,\ldots,k_N}\Phi_{k_1,\ldots,k_N}(\mathbf{r}_1,\ldots,\mathbf{r}_N). \tag{4.5}$$

That is, the $\Phi_{k_1,\ldots,k_N}$ for the non-interacting system are the basis states used to describe the interacting system.

Now these are rather clumsy expressions to carry around, so it would be desirable to have a more compact way of writing them. This may be gotten by noting that since all particles are indistinguishable, the essential information in (4.4) is just how many particles there are in each single-particle state. Therefore, we could equally well specify the state of the non-interacting system by writing Φ as

$$\Phi_{k_1,\ldots,k_N}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \Phi_{n_{p_1},n_{p_2},\ldots,n_{p_i},\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N) \tag{4.6}$$

For short, we shall represent this as

$$\Phi_{n_{p_1},n_{p_2},\ldots,n_{p_i},\ldots} \equiv |n_{p_1},n_{p_2},\ldots,n_{p_i},\ldots\rangle \tag{4.6'}$$

meaning: n_{p_1} particles in state ϕ_{p_1}, n_{p_2} in ϕ_{p_2}, etc., where $n_k=0$ or 1 by the Pauli principle. This is called '*occupation number* notation'. It is similar to the shell notation for atoms, where $(1s)^2(2s)^2(2p)^1$ means two electrons in the $1s$ state (one in the spin up and one in the spin down state), two in the $2s$ state, etc.

For the ground state in Fig. 4.1(a) we have in occupation number notation

$$\Phi_{k_1=p_1,\,k_2=p_2,\,k_3=p_3,\,k_4=p_4,\,k_5=p_5} = |1_{p_1},1_{p_2},1_{p_3},1_{p_4},1_{p_5},0_{p_6},0_{p_7},0_{p_8},\ldots,0,0,\ldots\rangle. \tag{4.7}$$

The excited state in Fig. 4.1(b) is

$$\Phi_{k_1=p_1,\,k_2=p_2,\,k_3=p_4,\,k_4=p_5,\,k_5=p_8} = |1_{p_1},1_{p_2},0_{p_3},1_{p_4},1_{p_5},0_{p_6},0_{p_7},1_{p_8},0_{p_9},\ldots\rangle. \tag{4.8}$$

For brevity, from now on we will drop the p's and just use the numerical subscripts. Then

$$\Phi = |n_1,n_2,n_3,\ldots,n_i,\ldots\rangle. \tag{4.9}$$

For example, (4.7) becomes

$$\Phi_0 = |1_1,1_2,1_3,1_4,1_5,0_6,0_7,0_8,\ldots\rangle.$$

It is important to note that just as the original Slater determinants form a complete orthogonal set of basis functions, so do the states in occupation number notation and we have

$$\begin{aligned}\langle n_1',\ldots n_i',\ldots|n_1,\ldots,n_i,\ldots\rangle &= \int d^3\mathbf{r}_1\ldots d^3\mathbf{r}_N\times\\ &\quad\times\Phi^*_{n_1',\ldots,n_i',\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\times\\ &\quad\times\Phi_{n_1,\ldots,n_i,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\\ &= \delta_{n_1'n_1}\ldots\delta_{n_i'n_i}\ldots\end{aligned} \tag{4.10}$$

Just as in (4.5), the $|n_1,\ldots,n_i,\ldots\rangle$ may be used as the basis states for describing the interacting system's wave function thus:

$$\Psi = \sum_{n_1,\ldots,n_i,\ldots} A_{n_1,\ldots,n_i,\ldots}|n_1,\ldots,n_i,\ldots\rangle. \tag{4.11}$$

Now in most cases of interest, only a few of the particles change their position from that in the ground state, since we deal primarily with only weakly excited states. Hence, carrying along all the unchanged 1's in a wave function like (4.8) is about as useful as taking along every piece of clothing one owns, on a two-day trip. The excess baggage may be avoided by regarding the ground state (4.7) as the 'zero' or so-called '*Fermi vacuum*' of our description, and recording in the $|\ldots\rangle$ only *changes* from the ground state. Thus, the ground state is written as though it has no particles in it:

$$\Phi_0 = |0\rangle \quad \text{('Fermi vacuum')} \tag{4.12}$$

corresponding to Fig. 4.1(c). The excited state of Fig. 4.1(b) according to this viewpoint is a *p*article (see (4.1)!) above ϵ_F and a hole below, as shown in Fig. 4.1(d), with the corresponding state vector

$$\Phi = |1_3^h,1_8^p\rangle \tag{4.13}$$

where h, p, stand for hole, *p*article. This is called 'particle–hole' notation.

Quantum mechanical operators have a new form in the occupation number formalism. Imagine that we have initially a single-particle system in its lowest energy eigenstate $\phi_1(\mathbf{r})$ ($\equiv\phi_{p_1}(\mathbf{r})$). In occupation number notation this is

$$\Phi_{\text{initial}} = \phi_1 = |1000\ldots\rangle. \tag{4.14}$$

If the system is now acted on by some perturbing operator $V(\mathbf{r},\mathbf{p})$, it may undergo a transition, say, to state ϕ_3, so that

$$\Phi_{\text{final}} = \phi_3 = |001000\ldots\rangle. \tag{4.15}$$

Thus, when written in this formalism, the effect of the operator V appears as the *destruction* of a particle in ϕ_1 and the *creation* of a particle in ϕ_3. This suggests that if we define two primitive operators—c_l (which is short for c_{p_l}), which destroys a particle in $\phi_l(\equiv\phi_{p_l})$ and $c_l^\dagger$ which creates a particle in ϕ_l—it may be possible to write all operators as various combinations of these primitive ones.

This is indeed the case. Look first at the detailed expression for the effect of the c's:

$$\begin{aligned}c_l|n_1,n_2,\ldots,n_l,\ldots\rangle &= n_l|n_1,n_2,\ldots,n_l-1,\ldots\rangle\\ c_l^\dagger|n_1,n_2,\ldots,n_l,\ldots\rangle &= (1-n_l)|n_1,n_2,\ldots,n_l+1,\ldots\rangle\end{aligned} \tag{4.16}$$

where the factors in front mean that c_l cannot destroy a particle in ϕ_l if there is no particle there to start with, and $c_l^\dagger$ cannot create another particle in an already occupied state. (A factor of ± 1 has been left out for simplicity—see chapter 7.) For example:

$$\begin{aligned}
&c_3|11111000\ldots\rangle = |1101100\ldots\rangle \\
&c_2|0000\ldots\rangle = 0 \\
&c_n|00\ldots1_j\ldots\rangle = \delta_{nj}|00\ldots\rangle \\
&c_3^\dagger|11111000\ldots\rangle = 0 \\
&c_2^\dagger|00\ldots\rangle = |0100\ldots\rangle \\
&c_m^\dagger|00\ldots0_m\ldots\rangle = |00\ldots1_m\ldots\rangle.
\end{aligned} \tag{4.17}$$

In the particle–hole notation, it is necessary to introduce hole creation and destruction operators, $b_l^\dagger$, b_l, and similarly *particle* operators $a_l^\dagger$, a_l, as follows: if $k_l < k_F$, then c_l destroys a particle under the Fermi level, thus creating a hole. Hence

$$\begin{aligned}
&\text{for } k_l > k_F, \quad c_l = a_l \quad (\textit{particle} \text{ destruction operator}) \\
&\qquad k_l < k_F, \quad c_l = b_l^\dagger \quad (\text{hole creation operator})
\end{aligned}$$

and

$$\begin{aligned}
&\text{for } k_l > k_F, \quad c_l^\dagger = a_l^\dagger \quad (\textit{particle} \text{ creation operator}) \\
&\qquad k_l < k_F, \quad c_l^\dagger = b_l \quad (\text{hole destruction operator}).
\end{aligned} \tag{4.18}$$

This change to *particle–hole* operators may be expressed compactly as the transformation

$$\begin{aligned}
c_l &= \theta_{k_l-k_F}a_l + \theta_{k_F-k_l}b_l^\dagger \\
c_l^\dagger &= \theta_{k_l-k_F}a_l^\dagger + \theta_{k_F-k_l}b_l
\end{aligned} \tag{4.19}$$

where

$$\theta_x = 1 \text{ for } x > 0; \quad \theta_x = 0 \text{ for } x < 0.$$

Simple examples of how the particle–hole operators work are:

$$\begin{aligned}
&a_l^\dagger|0\rangle = |1_l^p\rangle, \qquad a_l|1_l^p\rangle = \delta_{ll}|0\rangle, \qquad b_j^\dagger a_l^\dagger|1_m^p\rangle = |1_m^p, 1_l^p, 1_j^h\rangle, \\
&b_j^\dagger|0\rangle = |1_j^h\rangle, \qquad b_j|1_m^h\rangle = \delta_{jm}|0\rangle, \qquad a_l|0\rangle = b_l|0\rangle = 0, \\
&a_l^\dagger|1_l^p\rangle = 0, \qquad b_j^\dagger|1_j^h\rangle = 0.
\end{aligned} \tag{4.20}$$

In order to express other operators in terms of the c's (or a's and b's), it is simply required that: if $\mathcal{O}^{\text{old}}$ is the operator in the old notation, and $\mathcal{O}^{\text{occ}}$ is the same operator in the occupation number (or particle–hole) formalism, then $\mathcal{O}^{\text{occ}}$ must give the same matrix elements when sandwiched between states in occupation number (or particle–hole) formalism that $\mathcal{O}^{\text{old}}$ gave when sandwiched between Slater determinants. Consider first a one-particle case, where the Slater determinant is just ϕ_l. Then we must have

$$\langle 00\ldots1_l\ldots|\mathcal{O}^{\text{occ}}|\ldots1_j\ldots\rangle = \langle\phi_l|\mathcal{O}^{\text{old}}|\phi_j\rangle$$
$$\left(\equiv \int \phi_l^*(\mathbf{r})\mathcal{O}(\mathbf{r})\phi_j(\mathbf{r})\,d^3\mathbf{r} \equiv \mathcal{O}_{ij}\right). \tag{4.21}$$

A bit of Buddhistic contemplation shows that

$$\mathcal{O}^{\text{occ}} = \sum_{mn}\mathcal{O}_{mn}c_m^\dagger c_n \tag{4.22}$$

does the trick, since

$$\begin{aligned}
\langle\ldots1_l\ldots|\mathcal{O}^{\text{occ}}|\ldots1_j\ldots\rangle &= \sum_{mn}\mathcal{O}_{mn}\langle\ldots1_l\ldots|c_m^\dagger c_n|\ldots1_j\ldots\rangle \\
&= \sum_{mn}\mathcal{O}_{mn}\delta_{lm}\delta_{nj} = \mathcal{O}_{ij}
\end{aligned} \tag{4.23}$$

where (4.17) and (4.10) have been used. Equation (4.22) can be converted to particle–hole formalism by (4.18). This result turns out to hold also for systems with an arbitrary number of particles.

The Hamiltonian for an arbitrary system may be expressed in occupation number or particle–hole formalism. Suppose the system Hamiltonian in old Neanderthal notation describes a system in an external perturbing potential:

$$H_{\text{Neand.}} = \underbrace{\sum_l\left[\frac{p_l^2}{2m} + U(\mathbf{r}_l)\right]}_{H_0} + \underbrace{\sum_l V(\mathbf{r}_l)}_{H_1\ (\text{perturbation})} \tag{4.24}$$

and the single-particle states ϕ_k satisfy

$$\left[\frac{p^2}{2m} + U(\mathbf{r})\right]\phi_k = \epsilon_k\phi_k. \tag{4.25}$$

Then it is found that (see chapter 7):

$$\begin{aligned}
H_0 &= \sum_k \epsilon_k c_k^\dagger c_k = \sum_{k>k_F}\epsilon_k a_k^\dagger a_k + \sum_{k<k_F}\epsilon_k b_k b_k^\dagger \\
H_1 &= \sum_{m,n>k_F} V_{mn}a_m^\dagger a_n + \sum_{\substack{m>k_F \\ n<k_F}} V_{mn}a_m^\dagger b_n^\dagger + \sum_{\substack{m<k_F \\ n>k_F}} V_{mn}b_m a_n + \\
&\quad + \sum_{m,n<k_F} V_{mn}b_m b_n^\dagger.
\end{aligned} \tag{4.26}$$

For a system of mutually interacting particles with old Hamiltonian

$$H_{\text{old}} = \underbrace{\sum_i \frac{p_i^2}{2m}}_{H_0} + \underbrace{\tfrac{1}{2}\sum_{i,j} V(\mathbf{r}_i - \mathbf{r}_j)}_{H_1 \text{ (perturbation)}} \tag{4.27}$$

we find

$$H_0 = \sum_{k>k_F} \epsilon_k a_k^\dagger a_k + \sum_{k<k_F} \epsilon_k b_k b_k^\dagger, \quad \text{with} \quad \epsilon_k = k^2/2m$$

$$H_1 = \tfrac{1}{2}\sum_{k,l,m,n>k_F} V_{klmn} a_l^\dagger a_k^\dagger a_m a_n + \tfrac{1}{2}\sum_{\substack{k,l,m>k_F \\ n<k_F}} V_{klmn} a_l^\dagger a_k^\dagger a_m b_n^\dagger +$$

$$+ \cdots + \tfrac{1}{2}\sum_{k,l,m,n<k_F} V_{klmn} b_l b_k b_m^\dagger b_n^\dagger \tag{4.28}$$

with V_{klmn} as defined in (4.42).

It should be carefully remembered that in the case of systems with interaction, the wave functions are given by the linear combination (4.11).

4.4 Propagator for non-interacting Fermi system in external perturbing potential

Up to now we have worked with a propagator defined only for positive time differences, i.e., for $t_2 > t_1$. This was adequate for solving the super-simple quantum pinball problem, but fails when we try to use it on more complicated cases. To treat the general situation, it is necessary to extend the definition to times $t_2 < t_1$. This of course sounds peculiar, since it seems to describe a particle propagating backward in time. However, as explained in connection with (4.3), such 'time-machine' particles are not science fiction but simply removed particles or 'holes'. That is, a particle moving backward in time from t_1 to t_2 ($t_2 < t_1$) is just a hole moving forward in time from t_2 to t_1.

This leads us to the definition

$$iG(k_2, k_1, t_2 - t_1)_{t_2<t_1} \equiv iG^-(k_2, k_1, t_2 - t_1)$$

$$= (-1) \times \text{probability amplitude that if at time } t_2 \text{ we remove a particle in state } \phi_{k_2} \text{ from (i.e., if we add a hole in } \phi_{k_2} \text{ to) the interacting system in its ground state, then at time } t_1 \text{ the system will be in its ground state with a particle removed from (i.e., an added hole in) } \phi_{k_1}. \tag{4.29}$$

Analogous to (3.3), for $t_2 > t_1$ (but not for $t_2 = t_1$!), G^- is defined so that

$$iG^-(k_2, k_1, t_2 - t_1)_{t_2>t_1} = 0. \tag{4.30}$$

Thus, G^- is just the hole propagator. (The factor of (-1) here compared with (3.1) comes because we have fermions—see chapter 9. Note that G^- is called an 'advanced' propagator or Green's function.)

The use of the word hole in the sense of 'removed particle' is more general than the way it was used in §4.2. There we dealt with the non-interacting system, so a particle could be removed only from $k < k_F$ and therefore all holes had $k < k_F$. However, in the ground state of the interacting system, by (4.11) there is a finite probability of finding particles above k_F. Hence we can remove a particle or create a hole (in this more general sense) above $k = k_F$. If the 'hole propagator' G^- is, as above, defined as being the propagator for $t_2 < t_1$, then the free G_0^- has $k < k_F$ but the exact G^- can have any k.

In the case of a free hole, an argument like that in (3.8) applied to the single hole state in (4.3) yields (note that (3.8) and G_0^+ in (3.9) describe *particle* propagation, since $\epsilon_k > \epsilon_F$)

$$G_0^-(k, t_2 - t_1) = \begin{cases} i\theta_{t_1-t_2} e^{-i\epsilon_k(t_2-t_1)}, & \text{for } t_2 \neq t_1, \quad \epsilon_k < \epsilon_F \\ i, & \text{for } t_2 = t_1 \quad \text{(see (9.2), (9.4), end of appendix F)} \end{cases} \tag{4.31}$$

with Fourier transform

$$G_0^-(k, \omega) = \frac{1}{\omega - \epsilon_k - i\delta}, \quad \epsilon_k < \epsilon_F. \tag{4.32}$$

Suppose now that we turn on an external perturbing potential $V(\mathbf{r})$ (this is distinct from $U(\mathbf{r})$ which is part of the unperturbed Hamiltonian), and wish to find, say, the single-particle propagator $G^+(k_2, k_1, t_2 - t_1)$ or $G^+(k_2, k_1, \omega)$. This will be the sum of the amplitudes for all the ways the particle can move through the system interacting zero or more times with $V(\mathbf{r})$. Previously, we wrote down the series for the propagator and translated it into diagrams. Now we turn the trick and pull the hat out of the rabbit, i.e., write down the diagrams first, then translate them into the numerical series. To do this, we need a modified dictionary, analogous to Table 3.1 with downward directed lines for the hole propagators, as shown in Table 4.2. Observe the reversed time order for the hole propagator diagrams! This is of course due simply to the fact that $t_2 < t_1$ for holes. The reason why these diagrams are labelled 'Goldstone method' is discussed in §9.5.

The interaction amplitude, V_{kl}, merits some discussion. It is given by

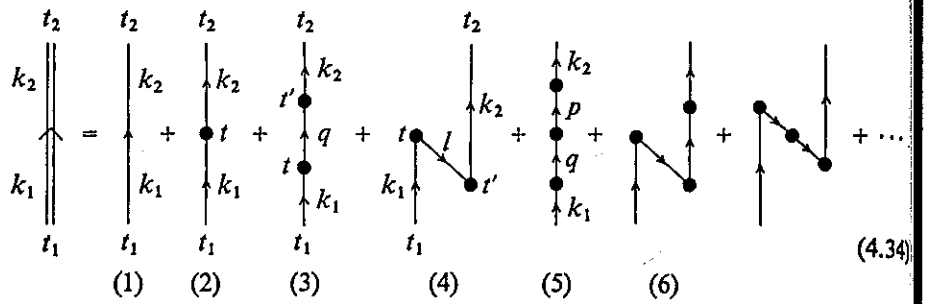
$$V_{kl} = \int d^3\mathbf{r} \phi_k^*(\mathbf{r}) V(\mathbf{r}, \mathbf{p}) \phi_l(\mathbf{r}). \tag{4.33}$$

The four possibilities shown in Table 4.2 mean: (*a*) scattering of a *particle* (remember (4.1)!) from state ϕ_l to ϕ_k, (*b*) the potential scatters a particle out of state ϕ_l, where $\epsilon_l < \epsilon_F$, into state ϕ_k, $\epsilon_k > \epsilon_F$, thus simultaneously creating a *particle* in ϕ_k and a hole in ϕ_l, (*c*), etc. [Note that these four possibilities correspond to the four interaction terms in the particle–hole Hamiltonian for this case (4.26).]

Of course, the particle which emerges in state **k** after interaction, is not necessarily the same particle which entered in state **l**, since this has no meaning

in a system of indistinguishable particles. Nevertheless, for the sake of verbal simplicity, it is customary to describe interactions *as if* particles were distinguishable; the reader should always bear in mind that this is just a manner of talking.

With the aid of Table 4.2, the diagrammatic series for G^+ may be drawn as the sum of all possible different diagrams which can be built up out of sequences of interaction dots connected by particle and hole lines, beginning in state k_1 and ending in state k_2:



(4.34)

(Note that the first diagram disappears if $k_2 \neq k_1$, by (3.9).) The physical significance of the hole lines in the diagrams may be understood by looking at the fourth diagram. A *particle* enters the system in state k_1 ($\equiv \phi_{k_1}$) at time t_1. At time t', the potential knocks a particle out of the state l into state k_2 thus creating a *particle* in k_2 and a hole in l. At time t, the *particle* in k_1 is knocked into the hole in l causing mutual annihilation; the *particle* in k_2 continues propagating until t_2.

It should be pointed out that many diagrams in this series violate the Pauli exclusion principle. For example, when $k_1 = k_2$, in diagram 4 we have two particles in the same state, k_1. The reason why such diagrams must be included is discussed at the end of Appendix G (see also §4.6).

[[It is amusing to do the 'book-keeping' on these processes by means of the particle–hole notation, with H_1 as in (4.26). We have the sequence:

(1) Put in *particle* in state k_1 at time t_1:

$$a^\dagger_{k_1}|0\rangle = |1^p_{k_1}\rangle$$

(2) At t', one of the terms in H_1 acts on system creating *particle* in k_2, hole in l:

$$V_{k_2 l}\, a^\dagger_{k_2} b^\dagger_l |1^p_{k_1}\rangle = V_{k_2 l}|1^p_{k_1}, 1^h_l, 1^p_{k_2}\rangle$$

(Note that if $k_2 = k_1$, we have $a^\dagger_{k_1}|1^p_{k_1}, 1^h_l\rangle$ which equals zero by (4.20). Nevertheless, the diagram which includes this process (number (4) in (4.34)) does not have the value zero! It is, as just mentioned, an exclusion-principle-violating diagram, and it must be kept (see §4.6).)

Table 4.2 *Diagram dictionary for many-fermion system in external perturbing potential (Goldstone method)*

(k,t)-space		(k,ω)-space	
Word	Diagram	Word	Diagram
$iG^+(k_2,k_1,t_2-t_1)$ (particle), see (3.2)	k_2,t_2 / k_1,t_1	$iG^+(k_2,k_1,\omega)$	k_2 / k_1, ω
$iG^-(k_2,k_1,t_2-t_1)$ (hole), see (4.29)	k_1,t_1 / k_2,t_2	$iG^-(k_2,k_1,\omega)$	k_1 / k_2, ω
$iG_0^+(k,t_2-t_1) = \theta_{t_2-t_1}\theta_{\epsilon_k-\epsilon_F}\exp[-i\epsilon_k(t_2-t_1)]$ ($=0$ for $t_2=t_1$) (free particle)	k: t_2 / t_1	$iG_0^+(k,\omega) = \dfrac{i\theta_{\epsilon_k-\epsilon_F}}{\omega-\epsilon_k+i\delta}$	k,ω
$iG_0^-(k,t_2-t_1) = -\theta_{t_1-t_2}\theta_{\epsilon_F-\epsilon_k}\exp[-i\epsilon_k(t_2-t_1)]$ ($=-1$ for $t_2=t_1$) (free hole)	k: t_1 / t_2	$iG_0^-(k,\omega) = \dfrac{i\theta_{\epsilon_F-\epsilon_k}}{\omega-\epsilon_k-i\delta}$	k,ω
$-iV_{kl}$ (interaction with external perturbation), see (4.33)	or, 4 possibilities: (a) k, l; (b) k, l; (c) l, k; (d) l, k	$-iV_{kl}$	or, 4 possibilities

(3) At t, H_1 acts again, destroying hole in l, particle in k_1:

$$V_{lk_1} b_l a_{k_1}[V_{k_2 l}|1^p_{k_1}, 1^h_l, 1^p_{k_2}\rangle] = V_{k_2 l} V_{lk_1}|1^p_{k_2}\rangle$$

(4) At t_2, take particle out:

$$a_{k_2}[V_{k_2 l} V_{lk_1}|1^p_{k_2}\rangle] = V_{k_2 l} V_{lk_1}|0\rangle.]] \tag{4.35}$$

The above diagram series may be written out in words by means of the dictionary Table 4.2. This gives in (k,t)-space (cancel the i's):

$$\begin{aligned} G^+(k_2,k_1,t_2-t_1) &= G_0^+(k_1,t_2-t_1)\,\delta_{k_1 k_2} \\ &\quad + \int_{-\infty}^{+\infty} dt\, G_0^+(k_2,t_2-t)\, V_{k_2 k_1}\, G_0^+(k_1,t-t_1) + \\ &\quad + \sum_{q>k_F} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \cdots + \cdots \end{aligned} \tag{4.36}$$

or in (k,ω)-space (leave out ω's for brevity):

$$\begin{aligned} G^+(k_2,k_1) &= \delta_{k_1 k_2} G_0^+(k_1) + G_0^+(k_1)\, V_{k_2 k_1}\, G_0^+(k_2) \\ &\quad + \sum_{q>k_F} G_0^+(k_1)\, V_{qk_1}\, G_0^+(q)\, V_{k_2 q}\, G_0^+(k_2) + \\ &\quad + \sum_{l<k_F} G_0^+(k_1)\, V_{lk_1}\, G_0^-(l)\, V_{k_2 l}\, G_0^+(k_2) + \cdots \end{aligned} \tag{4.37}$$

where we have remembered to sum over all possible intermediate states, q, l, etc., since, for example, the single diagram with q on it actually stands for an infinite number of diagrams, each one with a different value of q. (The notation $q>k_F$ is short for $\epsilon_q>\epsilon_F$, etc.)

[The time integrations in (4.36) are automatically restricted by the θ-functions found in G^+ and G^-. Thus, in the third diagram in (4.34) since all lines are particle propagators, we see that $t_1<t<t'<t_2$. In the fourth diagram, since the l-line is a hole propagator, t must be $>t'$, and we find: if $t_1<t<t_2$ then $-\infty<t'<t$, while if $t_2<t<\infty$, then $-\infty<t'<t_2$. (Strictly speaking, in the Goldstone method, diagrams are 'time-ordered' (see §9.5) so that for diagram (4), $t_1<t'<t$, $t_1<t<t_2$. There will be other diagrams like (4), but with $-\infty<t'<t_1$ and/or $t_2<t<\infty$, which may be added to (4) to obtain the stated region of integration.)

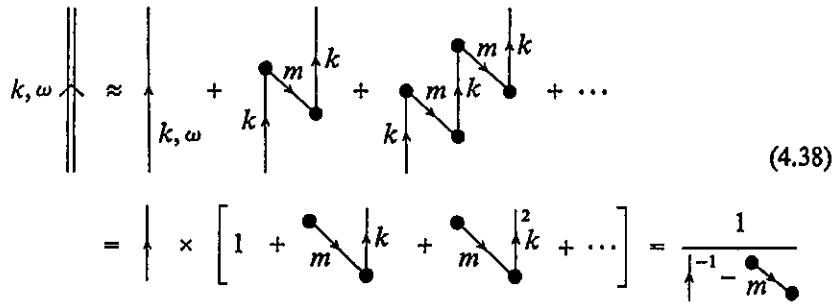
However, when the time integrations here are actually performed, one is dismayed to discover the page jumping with exponentials oscillating at ∞ just as in (3.12). The remedy is to change the integration limits from $\pm\infty$ to $\pm\infty(1-i\eta)$ where η is a positive infinitesimal like the δ in (3.12'): it is such that $\eta\times\infty=\infty$. The justification for these new limits lies in the rigorous derivation of the propagator expansion (see Appendix E, especially (E.11)).

One might imagine that these modified limits would cause trouble in Fourier transforming from (4.36) to (4.37). That is, we would expect that the limits $\pm\infty$ were required in order to get the δ-functions, like $\delta(\omega-\omega')$ in (2.23). However, one finds that the sort of integral which arises, i.e., of form

$$\int_{T_1}^{T_2} dt \exp(i\Delta\epsilon t),$$

where $T_1=-\infty(1-i\eta)$ and $T_2=+\infty(1-i\eta)$, is also a legitimate δ-function, so this causes no difficulty.]]

And now an easy example showing how to evaluate G^+ by partial summation. Suppose $k_1=k_2=k$ $(k>k_F)$, and the potential is such that V_{km} and V_{mk} $(m<k_F$—remember this is short for $\epsilon_m<\epsilon_F)$ are large, and all the other V's are small. Then the propagator in (4.34) may be approximated by the sum of the following diagrams:



(4.38)

or

$$\begin{aligned} G^+(k,\omega) &= \frac{1}{[G_0^+(k,\omega)]^{-1} - V_{km}\, V_{mk}\, G_0^-(m,\omega)} \\ &= \frac{1}{(\omega-\epsilon_k+i\delta) - \dfrac{|V_{km}|^2}{(\omega-\epsilon_m-i\delta)}}. \end{aligned} \tag{4.39}$$

This result is evidently not of the quasi particle form (3.16). However, by (3.14), the poles of G^+ give the excited state energies of the perturbed system. Thus, dropping the $i\delta$'s (they have no significance in this simple calculation) yields

$$\omega-\epsilon_k-\frac{|V_{km}|^2}{\omega-\epsilon_m}=0 \tag{4.40}$$

which gives

$$\begin{aligned} \omega = \epsilon_k' &= \frac{\epsilon_k+\epsilon_m}{2} + \tfrac{1}{2}\sqrt{\{(\epsilon_k-\epsilon_m)^2+4|V_{km}|^2\}} \\ &= \epsilon_m' = \frac{\epsilon_k+\epsilon_m}{2} - \tfrac{1}{2}\sqrt{\{(\epsilon_k-\epsilon_m)^2+4|V_{km}|^2\}}. \end{aligned} \tag{4.41}$$

These reduce respectively to ϵ_k, ϵ_m in the weak interaction case, when $V_{km}\to 0$, and are also valid in the strong interaction case when V_{km} is of the order of or greater than the separation between the levels, $\epsilon_k-\epsilon_m$. Note that it is necessary to go to infinite order to get (4.41). If we just go to *any finite order*, the poles are still at the unperturbed energies, ϵ_k, ϵ_m!

The result (4.41) will be recognized by experts as just the formula for the new energies of a single particle two-level system placed in a perturbing field. Of course, we could have predicted this result from the beginning since we've really got a single particle system here, because by assumption the particles don't interact with each other. Again, as mentioned in connection with the quantum pinball game, this should not be regarded as a demonstration that the 'powerful' diagram technique merely provides a complicated method for getting trivial results, but rather as a super-simple illustration of the general principles.

In the next section we go on to the real many-body problem.

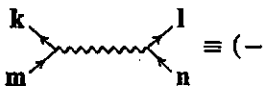
4.5 Interacting Fermi system

Imagine now that we've got a genuine many-body system consisting of N fermions interacting by means of two-body forces $V(|\mathbf{r}_i-\mathbf{r}_j|)$, depending just on the interparticle distance $|\mathbf{r}_i-\mathbf{r}_j|$. For simplicity, assume there are no external fields, so that the single particle states are just $\phi_k=\Omega^{-\frac{1}{2}}\exp(i\mathbf{k}\cdot\mathbf{r})$ with $\epsilon_k=k^2/2m$ as in (3.4) and (3.5). Our object is to construct diagrammatically the perturbation expansion of the propagator for this system, evaluate it by partial summation and examine the result for quasi particle behaviour.

The first thing we need is the transition probability amplitude for a process in which two particles, one in state ϕ_m, the other in state ϕ_n collide with each other and are scattered into states ϕ_k, ϕ_l respectively. Analogous to the interaction amplitude V_{kl} in (4.33), this is just the matrix element

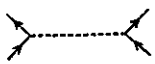
$$V_{klmn}=\int d^3\mathbf{r}\int d^3\mathbf{r}'\,\phi_k^*(\mathbf{r})\,\phi_l^*(\mathbf{r}')\,V(|\mathbf{r}-\mathbf{r}'|)\,\phi_m(\mathbf{r})\,\phi_n(\mathbf{r}')=V_{lknm}. \quad (4.42)$$

As we saw in (1.8) in $(\mathbf{r},t)$-space, such an interaction may be represented diagrammatically by a wiggly line:

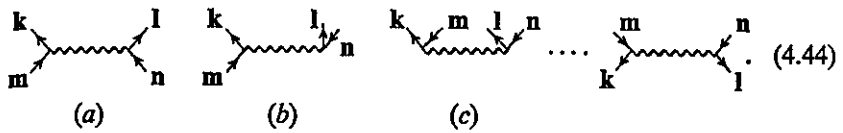


$$\equiv(-i)\tfrac{1}{2}V_{klmn}, \quad (4.43)$$

where the left intersection or 'vertex' shows the scattering of one particle from $\mathbf{m}$ to $\mathbf{k}$, and the right vertex shows the scattering of the other from $\mathbf{n}$ to $\mathbf{l}$. (Note: the majority of writers draw the above interaction with a dashed line:



However, we shall always use the wiggle (4.43).) [The $\frac{1}{2}$ comes from H_1 in (4.28). It is eliminated by (4.60).] Using the particle–hole description, this may be drawn in more detail, thus:



(4.44)

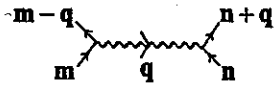
Diagram (*a*) just pictures ordinary scattering of two *p*articles from states $\mathbf{m},\mathbf{n}$ to $\mathbf{k},\mathbf{l}$. In (*b*) a *p*article in ϕ_m collides with a particle below the Fermi surface in state ϕ_n. It knocks the particle out of ϕ_n, thus creating a hole in ϕ_n and a *p*article above the Fermi surface in state ϕ_l. At the same time the original particle undergoes a transition to state ϕ_k. And so on. [Note that the diagrams (4.44) correspond precisely to the interaction terms in the Hamiltonian for this case, (4.28).]

☛ It is extremely important to note the labelling convention used in V_{klmn}: $\mathbf{k}$=line out of left vertex, $\mathbf{l}$=line out of right vertex, $\mathbf{m}$=line into left vertex, $\mathbf{n}$=line into right vertex. A mnemonic aid is to remember the tango dance step: left out, right out, left in, right in.

The interaction $V(|\mathbf{r}-\mathbf{r}'|)$ conserves linear and spin momentum since it depends only on $|\mathbf{r}-\mathbf{r}'|$, therefore cannot move the centre of mass of the two colliding particles or flip their spins. Thus

$$\mathbf{k}+\mathbf{l}=\mathbf{m}+\mathbf{n};\quad \sigma_k+\sigma_l=\sigma_m+\sigma_n. \quad (4.45)$$

If the arrows in (4.44) are interpreted as giving the direction of 'momentum flow', then (4.45) shows that the momentum flowing into the interaction equals the momentum flow out. It is convenient to incorporate this into the labelling as follows:

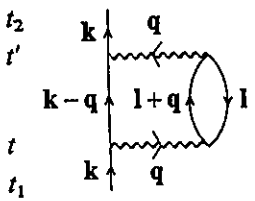


$$\equiv -i\times\tfrac{1}{2}V_{m-q,\,n+q,\,m,\,n}$$

$$=-i\times\tfrac{1}{2}V_q \quad (4.46)$$

where the form V_q is justified in (7.70). (Observe that the momentum transfer, $\mathbf{q}$, in (4.46) is defined as momentum into left vertex minus momentum out of left vertex. That is, for matrix element V_{klmn}, the momentum transfer is $\mathbf{q}=\mathbf{m}-\mathbf{k}$ ($=\mathbf{l}-\mathbf{n}$ by momentum conservation). The element V_{lknm}, corresponding to diagram (4.43) twisted through 180°, has momentum transfer $\mathbf{q}'=\mathbf{n}-\mathbf{l}=-\mathbf{q}$. Hence, since by (4.42) $V_{klmn}=V_{lknm}$, we have $V_q=V_{-q}$.) All this implies that no matter how complicated the chain of collision processes is,

the momentum at the beginning of the chain is equal to the momentum at the end. This can be seen, for instance, in the second-order diagram:



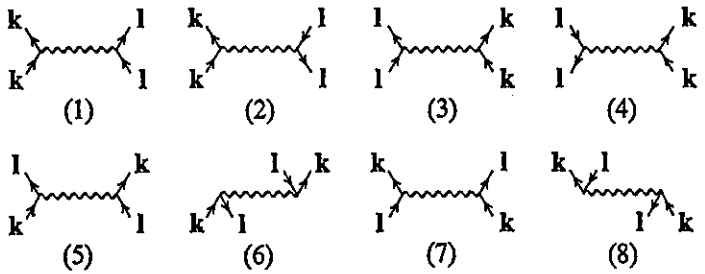
(4.47)

This is analogous to the flow of current in a network without sources or sinks, so that the flow of current into the network = current out. Hence it is only necessary to deal with propagators $G(\mathbf{k},\mathbf{l},t_2-t_1)$ such that $\mathbf{k}=\mathbf{l}$.

It is important to note here that although the collisions conserve momentum, they do not conserve energy. For example, at the lower interaction of (4.47) we see that the energy flow into the interaction (in units of $\hbar^2/2m$) is k^2+l^2, while the energy flow out is $(k-q)^2+(l+q)^2$. Hence we are dealing here with *virtual* scattering processes, not real ones.

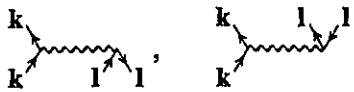
We may now construct the perturbation series for the single-particle propagator, G^+, as the sum of all possible different diagrams which can be built up out of sequences of interactions (4.43), connected by particle and hole lines, with a particle entering the system in state $\mathbf{k}$ and leaving in $\mathbf{k}$. One such sequence is just that in (4.47). It depicts a *p*article in $\mathbf{k}$ being scattered into $\mathbf{k}-\mathbf{q}$ and simultaneously knocking a particle out of $\mathbf{l}$ into $\mathbf{l}+\mathbf{q}$ (i.e., creating a *p*article in $\mathbf{l}+\mathbf{q}$ and a hole in $\mathbf{l}$). At later time t', the *p*article in $\mathbf{k}-\mathbf{q}$ knocks the *p*article in $\mathbf{l}+\mathbf{q}$ back into the hole state $\mathbf{l}$ (thus annihilating the *p*article–hole pair) and is itself scattered into state $\mathbf{k}$. This is a second-order process, because it involves two interactions.

There are also several first-order sequences which can occur. Although these are simpler than (4.47) because they involve only one interaction, they are more difficult to interpret physically. Let us see what first-order processes can be constructed using the interaction in (4.44). Since one particle enters in $\mathbf{k}$ and one leaves in $\mathbf{k}$, by conservation of momentum the only possibilities are



(4.48)

Such diagrams as



(4.49)

are not allowed since they have a *p*article and a hole in the same state, $\mathbf{l}$, which is impossible—by definition, *p*articles exist only above k_F and holes only below. It can also be shown that diagrams (1), (3), (5) and (7) above do not occur. [The argument for this requires use of the interaction Hamiltonian, H_1, as in (4.28). The term in H_1 corresponding to diagram (1) is

$$V_{klkl}a_l^\dagger a_k^\dagger a_k a_l. \tag{4.50}$$

When this acts on the state with one incoming *p*article in ϕ_k, we find

$$V_{klkl}a_l^\dagger a_k^\dagger a_k a_l|1_k^p\rangle = 0 \tag{4.51}$$

by (4.20). Diagrams (3), (5) and (7) are similarly eliminated. Note that the term in H_1 corresponding to diagram (2), for example, is

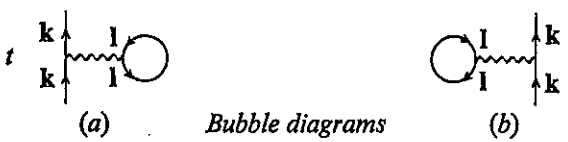
$$V_{klkl}b_l a_k^\dagger a_k b_l^\dagger \tag{4.52}$$

which gives, by (4.20):

$$V_{klkl}b_l a_k^\dagger a_k b_l^\dagger|1_k^p\rangle = V_{klkl}|1_k^p\rangle \neq 0.] \tag{4.53}$$

(Note: Let us not make the mistake of thinking that in diagrams (1)–(4) in (4.48), 'nothing has happened' just because the particles and holes emerge in exactly the same momentum state in which they entered. This would only be true if we were dealing with classical particles. In the present quantum case something has indeed happened, i.e., two particles in states $\mathbf{k},\mathbf{l}$ enter and interact with each other, but instead of being scattered into new states different from $\mathbf{k},\mathbf{l}$, they are simply scattered into the same states, $\mathbf{k},\mathbf{l}$. This is the same as what occurred in the quantum pinball game, where the potential $V_{M_{kk}}$ scattered the particle from the state $\mathbf{k}$ into the same state $\mathbf{k}$.)

The possible first-order processes may then be drawn using (4.48)—(2), (4), (6) and (8). This can be done in only one way, e.g., by in each case attaching the outgoing $\mathbf{l}$ line to the incoming one (otherwise we would have a *p*article and a hole entering and leaving the diagram, which would violate the definition of the single-particle propagator, or we would have to introduce more interaction lines, making it a higher-order process). Thus we find:



(4.54)

(4.55)

(c) *Open oyster diagrams* (d)

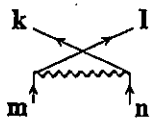
(closed oyster appears in (0.23))

The bubble processes can be physically interpreted as follows: a *particle* enters in **k**, knocks a particle out of state **l** ($|\mathbf{l}| < k_F$) at time t, then knocks the particle instantaneously back into **l** at time t, then continues freely in state **k**. Thus the hole which is created in **l** lasts only zero seconds, and there is no accompanying *particle*. Of course it is impossible to draw instantaneous processes like this, and the bubble picture is purely schematic. This process is also called '*forward scattering*', since the particle emerges in the same direction (i.e., momentum state) as it entered. (Note again that by the argument after (4.53), something has really 'happened' in these forward scattering processes!)

This bubble process undoubtedly sounds so bizarre that it may seem farfetched to consider it physical. The fact is that, while in the classical pinball case, each diagram described a real physical process, the quantum diagrams describe only what might be called '*quasi-physical*' processes. This will be discussed further in the next section, §4.6. At the end of Appendix G, it is proved rigorously that the bubble is a legitimate diagram.

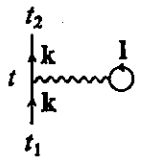
The open-oyster processes are just like the bubbles, except that a quick-change act occurs in which at time t the incoming *particle* simultaneously (*a*) strikes the particle in **l**, (*b*) creates an instantaneous hole in **l** and (*c*) is exchanged for the particle in **l**. Diagrams (4.55) are often called 'first-order *exchange diagrams*', and the process is referred to as an '*exchange scattering*'. The instantaneous hole lines in the bubble and open oyster are called '*non-propagating*' lines.

Note that the situation shown in (4.54, 55) is general, i.e., whenever the interaction (4.43) occurs in a diagram, there is also another diagram possible in which the two outgoing (or incoming) particles have exchanged momentum. This is usually drawn thus:



For example, diagram (5) in (4.63) is the exchange of diagram (4).

Let us see how one evaluates these diagrams. Consider first the bubbles. Using dictionary Table 4.2 and (4.43):

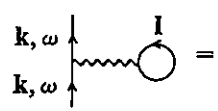


$$= (-1)\sum_{l<k_F}\int_{-\infty}^{+\infty} dt[iG_0^+(\mathbf{k}, t-t_1)]\times\left[-\frac{i}{2}V_{klkl}\right]\times$$
$$\times[iG_0^-(\mathbf{l}, t-t)]\times[iG_0^+(\mathbf{k}, t_2-t)], \tag{4.56}$$

where we have integrated over the 'intermediate' time, t, and summed over the 'intermediate' momentum, **l**, as in (4.36). (The extra factor of (-1) in front comes from the fact that the diagram contains one 'fermion loop', namely ◯. [A fermion loop is any set of directed lines, in a diagram, which can be traversed in the direction of the arrow, returning to the starting point without lifting pencil from the paper. For example, the **l**, **l**+**q** lines in (4.47) form a fermion loop.] This is one of the annoying 'phase factors' which comes out of the rigorous mathematical development of the theory (see end of Appendix G).) Note that an additional factor of (-1) appears because the propagator line for the bubble is:

$$iG_0^-(\mathbf{l}, t-t) = i\times ie^{-i\epsilon_l\times 0} = -1. \tag{4.57}$$

The Fourier transform of (4.56) may be taken just as was done in the pinball case (2.23). This yields

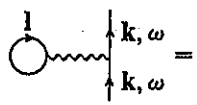


$$= (-1)[iG_0^+(\mathbf{k}, \omega)]^2\sum_{l<k_F}\left[-\frac{i}{2}V_{klkl}\right](-1). \tag{4.58}$$

The (-1) after V_{klkl} comes from (4.57) and is the value of the 'non-propagating' bubble line in $(\mathbf{k}, \omega)$-space as well as $(\mathbf{k}, t)$-space. Note that we cannot get (4.58) just by using the (k, ω) side of dictionary Table 4.2! This is because the bubble (and open oyster) diagrams are special cases.

It should be remarked here that if spin is included, then **k** is short for $\mathbf{k}, \sigma$ where σ is the spin quantum number (see p. 106), and $\mathbf{l}\equiv\mathbf{l}, \sigma'$. For a spin-independent interaction, (7.70) holds, and the sum over σ' then produces a factor 2 which multiplies (4.58).

In a similar fashion, the reversed bubble gives

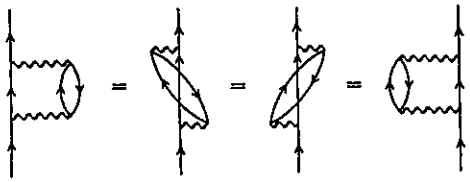


$$= (-1)[iG_0(\mathbf{k}, \omega)]^2\sum_{l<k_F}\left(-\frac{i}{2}\right)V_{lklk}(-1). \tag{4.59}$$

But by (4.42), $V_{klkl}=V_{lklk}$ so these two diagrams are equal. This is quite general and we may write:

> If we are given a diagram, and form a new diagram from it by twisting one or more of its interaction wiggles through 180 degrees, then the new diagram has the same value as the original one. Hence all twisted diagrams may be omitted if we just multiply (4.43) by a factor of 2. (4.60)

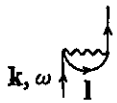
Thus, for instance, of the diagrams



(4.61)

it is only necessary to keep the first.

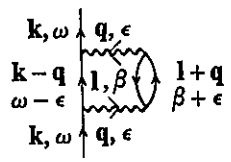
In a manner similar to (4.59), the open oyster gives



$$= [iG_0^+(\mathbf{k},\omega)]^2 \sum_{l<k_F} (-i)\, V_{lkkl}(-1). \qquad (4.62)$$

The factor of 2 recommended in (4.60) has been included. If spin is included, so $\mathbf{k}\equiv\mathbf{k},\sigma$, and $\mathbf{l}\equiv\mathbf{l},\sigma'$, then for a spin-independent interaction like (7.70), we find that $\sigma'=\sigma$. Hence there is *no* factor 2 from a spin sum, in contrast to the case of the bubble (4.58).

Observe that the *frequency* (or 'energy parameter'), ω, associated with the propagator line coming out of the interaction in (4.59, 62) is the same as that entering. This is a special case illustrating the general rule called '*conservation of frequency*'. It is the same thing we saw in the pinball model (2.23), (2.25), and results from the fact that the Hamiltonian is time-independent, so the propagators depend only on time differences. This gives rise to δ-functions similar to the $2\pi\delta(\omega'-\omega)$ in (2.23). Conservation of frequency may be incorporated into the labelling of diagrams in $\mathbf{k},\omega$-space, as shown in (4.62′)

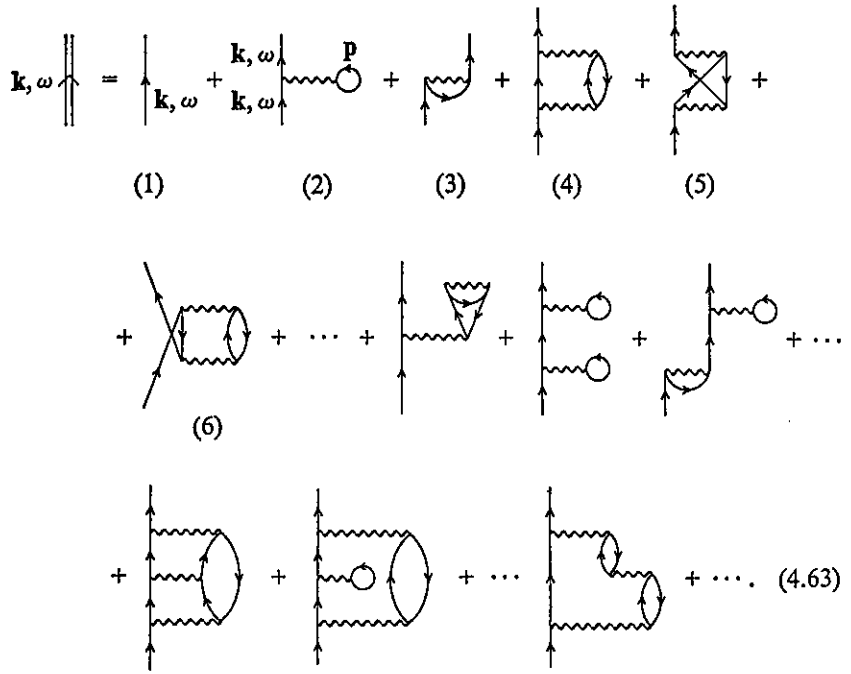


(4.62′)

All momenta and frequencies in this diagram, aside from those entering and leaving, are called 'intermediate'. Thus $\mathbf{q},\mathbf{l}$ and β,ϵ are the intermediate momentum and frequencies. Note that it is convenient to associate a frequency with the wiggly line, even though the interaction itself is independent of ω.

☛ Do not make the mistake of confusing the frequency of a line with the *particle energy*! For example, in the line $\mathbf{k},\omega$ the frequency is ω while the particle energy is $\epsilon_k=k^2/2m$. Also, the frequency is conserved while the particle energy is not.

Now we can collect the information in Table 4.2, equations (4.43, 57, 60) to produce an unabridged dictionary for the interacting many-body fermion system. This is shown in Table 4.3. The whole series for G^+ is then just the sum of all possible diagrams such as (4.47, 54), etc. Chapter 9 will show how to draw all the possibilities systematically, but here we will simply draw a few representative diagrams, written in $(\mathbf{k},\omega)$-space for simplicity:



(4.63)

Such diagrams are often called '*self-energy diagrams*' since they show the particle interacting with the many-body medium, which in turn acts back on the particle, altering its energy (see just after (0.5)). It should be noted that many writers draw these diagrams lying down, thus:

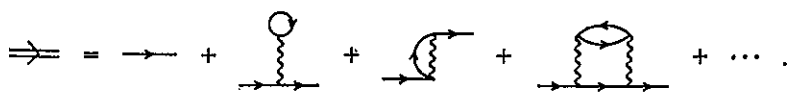


Table 4.3 *Diagram dictionary for interacting many-fermion system with no external potential (Goldstone method)*

$(\mathbf{k}, t)$-space		$(\mathbf{k}, \omega)$-space	
Word	Diagram	Word	Diagram
$iG^{\pm}(\mathbf{k}, t_2-t_1)$ (see (3.2), (4.29))	$\mathbf{k}$ t_2 t_1 + − $\mathbf{k}$ t_1 t_2	$iG^{\pm}(\mathbf{k}, \omega)$	$\mathbf{k}, \omega$ + − $\mathbf{k}, \omega$
$iG_0^{+}(\mathbf{k}, t_2-t_1) = \theta_{t_2-t_1} e^{-i\epsilon_k(t_2-t_1)}$	$\mathbf{k}$ t_2 t_1	$iG_0^{+}(\mathbf{k}, \omega) = \dfrac{i}{\omega-\epsilon_k+i\delta}$	$\mathbf{k}, \omega$
$iG_0^{-}(\mathbf{k}, t_2-t_1) = -\theta_{t_1-t_2} e^{-i\epsilon_k(t_2-t_1)}$	$\mathbf{k}$ t_1 t_2	$iG_0^{-}(\mathbf{k}, \omega) = \dfrac{i}{\omega-\epsilon_k-i\delta}$	$\mathbf{k}, \omega$
Non-propagating: $iG_0(\mathbf{k}, t_2-t_1) = -1, \ \lvert\mathbf{k}\rvert<k_F$ $= 0, \ \lvert\mathbf{k}\rvert>k_F$	$\mathbf{k}$ or $\mathbf{k}$	Non-propagating $iG_0(\mathbf{k}) = -1, \ \lvert\mathbf{k}\rvert<k_F$ $= 0, \ \lvert\mathbf{k}\rvert>k_F$	$\mathbf{k}$ or $\mathbf{k}$
Factor of -1	Each fermion loop. Example:	Factor of -1	Each fermion loop. Example:
$-iV_{klmn}$ or $-iV_q$ (see (4.42), (4.46))	$\mathbf{k}$ $\mathbf{l}$ t $\mathbf{q}$ $\mathbf{m}$ $\mathbf{n}$	$-iV_{klmn}$ or $-iV_q$	$\mathbf{k}$ $\mathbf{l}$ $\mathbf{q}, \epsilon$ $\mathbf{m}$ $\mathbf{n}$
$\sum_k, \int dt$	Each intermediate $\mathbf{k}, t$	$\sum_k, \int \frac{d\omega}{2\pi}$	Each intermediate $\mathbf{k}, \omega$

The diagrams may also be interpreted physically from another point of view. Look at the diagrams in $(\mathbf{k}, t)$-space at a particular time t_0:

At t_0 we see that besides the bare particle, there may exist in the many-body system two 'virtual' particles plus one hole created by second-order process *d*, or two particles and a hole created by second-order sequence *e*, and so on, with the particle plus three particle–hole pairs created during the eighth-order poodle process illustrating a typical higher-order case. That is, the diagrams show all the particles and holes which may be kicked up by the bare particle as it churns through the Fermi sea. Now, since the propagator given by (4.64) describes quasi particles (as will be proved in chapter 11) it follows that the diagrams reveal the content of the cloud of particles and holes surrounding the bare particle and converting it into a quasi particle.

Equation (4.63) may be translated into functions by Table 4.3, giving

$$G^{+}(\mathbf{k}, \omega) = G_0^{+}(\mathbf{k}, \omega) + (-1)\, G_0^{+}(\mathbf{k}, \omega)^2 \sum_{p<k_F} V_{kpkp}(-1) + \\ + G_0^{+}(\mathbf{k}, \omega)^2 \sum_{m<k_F} V_{kmmk}(-1) + \cdots . \tag{4.65}$$

4.6 The 'quasi-physical' nature of Feynman diagrams

In the classical pinball game, each individual diagram in the perturbation expansion of the propagator described a real physical process. Using 'physical intuition' based on the analogy to the classical case, we developed the diagrammatic perturbation expansion for the quantum propagator in a one-particle system (3.32), and in non-interacting and interacting many-particle systems, (4.34) and (4.63). Our intuitive methods are, in fact, similar to those used by Feynman when he first introduced diagrams into quantum electrodynamics (Feynman (1962), p. 167 ff.).

However, by now the reader is doubtless aware that Feynman diagrams describe processes which are considerably less 'real' than those described by the classical pinball diagrams. For example, in the case of a single particle in

an external potential, it was difficult to see how a particle could be scattered several times by a potential, despite the fact that it was in the potential the whole time. Later on, in the non-interacting fermion system, graphs appeared which violated the Pauli exclusion principle. And then, in the interacting case, we met the simple bubbles which seemed to elude any common-sense physical interpretation. Finally, we found that higher-order diagrams involved 'virtual', rather than real, processes.

Nevertheless, the situation is not as bad as it might seem at first sight. For, although the individual diagrams in quantum propagator expansions have unphysical properties, the sum as a whole does not. In fact, the full propagator, G^+, describes an actual physical experiment—for instance, the elastic scattering of a single nucleon by a nucleus in its ground state (Thouless (1961), p. 69). This means that the unphysical aspects arise because of the manner in which we have decomposed the propagator into a perturbation series. This is roughly analogous to breaking a sentence up into words: the individual words, even though they are meaningful, are not thoughts in themselves. It is only when they are put together to form the sentence that a thought emerges.

Because of the unphysical properties of Feynman diagrams, many writers do not give them any physical interpretation at all, but simply regard them as a mnemonic device for writing down any term in the perturbation expansion. However, the diagrams are so vividly 'physical-looking', that it seems a bit extreme to completely reject any sort of physical interpretation whatsoever. As Kaempffer (1965, p. 209) points out, one has to go back in the history of physics to Faraday's 'lines of force' if one wants to find a mnemonic device which matches Feynman's graphs in intuitive appeal. Therefore, we shall here adopt a compromise attitude, i.e., we will 'talk about' the diagrams as if they were physical, but remember that in reality they are only 'apparently physical' or '*quasi-physical*'.

There is still an important question left: the quantum propagator diagrams describe only quasi-physical processes, whereas the classical pinball diagrams describe real physical processes. How, then, can we justify obtaining the quantum series by analogy to the classical case? Evidently, the only satisfactory answer to this question would be to derive the diagram expansion directly from the Schrödinger equation. This was done at the end of chapter 3 in the single-particle case. It can also be done in the many-body case, but unfortunately the argument there is so long and labyrinthine that the average non-specialist tends to get completely lost in it. It is for this reason that we prefer to use the intuitive approach in the body of the text, and have postponed the rigorous derivation to the appendix. However, for those who feel extremely uncomfortable with intuitive arguments, we offer the following alternative:

IMPORTANT

Those readers who wish to see the rigorous derivation of the many-body diagrams before going any further, should leave the direct path through the book, and instead propagate along the following detour:

§4.6→—chapter 7 (second quantization)→—§9.1, 9.2 (mathematical definition of propagator)→—Appendices B through G (derivation of diagrams. Note: skip Appendix C, and all sections referring to 'vacuum amplitude' or 'finite temperature')→—§4.7→—etc.→—

All others should go on from here directly to §4.7.

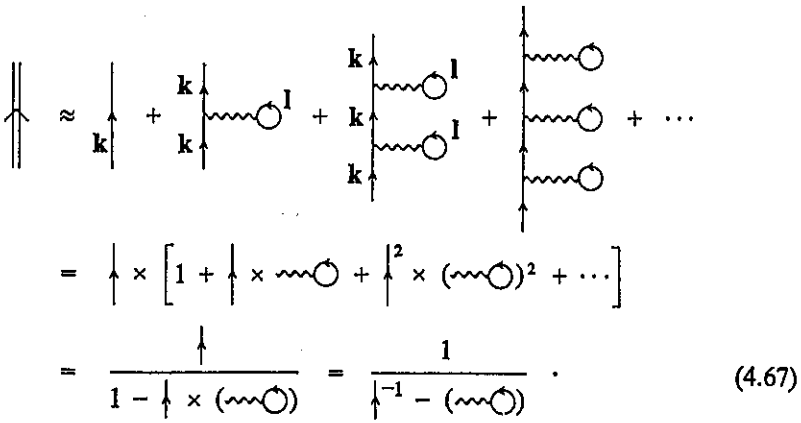
4.7 Hartree and Hartree–Fock quasi particles

We will now consider the simplest of all partial sum approximations for the propagator, i.e., the Hartree and the Hartree–Fock. Imagine we have a hypothetical system with no external potential and with an interaction between particles which is dominated by forward-scattering processes (i.e., both particles emerge from the interaction with the same momentum they had when they entered). We ask for the energy dispersion law of the elementary excitations (quasi particles) in this case. The procedure will be to calculate the propagator approximately by picking out the most important set of diagrams in (4.63) for this system, and sum over this set to infinite order.

Let us first write down the interaction, V_{klmn}, in (4.43, 44). This will be dominated by a large forward-scattering term, so we have

$$V_{klmn} = \delta_{mk}\delta_{nl}\underbrace{V_{klkl}}_{large} + \underbrace{W_{klmn}}_{small}(\mathbf{m} \neq \mathbf{k}, \mathbf{n} \neq \mathbf{l}) \tag{4.66}$$

Thus the most important interaction diagrams are the forward-scattering ones shown in (4.48 (1), ..., (4)). The diagrams which will dominate the series (4.63) will therefore be just those in which every interaction is of the forward-scattering type. A few trials reveal that the only diagrams of this sort are



(4.67)

those containing just bubbles, so that the propagator may be approximated by a partial summation over repeated bubbles (see (4.67)).

Using Table 4.3 and substituting for the propagators, this becomes

$$iG^+(\mathbf{k},\omega) = \frac{1}{[iG_0^+(\mathbf{k},\omega)]^{-1} - (-1)\sum\limits_{l<k_F}(-iV_{klkl})(-1)} \tag{4.68}$$

or

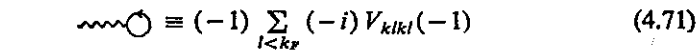
$$G^+(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_k - \sum\limits_{l<k_F} V_{klkl} + i\delta}. \tag{4.69}$$

Comparing with (3.16) reveals that we have here a live many-body quasi particle with energy dispersion law and lifetime:

$$\epsilon_k' = \epsilon_k + \sum_{l<k_F} V_{klkl}; \quad \tau_k = 1/\delta = \infty. \tag{4.70}$$

The quantity $\sum\limits_{l<k_F} V_{klkl}$ is the 'self-energy' of the particle as described just after (0.5). If spin is included (see after (4.58)) there is a factor 2 multiplying V_{klkl}.

This result has a simple physical meaning. First we note that (4.67) has exactly the same form as the diagram series (3.33) for a single particle moving through an external potential, with



(4.71)

playing the same role as

(4.72)

Thus, (4.71) can be interpreted as a transition probability for $\phi_k \to \phi_k$ scattering caused by an 'effective external potential', v_{eff}. We can find v_{eff} by writing out (4.71) in detail, using (4.42):

$$\sum_{l<k_F} V_{klkl} = \int d^3\mathbf{r}\,\phi_k^*(\mathbf{r})\underbrace{\left\{\sum_{l<k_F}\int |\phi_l(\mathbf{r}')|^2 V(\mathbf{r}-\mathbf{r}')\,d^3\mathbf{r}'\right\}}_{v_{\text{eff}}}\phi_k(\mathbf{r}). \tag{4.73}$$

Comparing with (4.33) shows that the quantity in brackets is just v_{eff}. Since $|\phi_l(\mathbf{r}')|^2$ is the density at point $\mathbf{r}'$ of a particle in ϕ_l, v_{eff} is evidently the average potential at point $\mathbf{r}$ due to all the particles in the Fermi sea. (In the present case, since the ϕ_l are plane waves, v_{eff} is independent of $\mathbf{r}$.)

We now recall that for the quantum pinball propagator, the quasi particle energy (3.38) could be obtained both by the diagram method and directly

from the Schrödinger equation using Hamiltonian (3.20). In the present case, it's easy to write a Schrödinger equation with energy eigenvalues ϵ_k' by just using v_{eff} as external potential:

$$\left[\frac{p^2}{2m} + v_{\text{eff}}(\mathbf{r})\right]\phi_k(\mathbf{r}) = \epsilon_k'\phi_k(\mathbf{r}). \tag{4.74}$$

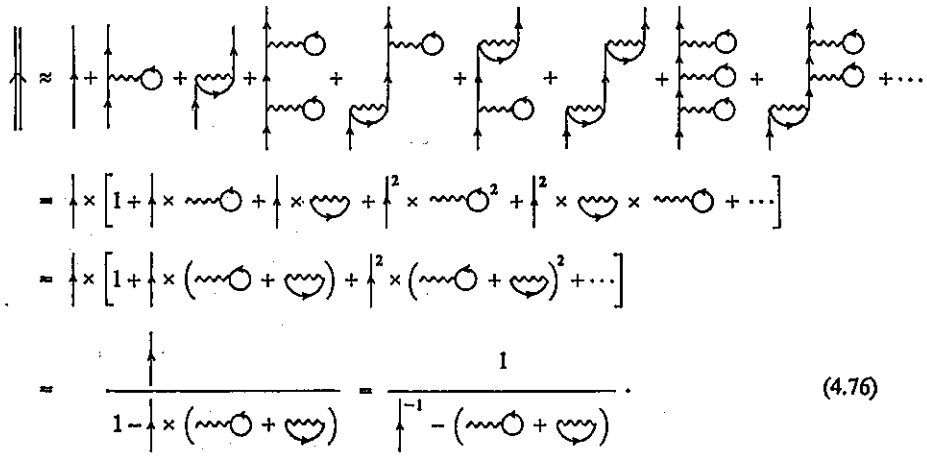
It is easily checked that this is correct by multiplying both sides by $\phi_k^*(\mathbf{r})$ and integrating—the result is just (4.70).

In our intuitive argument for (4.74), the ϕ_k were given (plane waves). However, if we regard them as eigenfunctions to be solved for, then (4.74) is just the famous Hartree equation. Remember that by (4.73), v_{eff} is a function of all the ϕ_k's. This means that we must calculate ϕ_k *self-consistently*, i.e., put an assumed ϕ_k in v_{eff}, find a new ϕ_k from (4.74), put the new ϕ_k in v_{eff}, calculate a newer ϕ_k, etc., until ϕ_k stops changing appreciably. In the present case with no external potential, we find immediately that the correct ϕ_k is just a plane wave. However, in a system with an external potential, like an atom, or a molecule the whole self-consistent procedure must be carried out. In such cases, the ϕ_k may correspond to atomic or molecular orbitals, and V may be interpreted as scattering between orbitals. (See §11.1 for further discussion.)

From here, it is only a baby step away to the quasi particle in Hartree–Fock (HF) approximation. Imagine that exchange scattering is just as important as forward scattering in our hypothetical system, i.e., that

$$V_{klmn} = \delta_{mk}\delta_{nl}V_{klkl} + \delta_{ml}\delta_{nk}V_{kllk} + \text{small terms}. \tag{4.75}$$

Then the open oysters must also be included in the approximation for the propagator, and the partial sum carried out as in (3.39):



(4.76)

Translating by means of dictionary Table 4.3 yields

$$G^+(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_k - \sum_{l<k_F}(V_{klkl} - V_{lkkl}) + i\delta}. \tag{4.77}$$

(If spin is included, multiply V_{klkl} by 2.) This also has quasi particle form with

$$\epsilon_k' = \epsilon_k + \sum_{l<k_F}(V_{klkl} - V_{lkkl})$$
$$\tau_k = \infty. \tag{4.78}$$

This is the quasi particle energy and lifetime in HF approximation. The V_{lkkl} is the well-known 'exchange term'. Analogous to what was done in the Hartree case, we can here construct a Schrödinger equation including the effective external 'exchange' potential; this turns out to be the Hartree–Fock equation. (Note that plane waves are the self-consistent solution of the HF equation in the present case with no real external potential, just as with the Hartree equation (4.74).) It should be mentioned that the lifetime here is infinite because of the crudeness of the HF approximation. Better approximations, which include sums over diagrams like (4.47), produce finite lifetimes.

4.8 Hartree–Fock quasi particles in nuclear matter

Real-life physical systems have interactions considerably more complicated than the hypothetical 'forward plus exchange scattering' model in the previous section. Nevertheless, the HF can be used as a very crude 'first approximation' to the propagator, as we show now for the case of nuclear matter.

Nuclear matter is *not* matter in a nucleus! It is a *hypothetical* stuff concocted in the following way (see Thouless (1961), p. 20, for details): On the basis of the 'liquid drop' model of the nucleus, Weizsäcker constructed the famous 'semi-empirical mass formula' for nuclear binding energy:

$$E(N,Z) = \underbrace{-a_1 A}_{\substack{\text{nuclear}\\ \text{forces}}} + \underbrace{a_2 A^{\frac{2}{3}}}_{\substack{\text{surface}\\ \text{correction}}} + \underbrace{a_3 Z^2 A^{-\frac{1}{3}}}_{\substack{\text{Coulomb}\\ \text{forces}}} + \underbrace{\tfrac{1}{4}a_4(N-Z)^2/A}_{\substack{\text{Pauli principle}\\ \text{correction}}} \tag{4.79}$$

where N and Z = number of neutrons and protons respectively, $A = N+Z$ and the a_i's are constants determined by fitting (4.79) to known nuclear masses. In the first term, $-a_1$ is the binding energy of a single nucleon, well inside the nucleus (i.e., not near the surface), due to the attractive nuclear forces—it is about $-15{\cdot}9$ MeV. The second, third and fourth terms are respectively corrections due to the presence of the nuclear surface, Coulomb forces between protons, and the effect of the exclusion principle.

If there were no Coulomb forces, and if the number of nucleons was so large that the nucleus was the size of, say, a coconut (making the surface term negligible in comparison with the first term) and if $N=Z$, then we would have a simple system with binding energy proportional to the number of nucleons, A. This hypothetical system consisting of a huge number of protons and an equal number of neutrons interacting by purely nuclear forces (no Coulomb forces) is called *nuclear matter*. It is of great interest because a calculation of the binding energy of nuclear matter, using some model of the nuclear force, is evidently a calculation of $-a_1$, and can be compared with the experimental value of $-15{\cdot}9$ MeV.

We will assume that the nuclear interaction has the form of a simple Yukawa potential ($V_0 < 0$)

$$V = +aV_0 \frac{e^{-|\mathbf{r}-\mathbf{r}'|/a}}{|\mathbf{r}-\mathbf{r}'|}. \tag{4.80}$$

(Such a purely attractive interaction is clearly science-fiction, since it would cause the nuclear matter to collapse to a point. This can be prevented by adding a 'hard core' to the potential, as described in §12.4.) The quantity a ($\sim 10^{-13}$ cm) is called the 'range' of the interaction, since the exponential becomes very small for $|\mathbf{r}-\mathbf{r}'| > a$.

The quasi particle energy in HF approximation may be calculated using (4.78, 80) (Brown (1972)). Noting that the density of points in $\mathbf{k}$-space is $\Omega/(2\pi)^3$, where Ω is the normalization volume, (see after (3.64)), we may convert from a sum to an integral using

$$\sum_l \to \Omega \int \frac{d^3\mathbf{l}}{(2\pi)^3} \tag{4.81}$$

so that (multiply V_{klkl} by 2 if spin is included)

$$\epsilon_k' = \frac{k^2}{2m} + \Omega \int_{|\mathbf{l}|<k_F} \frac{d^3\mathbf{l}}{(2\pi)^3}(V_{klkl} - V_{lkkl}). \tag{4.82}$$

The transition matrix element V_{klmn} is (using (3.5), (4.42, 45, 80))

$$V_{klmn} = +\frac{V_0}{\Omega^2}\int\int d^3\mathbf{r}\, d^3\mathbf{r}'\, e^{-i(\mathbf{k}\cdot\mathbf{r}+\mathbf{l}\cdot\mathbf{r}'-\mathbf{m}\cdot\mathbf{r}-\mathbf{n}\cdot\mathbf{r}')}\frac{e^{-|\mathbf{r}-\mathbf{r}'|/a}}{|\mathbf{r}-\mathbf{r}'|/a}$$
$$= \frac{1}{\Omega}\frac{4\pi V_0 a^3 \delta_{k+l,\,m+n}}{[1+(\mathbf{k}-\mathbf{m})^2 a^2]} = \frac{1}{\Omega}\frac{4\pi V_0 a^3 \delta_{k+l,\,m+n}}{[1+(k^2+m^2-2km\cos\theta)a^2]} \tag{4.83}$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{m}$ and we have used that $\Omega \gg a^3$. Hence

$$V_{klkl} = +\frac{4\pi V_0 a^3}{\Omega}, \quad V_{lkkl} = +\frac{1}{\Omega}\frac{4\pi V_0 a^3}{[1+(l^2+k^2-2kl\cos\theta)a^2]}. \tag{4.84}$$

Substituting these expressions in (4.82), we find that the V_{klkl} integral is trivial and yields $2V_0a^3k_F^3/3\pi$. The V_{lkkl} integral is first integrated over ϕ and θ, which yields terms involving $(k+l)a$ and $(k-l)a$. The remaining l-integration is easily carried out with the aid of the substitutions $y=(k+l)a$, and $z=(k-l)a$, and we obtain for the quasi particle energy

$$\epsilon_k' = \frac{k^2}{2m} + \frac{2V_0a^3k_F^3}{3\pi} - \frac{V_0}{2\pi}[F(ka+k_Fa)-F(ka-k_Fa)], \tag{4.85}$$

where

$$F(z) = \frac{1}{2ka}[1+z^2][\ln(1+z^2)-1] - [z\ln(1+z^2)-2z+2\tan^{-1}z] \tag{4.86}$$

This expression can be evaluated to find the effective mass in the limit when ka and k_Fa are both $\ll 1$, so that $z \ll 1$. In order to get a non-vanishing contribution from $[F(ka+k_Fa)-F(ka-k_Fa)]$, it is necessary to expand the logarithm and $\tan^{-1}$ functions up through order z^6. Keeping only terms up through order k^2 we find:

$$\epsilon_k' \approx \frac{2V_0a^5k_F^5}{5\pi} + \left[\frac{1}{2m} + \frac{2V_0a^5k_F^3}{3\pi}\right]k^2, \tag{4.87}$$

from which we see that the effective mass is

$$m^* = \frac{m}{1+\dfrac{4mV_0a^5k_F^3}{3\pi}}. \tag{4.88}$$

4.9 Quasi particles in the electron gas, and the random phase approximation

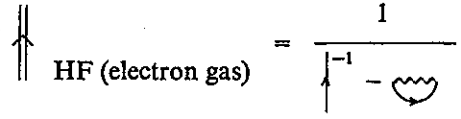
A real metal consists of $\sim 10^{23}$ positively charged ions arranged in the form of a regular lattice, with $\sim 10^{23}$ electrons moving more or less freely among these ions. The ions execute oscillations about their equilibrium positions ('lattice vibrations'). Such a complicated system poses a nasty problem for the many-body physicist. To make life easier, he often postulates a utopian metal in which the ions are motionless, and the positive ion charge is smeared out to form a fixed uniform positive background against which the electrons move. The electrons are assumed to interact by purely Coulomb forces. This theoretician's pipe dream is called the 'electron gas'. (See Fig. 0.7).

Let us first examine the electron gas in the HF approximation. The Coulomb interaction and its transition matrix element are just the Yukawa interaction (4.80) (with $V_0>0$) and its matrix element (4.83) with $V_0a=e^2$, $a\to\infty$, i.e.:

$$\text{(a) } V(\mathbf{r},\mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}, \qquad \text{(b) } V_{klmn} = \frac{4\pi e^2}{|\mathbf{k}-\mathbf{m}|^2}, \tag{4.89}$$

where spins are left out for simplicity, and we take $\Omega=1$ cm^3. That is, the Coulomb interaction has the form of a Yukawa interaction with 'infinite range'. Alternatively, one often says that the Yukawa potential has the form of a 'shielded' Coulomb potential, the $\exp(-r/a)$ in (4.80) being the 'shielding factor'. Note also that (4.89) becomes infinite for $\mathbf{k}=\mathbf{m}$ whereas (4.83) remains finite.

The quasi particle energy may be evaluated in exactly the same way as for the nuclear matter case. There is a slight simplification because of the fact that the bubble term in (4.76) is cancelled by the positive charge background (see §10.4), so that



(4.90)

The expression for the quasi particle energy turns out to be (take limit of (4.85), (4.86) when $V_0a=e^2$ and $a\to\infty$):

$$\epsilon_k' = \frac{k^2}{2m} - \frac{e^2k_F}{2\pi}\left[2+\frac{(k_F^2-k^2)}{kk_F}\ln\left|\frac{k+k_F}{k-k_F}\right|\right]. \tag{4.91}$$

We are mainly interested in quasi particles near k_F, since it is primarily these which take part in physical processes. For $|\mathbf{k}|$ near k_F, the effective mass may be found by expanding ϵ_k' about k_F:

$$\epsilon_k' = \epsilon_{k_F}' + \left(\frac{\partial\epsilon_k'}{\partial k}\right)_{k_F}(k-k_F)+\cdots, \tag{4.92}$$

where $k=|\mathbf{k}|$.

For the non-interacting system

$$\epsilon_k = \frac{k_F^2}{2m} + \frac{k_F}{m}(k-k_F)+\cdots. \tag{4.93}$$

Comparing (4.92) and (4.93), we may regard the effective mass as given by

$$\frac{k_F}{m^*} = \left(\frac{\partial\epsilon_k'}{\partial k}\right)_{k_F} \quad \text{or} \quad m^* = k_F\Big/\left(\frac{\partial\epsilon_k'}{\partial k}\right)_{k_F}. \tag{4.94}$$

For ϵ_k' as in (4.91) we obtain

$$m^*_{\text{HF (electron gas)}} = 0! \tag{4.95}$$

This is of course an absurd result, and it disagrees with experiments, all of which show m^* to be of the same order of magnitude as m.

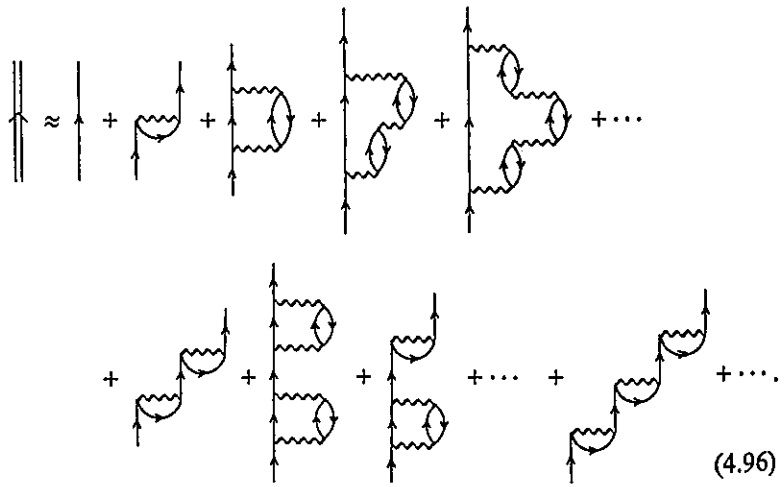
The reason why the Coulomb interaction produces zero effective mass at the Fermi surface, whereas the Yukawa interaction does not, can be traced back to the fact that the Coulomb interaction is infinite for zero momentum transfer, as was pointed out after (4.89). The HF approximation is not adequate to handle such singular interactions.

The physical reason for the inadequacy of HF lies in the fact that it treats the effect of all the other particles on the test particle by means of a time-independent average potential. But we know from §0.2 that the quasi particle is a bare particle plus a cloud which in a sense 'follows' the bare particle. The HF approximation thus gives us what might be called the 'static' part of this cloud, but misses out on the 'moving' part.

The usual way of putting this is to say that the HF neglects 'correlations', which means that it neglects that movement of the other particles which 'is correlated with' (i.e., 'follows') the movement of the bare particle. As mentioned in §0.2, we would expect that these correlations would have the effect of 'shielding' the interaction between particles, making it much weaker. The diagram method which we discuss now (very briefly) gives us the way to calculate this shielding effect. (It should be observed that although we consider only the electron gas here, this is the same sort of problem one has to deal with when trying to improve on HF calculations of atoms and molecules.)

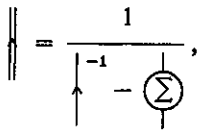
How is it possible to take account of correlations diagrammatically? Evidently the correlation effects must lie in those diagrams which were omitted in the HF approximation. Of course it is impossible to take account of all the omitted diagrams, but we can at least sum over the most important ones.

It turns out (as will be shown in §10.4) that in the limit of a high density electron gas, the most important diagrams are those occurring in the following approximation for G:



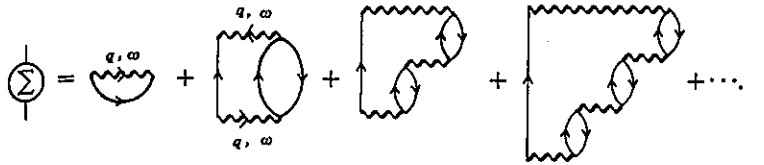
(4.96)

These diagrams may be summed to infinity and it is found that (see chapter 10)



(4.97)

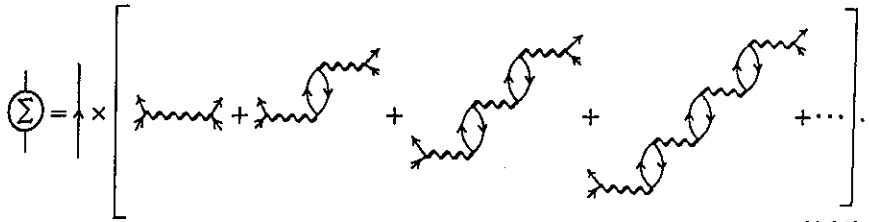
where $\sum$ (the self energy) is given by



(4.98)

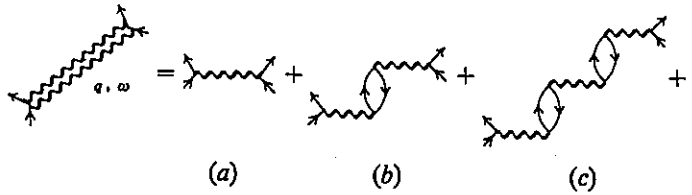
The diagrams in (4.98) are called 'ring' diagrams because of their ring-like structure. For historical reasons, this approximation for G is called the 'Random Phase Approximation' or 'RPA'.

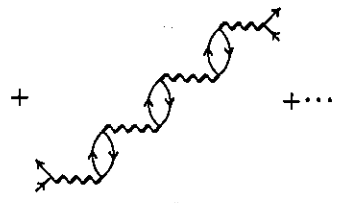
In order to interpret (4.98), we twist the top interaction wiggle in each diagram through 180° (this has no effect on the value—see (4.61)), and factor out a free propagator:



(4.99)

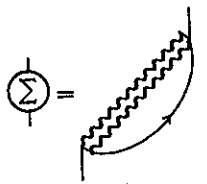
The series in brackets





(4.100)

is called the 'effective interaction'. The reason for this is as follows: Diagram (*a*) shows the direct or 'bare' interaction between two particles. Diagram (*b*) shows the first particle creating a particle–hole pair in the system, and the second particle interacting with this pair. There is thus an indirect or 'effective' interaction between two particles via the many-body system. The higher order diagrams describe interactions which are more and more indirect. We may thus write $\sum$ in terms of the effective interaction:



(4.101)

which shows an electron interacting with itself via the effective interaction.

We may obtain further insight into the nature of the effective interaction by carrying out the sum (4.99). In the limit when $\omega=0$ and q is small, this yields (see chapter 10):

$$V_{\text{eff}}(q)=\frac{4\pi e^2}{q^2+\lambda^2} \tag{4.102}$$

This has the same form as (4.83), so that, assuming it is true for all q, it must correspond to an effective interaction having the same **r**-dependence as the Yukawa potential in (4.80):

$$V_{\text{eff}}(\mathbf{r}) = 4\pi e^2 \frac{e^{-\lambda r}}{r}. \tag{4.103}$$

In contrast to the Coulomb interaction, which is 'long range', dropping off as $1/r$, this drops off exponentially for $r \gg \lambda^{-1}$ so it has only a short range $\sim\lambda^{-1}$ cm. It is referred to as a 'shielded' or 'screened' interaction.

Such a screened interaction is just what we would expect physically on the basis of the argument in §0.2. The real electron repels other electrons from it; this exposes the positive charge background so that the electron is effectively 'followed' by a positive charge cloud of width λ^{-1}. This turns it into a quasi electron because the positive cloud 'screens' the electron's own charge, thus drastically reducing its interaction with the other particles of the system at distances greater than λ^{-1}.

Since (4.101) with V_{eff} as in (4.102) has the same form as the HF self-energy in (4.90), the quasi particle energy is easily calculated by placing $V_{\text{eff}}(\mathbf{k}-\mathbf{l})$ into (4.82), with the V_{klkl} term equal to zero:

$$\epsilon_k' = \frac{k^2}{2m} - \int_{|\mathbf{l}|<k_F} \frac{d^3\mathbf{l}}{(2\pi)^3} \frac{4\pi e^2}{[(\mathbf{k}-\mathbf{l})^2+\lambda^2]}. \tag{4.104}$$

The calculation of the effective mass then goes just as for the Yukawa potential. In the simple case of large λ (i.e., $k_F\lambda^{-1}\ll 1$, a condition which is not actually satisfied in the electron gas), it is found that parallel to (4.88),

$$m^* = \frac{m}{1+\frac{16}{3}\frac{m\pi e^2}{\lambda^5}k_F^3} \tag{4.105}$$

which is evidently finite. Thus the inclusion of the correlation (screening) effects represented by the ring diagrams has produced a physically reasonable result. (The result for m^* in RPA when $\omega\neq 0$ and **q** is not small appears in §10.4.)

Exercises

4.1 In a system of free particles, a hole is created in the single-particle state $\phi_k(\mathbf{r})=\Omega^{-1/2}e^{i\mathbf{k}\cdot\mathbf{r}}$. What is the momentum of the hole?

4.2 For the five-particle system in Fig. 4.1:

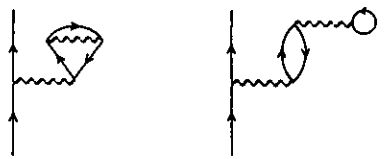
(*a*) Evaluate $c_3^\dagger c_5^\dagger c_4 c_6^\dagger c_3|11111000\ldots\rangle$.

(*b*) Write $|1101100100\ldots\rangle$ in particle–hole notation.

(*c*) Find $\sum_k \epsilon_k c_k^\dagger c_k|1111100\ldots\rangle$.

4.3 Suppose we have a non-interacting system with external perturbing potential such that V_{km}, V_{mk}, V_{kl}, V_{lk} ($m<k_F$, $l>k_F$, $k>k_F$) are large, and all other V's are small. Find $G^+(k_1=k, k_2=k, \omega)$.

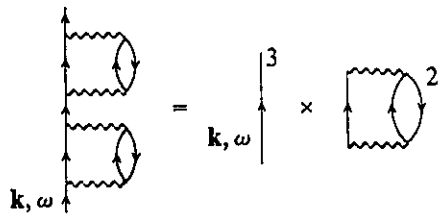
4.4 Show that for a system of fermions with a momentum-conserving interaction, the following diagrams are not allowed:



4.5 Consider diagram 5 on the right-hand side of (4.63).
(*a*) Label it, showing momentum conservation explicitly in the labelling.
(*b*) Show that the scattering processes at each interaction are virtual.

4.6 Translate (4.62′) into functions. What variables does it depend on?

4.7 Show that:



4.8 Suppose we have a hypothetical system in which the most important scattering processes are the forward and exchange scattering of (4.58), (4.62) and the double scattering in (4.62'). Find an approximate expression for the propagator by partial summation. Do not attempt to evaluate the integrals!

4.9 Verify in detail equations (4.83) through (4.88).

4.10 Verify (4.91).

4.11 We have a system of N non-interacting Fermi particles. (*a*) They are acted upon by an external perturbing potential such that $V_{kl}=A$ for all k, l. Find the propagator $G^+(\mathbf{q}, \mathbf{p}, \omega)$, $p>k_F$, $q>k_F$, by summing exactly over all diagrams. (*b*) Generalize your result to the case where V_{kl} has the form: $V_{kl}=Af_kf_l$ (factorizable potential).

Chapter 5

Ground State Energy and the Vacuum Amplitude or 'No-particle Propagator'

5.1 Meaning of the vacuum amplitude

One of the first many-body problems to be tackled by the field theoretical diagram techniques was that of finding the ground state energy, E_0, of a system of interacting fermions. This quantity is directly related to experimentally measured properties—such as for example the cohesive energy in a metal or the binding energy in nuclear matter. Calculating it theoretically is a tough job. The interactions are large and hard to handle, and naïve approaches simply drown one in a deluge of infinities. Thus in the nuclear case, because of the hard core interaction, one gets $V_{klmn}=\infty$ making the interaction Hamiltonian infinite. The electron gas is equally psychotic, yielding ∞ for every order of perturbation theory higher than first.

The diagrammatic methods to be discussed in this chapter provide a neat way of handling such delinquents as the above nuclear and electron interactions. In both cases, we can perform a partial sum over an infinite series of infinite terms and get a finite result! In order to do this, it is necessary to have a general way of writing down the nth-order term in the ordinary perturbation series for E_0, i.e., in

$$E_0 = W_0+\langle\Phi_0|H_1|\Phi_0\rangle+\sum_{m\neq 0}\frac{\langle\Phi_0|H_1|\Phi_m\rangle\langle\Phi_m|H_1|\Phi_0\rangle}{W_0-W_m}+\cdots \qquad (5.1)$$

where W_0, W_m are the ground and excited state energies of the unperturbed Hamiltonian, and Φ_0, Φ_m are the corresponding wave functions. The general term is hard to obtain from the time-independent theory usually used to get (5.1). However, there is a time-dependent technique which gives a pictorial recipe for finding the desired nth-order term; this is the method of the vacuum amplitude expansion.

The *vacuum amplitude*, $R(t)$, is defined as follows: Let Φ_0 be the ground state of the unperturbed system as defined in (4.12) (i.e., Φ_0 is the 'Fermi vacuum'). Then $R(t)$ is the probability amplitude that if the system is in Φ_0 at time 0, and the external potential and/or interactions between particles are allowed to act, then the system will be in Φ_0 at time t. That is, $R(t)$ is the 'Fermi vacuum to Fermi vacuum transition amplitude'.