Notes on Feynman Diagrams in Many-body Problems

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Contents

看山不是山，看水不是水。

1 General Introduction to Feynman Diagram in Many-body Problem

1.1 A Brief Intro to Quasi-particle

Quasi particles arise from the fact that when a real particle moves through the system, it pushes or pulls on its neighbours and thus becomes surrounded by a **'cloud' of agitated particles**.

The particle cloud "shields" or "screens" the real particles so that quasi particles interact only weakly with one another. The presence of the cloud also makes the properties of the quasi particle different from that of the real particle-it may have an "**effective mass**" different from the real mass, and a "**lifetime**". These properties of quasi particles are directly observable experimentally. It should be remarked that the quasi particle is in an excited energy level of the many-body system. Hence it is referred to as an '**elementary excitation**' of the system. We now consider some examples of quasi particles.

1. Quasi ion in a classical liquid

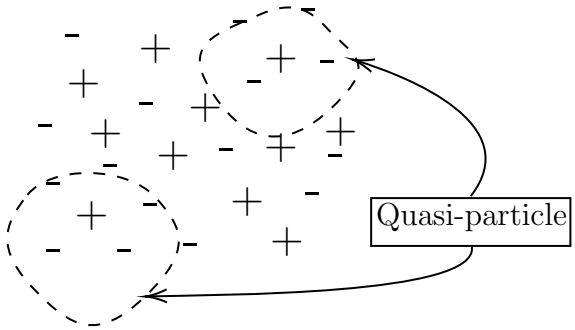


Figure 1.1: Quasi particles in a Liquid of Positive and Negative Ions

From Fig.1.1, we know, from more powerful terminology of QFT:

"bare" particle + "clothing"/"cloud" = "dressed"/"renormalized" particle

For example, in quantum electrodynamics a 'bare' electron interacting with a field of photons acquires a cloud of virtual photons around it, converting it into the 'dressed' electron. In a similar manner, the interaction between real particles is called the 'bare' interaction, while the weak interaction between quasi particles is referred to as the 'effective' or "dressed" or "renormalized" interaction. It should be noted that each bare particle is simultaneously the 'core' of a quasi particle and a transient 'member' of the cloud of several other quasi particles.

The free quasi particles have a new energy law as

$$\epsilon' = \frac{p^2}{2m^*} \quad \text{instead of} \quad \epsilon = \frac{p^2}{2m}$$

where m^* is the effective mass. The difference

$$\epsilon_{quasi} - \epsilon_{bare} = \epsilon_{self}$$

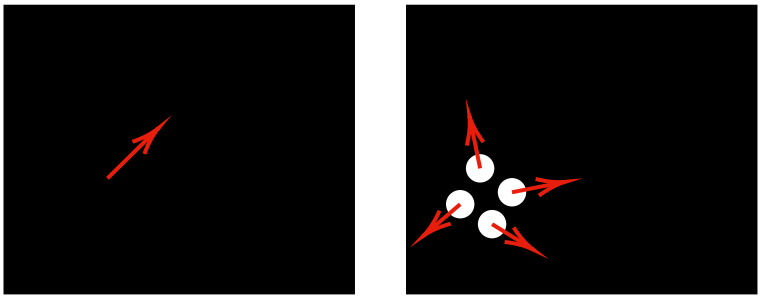
is called **"self-energy"** of the quasi particle.

2. Quantum System: quasi electreon in electron gas

The ' electron gas' is a simple model often used to describe many-body effects in metals. It consists of a box containing a large number of electrons interacting by means of the Coulomb force. In addition, there is a uniform, fixed, positive charge 'background' put into the box in order to keep the whole system electrically neutral. In the ground state, the electrons are spread out uniformly in the box.

Suppose now that we have a single, well-localized electron which we shoot into the electron gas Because of the repulsive Coulomb interaction between electrons, this extra electron repels other electrons away from it, so we get an empty space near the extra electron, and repelled electrons further away(Fig.1.2). This empty region may be viewed in a more detailed or microscopic way as composed of 'holes' in the electron gas. That is, the extra electron has

"lifted out" electrons from the uniform charge distribution in its vicinity, thus creating 'holes' in this charge distribution, and has 'put down' these lifted-out electrons further away.



(a)"Empty" region near the electron (b)Lifted-out electrons create "holes"

Figure 1.2: Extra Electron Pushes Other Electrons Away

3. Bogoliubov quasi particles ("bogolons")

These are the elementary excitations in a superconductor. We include them here since they are called quasi particles, but actually their structure is quite different from the 'particle plus cloud' picture described above. They consist of a linear combination ofan electron in state $(+k, \uparrow)$ and a hole $'$ in $(-k, \downarrow)$.

1.2 A Brief Intro to Collective Excitations

As we have seen, the quasi particle consists of the original real, individual particle, plus a cloud of disturbed neighbours. It behaves very much like an individual particle, except that it has an effective mass and a lifetime. But there also exist other kinds of fictitious particles in many-body systems, i.e., 'collective excitations'. These do not centre around individual particles, but instead involve collective, wavelike motion of all the particles in the system simultaneously. Here are some examples:

1. Plasmons

If a thin metal foil is bombarded with high energy electrons, it is possible to set up sinusoidal oscillations in the density of the electron gas in the foil. This is known as a 'plasma wave', and it has a frequency ω_p and wavelength λ_p. The plasma wave may be visualized as built up of 'holes' in the low-density regions and extra electrons in the high-density regions. Just as light waves are quantized into units having energy $E = \hbar\omega$ called photons, plasma waves are quantized into units with energy $E_p = \hbar\omega_p$ called plasmons.

2. phonons

Sound waves are sinusoidal oscillations in the crystal lattice ofa solid. They are quantized into collective excitations called 'phonons'.

3. Magnons

In ferromagnets there are regular fluctuations in the density of spin angular momentum known as spin waves. The collective excitation here is the spin wave quantum known as the 'magnon".

1.3 Propagators-the Keys to the Many-body Problem

The idea behind the propagator method is this: the detailed description of a many-body system requires in the classical case the position of each particle as a function of time, or in the quantum case, the time dependent wave function of the whole system. Fortunately, it turns out that **in order to find the important physical properties of a system it is not necessary to know the detailed behaviour of each particle in the system, but rather just the average behaviour of one or two typical particles.** The quantities which describe this average behaviour are the *one-particle propagator* and *two-particle propagator* respectively, and physical properties may be calculated directly from them.

One-particle propagator: we put a particle into the interacting system at point r_1 at time t_1 and let it move through the system colliding with the other particles for a while (i.e., let it "propagate" through the system). Then the one-particle propagator is the probability (or in quantum systems, the probability amplitude) that the particle will be observed at the point r_2 at time t_2. (Note that instead of putting the particle in at a definite point, it is sometimes more convenient to put it in with definite momentum, say p_1, and observe it later with momentum p_2.) The single-particle propagator yields directly the energies and lifetimes of quasi particles. It also gives the momentum distribution, spin and particle density and can be used to calculate the ground state energy.

Two-particle propagator: the probability amplitude for observing one particle at r_2, t_2 and another at r_4, t_4 if one was put into the system at r_1, t_1 and another at r_3, t_3. This also has a wide variety of talents, giving directly the energies and lifetimes of collective excitations, as well as the magnetic susceptibility, electrical conductivity, and a host of other non-cquilibrium properties.

1.4 Calculate Propagator:the drunk man example

With the aid of Feynman diagrams, we expand the propagator in an infinite series and evaluate the series approximately. This can be carried out in a general, systematic, and picturesque way.

Just to get an idea of what these diagrams are, consider the following simple example. A man who has had too much to drink, leaves a party at point 1 and on the way to his home at point 2, he can stop off at one or more bars-Alice's Bar (A), Bardot Bar (B), Club Six Bar (C), ... , etc. He can wind up either at his own home 2, or at any one of his friends' apartments, 3, 4, etc. We ask for the probability, P(2, I), that he gets home. This

probability, which is just the propagator here (with time omitted for simplicity), is the sum of the probabilities for all the different ways he can propagate from I to 2 interacting with the various bars.

The first way he can prophgate is ' freely' from 1 to 2, i.e., without stopping at a bar. Call the probability for this free propagation $P_0(2,1)$

The second way he can propagate is to go freely from 1 to bar A (the probability for this is $P_0(A,1)$), then stop off at bar A for a drink (call the probability for this $P(A)$), then go freely from A to 2 (probability $= P_0(2,A)$). Assume for simplicity that the three processes here are independent. Then the total probability for this second way is the product of the probabilities for each process taken separately, i.e., $P_0(A,1) \times P(A) \times P_0(2,A)$. (This is like the case in coin-tossing: since each toss is independent, the probability of first tossing a head, then a tail, equals the probability of tossing a head times the probability of tossing a tail.)

The third way he can propagate is from 1 to B to 2, with probability $P_0(B,1)P(B)P_0(2,B)$. Or he could go from 1 to C to 2, etc., or from 1 to A to B to 2, or from 1 to A, come out of A, go back into A, then go to 2, and so on. The total probability, $P(2,1)$ is then given by the sum of the probabilities for each way, i.e., the infinite series:

$$\begin{aligned} P(2,1) =& P_0(2,1) + P_0(A,1)P(A)P_0(2,A) + P_0(B,1)P(B)P_0(2,B) + \cdots \\ &+ P_0(A,1)P(A)P_0(B,A)P(B)P_0(2,B) + \cdots \end{aligned}$$

This is an example of a 'perturbation series', since each interaction with a bar "perturbs" the free propagation of the drunken man. Represent this series using the following dictionary:

Word	Picture	Meaning
$P(2,1)$		probability of propagation from 1 to 2
$P_0(s,r)$		probability of free propagation from r to s
$P(X)$		probability of stopping of at bar X for a drink

Figure 1.3: Diagram dictionary for drunken man

The perturbation series in diagrams for this drunken man propagator is therefore

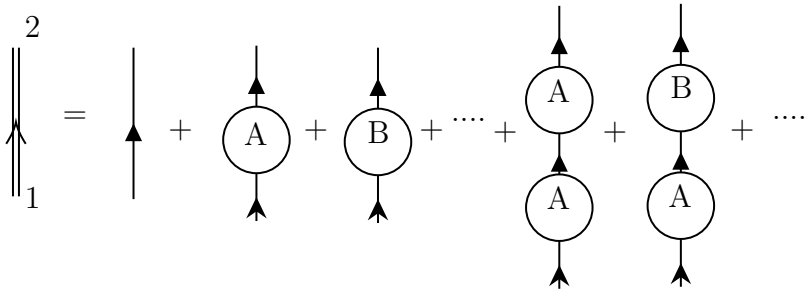


Figure 1.4: Drunken man series

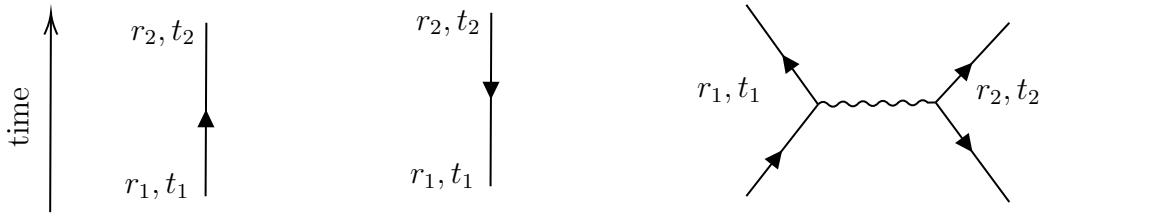
1.5 Single-particle propagator for system of many interacting particles

We now describe a second-order propagation process as following:

- At time t_1, extra particle enters system
- At time t, extra particle interacts with a particle (through virtual photon) in the system, lifting it out of its place, creating a "hole" in the system
- The extra particle, plus the "hole" and the "lifted-out" particle(particle-hole pair) travel through the system

- At time t', the extra particle interacts with "lifted-out" particle, knocking it back into the hole, thus destroying the particle-hole pair.
- At time t_2, the extra particle moves out of the system.

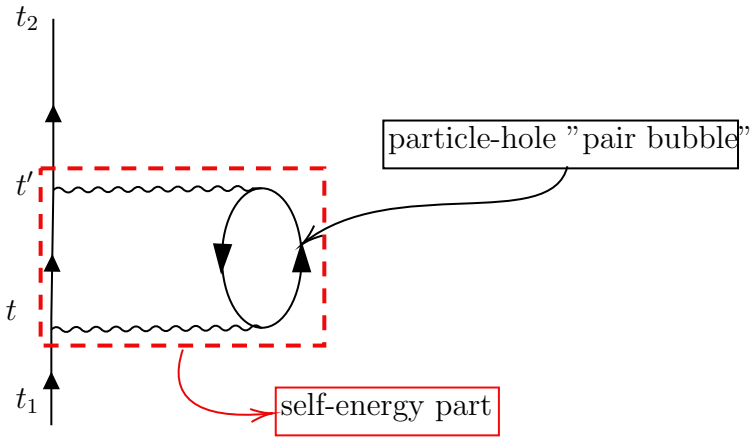
We use the following diagram elements here.Note that the hole is drawn as a particle moving backward in time.



propagator for particle propagator for hole probability amplitude for a particle interacting with another particle

Figure 1.5: Diagram elements for second-order propagation

Then the probability amplitude for the above sequence of events can be represented by the diagram

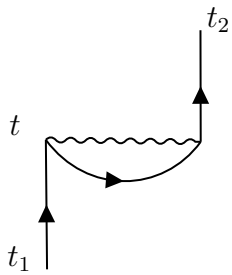


where we have a so-called "self-energy part" because it shows the particle interacting with itself via the particle-hole pair it created in the many-body medium.

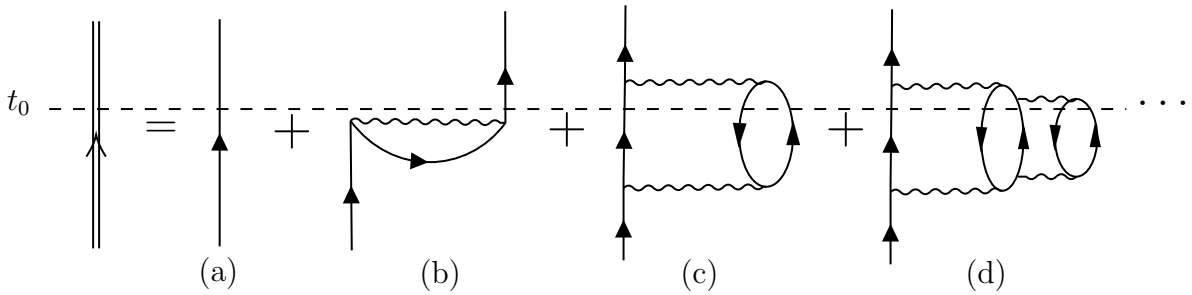
Another sequence of events which can occur involves only one interaction (i.e., a 'first-order ' process). It is a quick-change act in which the incoming electron at point r interacts with another electron at point r' and changes place with it. This is analogous to billiard ball 1 striking billiard ball 2 and transferring all its momentum to 2. The process sequence is:

- Extra particle enters at time t_1
- At time t, the particles is at point r. It interacts with a particle at r'(through virtual photon) and changes place with it.
- Extra particle leaves at time t_2

with a "open oyster" diagram as below:



We can see the direct connection between the one-particle propagator and the quasi particle by looking at all the diagrams at a particular time t_0 (dashed line)

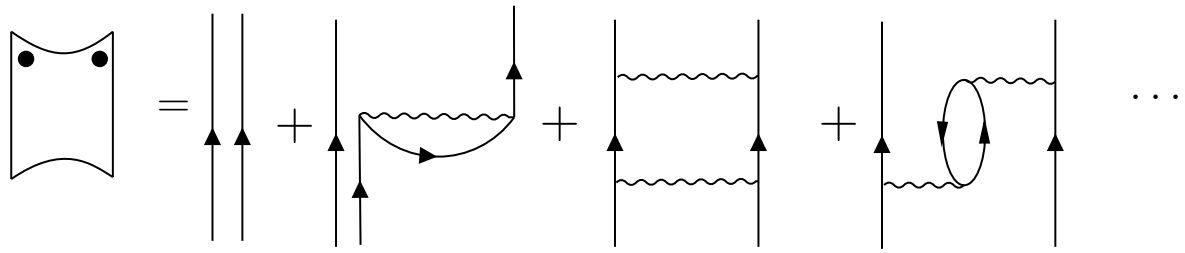


At t_0, we see that various situations may exist: there may be just the bare particle (a), or there may exist two particles plus one hole created by the second order sequence (c), or

three particles plus two holes in (d), etc. That is, the diagrams show all the configurations of particles and holes which may be kicked up by the bare particle as it churns through the many-body system. Thus, **the diagrams reveal the content of the ever-changing cloud of particles and holes surrounding the bare particle and converting it into a quasi particle.**

1.6 The two-particle propagator and the particle-hole propagator

The two-particle propagator is the sum over the probability amplitudes for all the ways two particles can enter the system, interact with each other and with the particles in the system, then emerge again. The diagram series for it is (note that the dots on the diagram for the two-particle propagator show the points at which directed lines emerge):



1.7 No-particle amplitude (vacuum amplitude)

The ground state energy of a many-body system may be obtained directly from the no-particle propagator, or ' vacuum amplitude'. This is the sum of amplitudes for all the ways the system can begin at time t_1 with no extra or lifted-out particles, or holes in it (this is the undisturbed or ' Fermi vacuum' state), have its particles interact with each other, and wind up at t2 with no extra or lifted-out particles, or holes. The simplest process is where nothing at all happens-the system just sits there. A first-order process occurs in which two particles change places with each other (vacuum bubble in QFT).

2 Classical Quasi Particles

2.1 The Classical Quasi Particle Propagator

Quasi particles in a system may be tracked down by means of the single particle Green's function or 'propagator'. Let us see what this is in the classical case. Imagine we have a many-body system, and we consider the motion of one particle in it under the influence of a constant external force $\mathbf{F}$ applied to it. Suppose the particle begins at r_1 at time t_1. If there are no collisions with other particles, the movement or 'propagation' of the particle to the point $\mathbf{r_2}$ at time t_2 is described by

$$r_2 - r_1 = \frac{1}{2}\left(\frac{F}{m}\right)(t_2 - t_1)^2 \tag{2.1}$$

But in the interacting case, collisions take place, and the particle will follow a highly irregular path not described by the eqn. above. The best one can do in this situation is to **talk about the probability of the particle going from one point to another.** This leads us to define the classical propagator: $P(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1)$ as probability density (= probability per unit volume) that if a particle at rest is put into the system at point $\mathbf{r}_1$ at time t_1, then it will be found at $\mathbf{r}_2$ at later time t_2.

It will be convenient, when we later take the Fourier transform, to have P defined also for $t_2 < t_1$:

$$P(r_2, t_2, r_1, t_1) = 0, \text{ for } t_2 < t_1 \tag{2.2}$$

In Fig.2.1 is a graph showing a qualitative picture of this propagator in the interacting and non-interacting cases. Probability density is plotted on the vertical axis, and t_2 and an arbitrary component of $\mathbf{r}_2$ on the horizontal axes. In the absence of interactions, P will be a surface which is zero everywhere except on the line $r_2 - r_1 = \frac{1}{2}(F/m)(t_2 - t_1)^2$, where it equals ∞, i.e., the Dirac δ-function:

$$P_0(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1) = \delta\left[(\mathbf{r}_2 - \mathbf{r}_1) - \frac{1}{2}\left(\frac{\mathbf{F}}{m}\right)(t_2 - t_1)^2\right] \tag{2.3}$$

This propagator in the absence of interactions is called the free propagator.

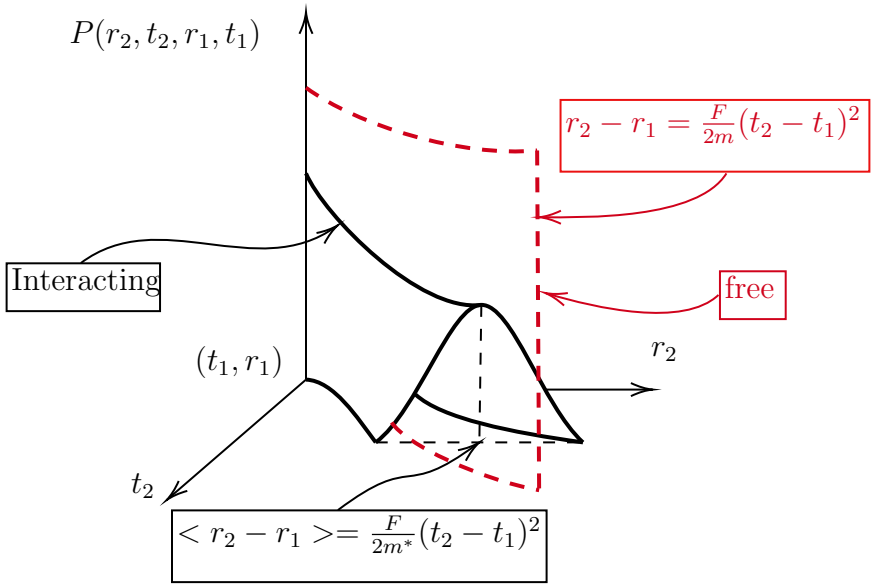


Figure 2.1: The classical propagator

If interactions between particles are now allowed to occur, this surface will **spread out**, as shown qualitatively. If we examine $\langle \mathbf{r}_2 - \mathbf{r}_1 \rangle$, the position of the maximum value of P in the interacting case, we see that for some types of interaction we might find that

$$\langle \mathbf{r}_2 - \mathbf{r}_1 \rangle = \frac{1}{2}\left(\frac{\mathbf{F}}{m^*}\right)(t_2 - t_1)^2 \qquad \text{for } P = \text{ maximum} \tag{2.4}$$

If this is true, then $\langle r_2 - r_1 \rangle$ behaves as the co-ordinate of a quasi particle of effective mass m^*. Look now at the maximum height of P as a function of t_2 Because of the 'spreading out' of the particle position, $P_{\max}$ will first fall infinitely rapidly from its value of ∞ at $t_2 = t_1$, then more slowly. If this slower decay is exponential:

$$P_{\max}(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1) \propto e^{-(t_2 - t_1)/\tau} \tag{2.5}$$

then τ may be identified as the quasi particle lifetime; it clearly must be fairly large if the quasi particle picture is to be useful. Thus, if we calculate P and find that it shows the above behaviour, then the system is describable in terms of quasi particles and their lifetime and effective mass may be determined.

2.2 Calculation of the Propagator by means of diagrams

The actual calculation of the propagator P is quite complicated, but it is easy to illustrate all the principles involved with the aid of a simple analogue example in which the many-body system is replaced by **a set of fixed scattering centres**(e.g. A,B,C,D,E,F,G etc). A pinball is injected at the point r_1, at time t_1 and propagates through the system, being scattered at the various centres. We ask for the probability $P(\mathbf{r}_2, t_2, \mathbf{r}_1, t_1)$ that the particle reaches the point r_2 at time t_2.

The scattering mechanism is assumed to be such that (1) if the pinball strikes the scattering point A, then there is probability $P(A)$ that it is scattered and $1 - P(A)$ that it will go straight through without scattering, (2) the probability distribution of pinball paths and velocities after scattering at A must be independent of the pinball path and velocity before scattering that is, the pinball loses its ' memory" of how it got to A.

For the sake of simplicity, let us leave time out of the argument to begin with, and consider just $P(\mathbf{r}_2, \mathbf{r}_1)$; this is the probability that if the particle begins at r_2 it will finish at r_2 regardless of the time. From the definition of probability, $P(\mathbf{r}_2, \mathbf{r}_1)$ is the sum of the probabilities for all the different ways the particle can go through which begin at r_1 and wind up at r_2. For example, the probability that the pinball will first hit scattering point G and then end up at r_2 is:

$$P\left\{(\mathbf{r}_1 \to \mathbf{r}_G),\ (\text{scattered at } \mathbf{r}_G), (\mathbf{r}_G \to \mathbf{r}_2)\right\} = P_0(\boldsymbol{r}_G, \mathbf{r}_1) P(G) P_0(\mathbf{r}_2, \mathbf{r}_G) \tag{2.6}$$

The total probability, $P(r_2, r_1)$, is just the sum of the probabilities for the various paths. Thus we find

$$\begin{aligned} P(\mathbf{r}_2, \mathbf{r}_1) &= P_0(\mathbf{r}_2, \mathbf{r}_1) + P_0(\mathbf{r}_0, \mathbf{r}_1) P(M) P_0(\mathbf{r}_2, \mathbf{r}_0) + P_0(\mathbf{r}_M, \mathbf{r}_1) P(M) P_0(\mathbf{r}_2, \mathbf{r}_M) + \\ &+ P_{\mathrm{o}}(\mathbf{r}_{\boldsymbol{\sigma}}, \mathbf{r}_1) P(G) P_{\mathrm{o}}(\mathbf{r}_{\boldsymbol{G}}, \mathbf{r}_\sigma) P(G) P_0(\mathbf{r}_2, \mathbf{r}_\sigma) + \cdots \end{aligned} \tag{2.7}$$

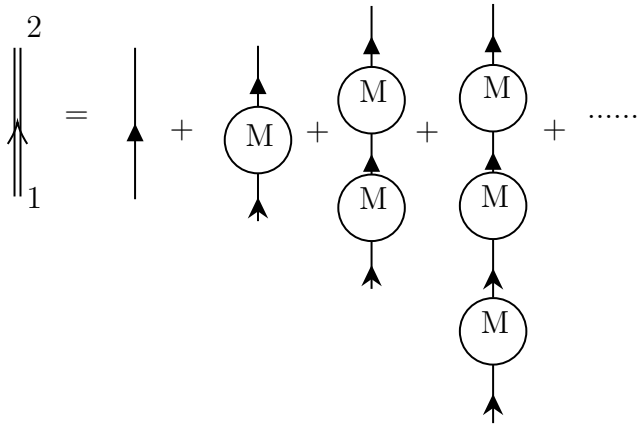
where M, and G are different scattering points.

How can this series be evaluated? If we assume that the P_0 's are large, say $\sim \frac{1}{2}$ or so, and the various interaction $P(A)$'s are small, say $\sim \frac{1}{10}$, then the higher order diagrams

(i.e., note that by order here we mean the total number of interactions) will give successively smaller contributions, and just as in ordinary perturbation theory, we can get an approximate solution by simply summing the series up through the first-or second-order terms. Thus, the zeroth-order approximation would be just the unperturbed case where the particle propagates freely from $\mathbf{r}_1$ to $\mathbf{r}_2$. When we add the possibility of a perturbing (scattering) interaction with the various scattering points once each, we get the first-order approximation.

Allowing two interactions gives the second-order approximation and so on. If, on the other hand, one or more of the interaction terms $P(A)$ is large (i.e., strong scattering at A) this method is not practical, since the series converges too slowly, and the summation must be carried out to extremely high orders to give a good result.

However, there is another kind of approximation where we do not stop at low order interactions, but instead sums over important diagrams to infinite order. Suppose for example, that only $P(M)$ is large and all the other $P(X)$ are small. Then the "M" diagrams will dominate, and the series may be approximated by the sum over just repeated "M"s, thus:



Translating each element of the diagrams into the appropriate probability, it is easy to write down the corresponding series:

$$P(\mathbf{r}_2, \mathbf{r}_1) \approx P_0(\mathbf{r}_2, \mathbf{r}_1) + P_0(\mathbf{r_M}, \mathbf{r}_1) P(M) P_0(\mathbf{r}_2, \mathbf{r}_M) + \\ + P_0(\mathbf{r}_M, \mathbf{r}_1) P(M) P_0(\mathbf{r}_M, \mathbf{r}_M) P(M) P_0(\mathbf{r}_2, \mathbf{r}_M) + \cdots$$

and

$$P(\mathbf{r}_2,\mathbf{r}_1) \approx P_0(\mathbf{r}_2,\mathbf{r}_1) + P_0(\mathbf{r}_M,\mathbf{r}_1)\,P(M)P_0(\mathbf{r}_2,\mathbf{r}_M) \times$$
$$\times\left[1 + P(M)P_0(\mathbf{r}_M,\mathbf{r}_M) + P(M)^2 P_0(\mathbf{r}_M,\mathbf{r}_M)^2 + \cdots\right]$$
$$= P_0(\mathbf{r}_2,\mathbf{r}_1) + \frac{P_0(\mathbf{r}_M,\mathbf{r}_1)\,P(M)P_0(\mathbf{r}_2,\mathbf{r}_M)}{1 - P(M)P_0(\mathbf{r}_M,\mathbf{r}_M)}$$

This new approximation, involving the summation of a perturbation series to infinite order over a selected class of repeated diagrams (i.e., terms) is called' partial summation' or' selective summation'. It is drastically different from the ordinary perturbation approximation.

The above diagram technique may easily be extended to the time-dependent propagator, $P(\mathbf{r}_2,\mathbf{r}_1,t_2-t_1)$. (We have written t_2-t_1 since the force is time independent so the propagators can depend only on time differences.) Let $P_0(\mathbf{r}_j,\mathbf{r}_i,t_j-t_i)$ = probability that if the particle leaves the point $\mathbf{r}_i$ at time t_i then it arrives at r_j at time t_j without undergoing any interaction on the way (this is the 'free propagator'). Let $P(A)$ be the interaction term, assumed instantaneous for simplicity. Then, we have

$$\begin{aligned} P(\mathbf{r}_2,\mathbf{r}_1,t_2-t_1) =& P_0(\mathbf{r}_2,\mathbf{r}_1,t_2-t_1) + \\ &+ \int_{t_1}^{t_2} dt_G P_0(\mathbf{r}_G,\mathbf{r}_1,t_G-t_1)\,P(G)P_0(\mathbf{r}_2,\mathbf{r}_G,t_2-t_G) + \\ &+ \int dt_M \cdots + \iint + \cdots + \iiint + \cdots + \cdots \end{aligned} \tag{2.8}$$

The integrals parading through this expansion can be removed by noticing that they all have the form of "folded" products. This means they can be converted into simple products by a Fourier transformation. Suppose we define the transformed propagator, $P_0(\mathbf{r}_j,\mathbf{r}_i,\omega)$ by

$$P_0(\mathbf{r}_j,\mathbf{r}_i,t_j-t_l) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega e^{-i\omega(t_j-t_i)} P_0(\mathbf{r}_j,\mathbf{r}_i,\omega) \tag{2.9}$$

with a similar expression for $P(\mathbf{r}_j,\mathbf{r}_l,\omega)$. Then the first two terms of (2.8) become (note that we can integrate over t_G from $-\infty$ to $+\infty$ because condition (2.2) automatically limits the integral to the region $t_1 \to t_2$):

$$P_0(\mathbf{r}_2,\mathbf{r}_1,t_2-t_1) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega e^{-i\omega(t_2-t_1)} P_0(\mathbf{r}_2,\mathbf{r}_1,\omega)$$

$$\int_{-\infty}^{+\infty} dt_G P_0(\mathbf{r}_G,\mathbf{r}_1,t_G-t_1)\,P(G)P_0(\mathbf{r}_2,\mathbf{r}_G,t_2-t_G) =$$
$$= \int_{-\infty}^{+\infty} dt_G \left[\tfrac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega' e^{-i\omega'(t_G-t)} P_0(\mathbf{r}_G,\mathbf{r}_1,\omega')\right] \times$$
$$\times P(G) \times \left[\tfrac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega e^{-i\omega(t_2-t_G)} P_0(\mathbf{r}_2,\mathbf{r}_G,\omega)\right] =$$

$$= \frac{1}{(2\pi)^2} \int_{-\infty}^{+\infty} d\omega \int_{-\infty}^{+\infty} d\omega' P_0\left(\mathbf{r}_G, \mathbf{r}_1, \omega'\right) \times$$
$$\times P(G) P_0\left(\mathbf{r}_2, \mathbf{r}_G, \omega\right) e^{+i(\omega' t_1 - \omega t_2)} \int_{-\infty}^{+\infty} dt_G e^{-it_0(\omega' - \omega)}$$

Since

$$2\pi\delta\left(\omega' - \omega\right) = \int_{-\infty}^{+\infty} dt_G e^{-it_G(\omega' - \omega)} \tag{2.10}$$

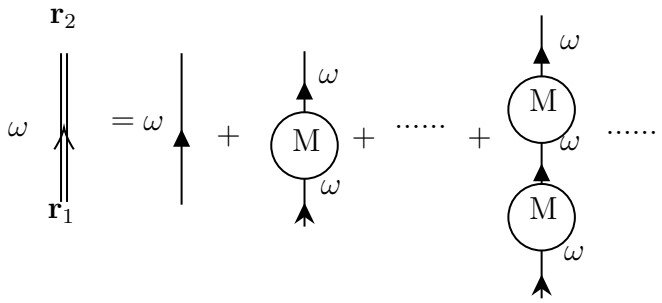
we have

$$\int_{-\infty}^{+\infty} dt_G P_0\left(\mathbf{r}_G, \mathbf{r}_1, t_G - t_1\right) P(G) P_0\left(\mathbf{r}_2, \mathbf{r}_G, t_2 - t_G\right) =$$
$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{-i\omega(t_2 - t_1)} P_0\left(\mathbf{r}_G, \mathbf{r}_1, \omega\right) P(G) P_0\left(\mathbf{r}_2, \mathbf{r}_G, \omega\right) \tag{2.11}$$

Continuing thus, and finally taking the inverse transform, yields

$$P\left(\mathbf{r}_2, \mathbf{r}_1, \omega\right) = P_0\left(\mathbf{r}_2, \mathbf{r}_1, \omega\right) + P_0\left(\mathbf{r}_G, \mathbf{r}_1, \omega\right) P(G) P_0\left(\mathbf{r}_2, \mathbf{r}_G, \omega\right) + \cdots \tag{2.12}$$

Thus, the diagrammatic series is



3 Quantum Quasi Particles and the Quantum Pinball Propagator

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

$$G(2,1) = G(\text{ process 1}) + G(\text{ process 11}) + \cdots$$

so that the corresponding probability is given by

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

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.

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):

$$iG\left(\mathrm{r}_2, \mathrm{r}_1, t_2 - t_1\right)_{t_2 > t_1} = iG^+\left(\mathrm{x}_2, \mathrm{r}_1, t_2 - t_1\right) \tag{3.1}$$

probability amplitude that if at time t_1 we add a particle at point r_1 to the interacting system in its ground state, then at time t_2 the system will be in its ground state with an added particle at $\mathbf{r}_2$

The i factor is purely for decoration (a matter of convention) and the $+$ superscript denotes $t_2 > t_1$. The probability corresponding to the amplitude is

$$P\left(\mathbf{r}_2, \mathbf{r}_1, t_2 - t_1\right) = G^+\left(r_2, \mathbf{r}_1, t_2 - t_1\right)^* G^+\left(\mathbf{r}_2, \mathbf{r}_1, t_2 - t_1\right)$$

Note that it is not necessarily the 'same' particle which is observed at 12, since this has no meaning in the systems of identical particles with which we shall generally deal. The

quantity G^+ 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 $t_2 \leqslant t_1$.

It is actually more convenient to work with an equivalent definition of G in terms of arbitrary single-particle eigenstates, $\phi_k(r)$, instead of position eigenstates. Then we have $iG^+(k_2, k_1, t_2 - t_1)_{t_2>t_1}$ =probability amplitude that if at time t_1 we add a particle in $\phi_{k_1}(r)$ to the interacting system in its ground state, then at time t_2 the system will be in its ground state with an added particle in $\phi_{k_2}(r)$. For $t_2 \leqslant t_1, G^+$ is defined so that:

$$iG^+(k_2, k_1, t_2 - t_1)_{t_2 \leq t_1} = 0 \tag{3.2}$$

A convenient choice for $\phi_k(r)$ is the eigenstates of the unperturbed single particle Hamiltonian, which we will call H_0 :

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

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

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

and

$$H_0 = -\frac{\nabla_r^2}{2m}, \quad \phi_k(r) = \frac{1}{\sqrt{\Omega}}e^{ik\cdot r}, \quad \epsilon_k = \frac{k^2}{2m} \tag{3.3}$$

where Ω is normalization volume and spin is neglected for simplicity. 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 $\phi_{k,}(\mathrm{r})$. Then we have:

$$\psi(\mathbf{r}, t_1) = \phi_{\mathbf{k}_2}(\mathbf{r})$$

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

$$\psi(\mathbf{r}, t_2) = \phi_{k_1}(\mathbf{r})e^{-i\varepsilon_{k1}(t_2 - t_1)} \tag{3.4}$$

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

$$\int d^3\mathbf{r}\psi(\mathbf{r}, t_2)\,\phi^*_{k_2}(\mathbf{r}) = e^{-i\exp(l_2-t_1)}\int \underbrace{d^3\mathbf{r}\phi_{k_1}(\mathbf{r})\phi^*_{k_2}(\mathbf{r})}_{\delta_{k_2k_1}} \tag{3.5}$$

whence, by definition

$$G_0^+(k, t_2-t_1) = \begin{cases} -i\theta_{12-t_1}e^{-i\epsilon_{k_1}(t_2-t_1)}, & \text{for } t_2 \neq t_1 \\ 0, & \text{for } t_2 = t_1 \end{cases} \tag{3.6}$$

where

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

Note that for fermions, all levles up to ϵ_F(=Fermi energy) are fileed, so we can only propagate a particle with $\epsilon_{k_1} > \epsilon_F$. The Fourier transform of (3.6) is

$$\begin{aligned} G_0^+(k,\omega) &= -i\int_{-\infty}^{+\infty} d(t_2-t_1)\,\theta_{t_2-t_1}e^{i\omega(t_2-t_1)}e^{-i\epsilon_k(t_2-t_1)} \\ &= (-1)\frac{e^{i(\omega-\epsilon_k)(t_2-t_1)}}{\omega-\epsilon_k}\Big|_0^\infty = \frac{1}{\omega-\epsilon_k} - \frac{e^{i(\omega-\epsilon_k)\infty}}{\omega-\epsilon_k} \end{aligned} \tag{3.7}$$

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 (3.6) becomes:

$$G_0^+(k, t_2-t_1) = -i\theta_{t_2-t_1}e^{i(\epsilon_k - i\delta)(t_2-t_1)} \tag{3.8}$$

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 3.8 is placed in 3.7 we find

$$G_o^+(k,\omega) = \frac{1}{\omega-\epsilon_k+i\delta} \tag{3.9}$$

From 3.9 we see the pole is at $\omega = \epsilon_k$, the eigenvalue for the eigenstate ϕ_k. It turns out this observation is quite general, even for interacting propagator, $G^+(k, l; \omega)$:

The poles of $G^+(k,l,\omega)$, the fourier transform of the single-particle propagator, corresponds to the excited energy of (N+1)-particle system **minus the ground state energy of N-particle system**.

Also from 3.9, we have the particle lifetime τ as $\delta^{-1} = \infty$, which makes sense because we only consider one free particle here. This observation can also be extended to interacting system where the propagator has the form of

$$G^+ = \frac{1}{\omega - \epsilon'_k + i\tau_k^{-1}} \tag{3.10}$$

where τ_k is the quasi-particle lifetime at the state of ϵ_k.

In a Fermi system, because of the Pauli's principle, each state can only be occupied by one fermion. If a state is partially occupied by a fermion, the possibility of adding another fermion at the same state will be less than 1. Hence we have to multiply the propagator by a factor $Z_k \leq 1$:

$$G^+_{\substack{\text{quasi} \\ \text{particle}}}(k, t_2 - t_1) = -iZ_k e^{-i\epsilon'_k(t_2-t_1)} e^{-(t_2-t_1)/\tau_k} \tag{3.11}$$

$$G^+_{\substack{\text{quasi} \\ \text{particle}}}(k, \omega) = \frac{Z_k}{\omega - \epsilon'_k + i\tau_k^{-1}} \tag{3.12}$$

The poles in the equation above are

$$\omega = \epsilon'_k - i\tau_k^{-1} \tag{3.13}$$

We can still interpret these poles as the excited energy levels even though they are imaginary numbers. For free particles, we have eigenstates as:

$$\psi_k(x) = \phi_k(x) e^{-i\epsilon_k t}$$

When the weak interaction is turned on, the particle decays out of state "k", we have

$$\psi_k(x) \approx \phi_k(x) e^{-i\epsilon'_k t} e^{-t/\tau_k} = \phi_k(x) e^{-i(\epsilon'_k - i\tau^{-1})t}$$

3.1 Quantum Pinball Game

Like the classical pinball game, we now consider the quantum version of the game where the "scattering centers" are now "scattering fields/potentials". Let's assume that a perturbative potential that interacts with free particle has a form of:

$$V(\mathbf{p}) = V_M + V_L = Mp^2 + Lp^4 = -M\nabla_r^2 + L\nabla_r^4 \tag{3.14}$$

where $M \geqslant L$. By solving the Schrodinger equation we have the Hamiltonian as

$$H = (\frac{1}{2m} + M + Lp^2)p^2$$

with

$$\epsilon'_k = (\frac{1}{2m} + M + Lk^2)k^2$$

and $\phi_k(x) = \frac{1}{\sqrt{\Omega}} e^{-i\mathbf{k}\cdot\mathbf{r}}$.Now let us solve for the eigenvalues in a propagator way.

The simplest way the particle can propagate through the system is without interaction, which has a propability amplitude as $G^+(k, t_2 - t_1)$. 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. The probability amplitude in this case is just the product of the probability amplitude for each independent process:

$$G_0^+(k_1, t_M - t_1)V_M G_0^+(k_1, t_2 - t_M)$$

V_M can be obtained from 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:

$$\dot{c}_p(t) = -i \sum_l V_{pl} c_l e^{i(\epsilon_p - \epsilon_l)(t - t_o)} \tag{3.15}$$

where V_{pl} is just the element of S matrix. Hence the probability amplitude per unit time that the system undergoes a transition from ϕ_{k_1} to $\phi_p = \phi_{k_2}$, at time t_M is:

$$\begin{aligned} \dot{c}_{k_2}(t = t_M) = -iV_{M_{k_2 k_1}} = -i \int d^3\mathbf{r} \phi^*_{k_2}(r) V_M \phi_{k_1}(r) = \\ = +iM \int d^3\mathbf{r} \phi^*_{k_2} \nabla^2 \phi_{k_1} = -iMk_1^2 \delta_{k_2 k_1} \end{aligned} \tag{3.16}$$

Thus the probability amplitude for this first-order scattering is

$$\begin{bmatrix}\text{probability}\\ \text{amplitude}\end{bmatrix}_{t_1\to t_M\to t_2} = i\int_{-\infty}^{+\infty} dt_M G_0^+\left(\mathbf{k}_1, t_M - t_1\right) V_{M_{k_2k_1}} G_0^+\left(\mathbf{k}_2, t_2 - t_M\right) \tag{3.17}$$

Similarly for V_L, we have

$$-iV_{L_{k_1k_2}} = -iLk_1^4\delta_{k_2k_1}$$

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:

$$\begin{aligned} G^+\left(\mathbf{k}, t_2 - t_1\right) = G_0^+\left(\mathbf{k}, t_2 - t_1\right) &+ \int_{-\infty}^{+\infty} dt_M G_0^+\left(\mathbf{k}, t_M - t_1\right) V_M G_0^+\left(\mathbf{k}, t_2 - t_M\right) \\ &+ \int_{-\infty}^{+\infty} dt_L G_0^+\left(\mathbf{k}, t_L - t_1\right) V_L G_0^+\left(\mathbf{k}, t_2 - t_L\right) + \\ &+ \int dt_M dt'_M \cdots + \int dt_M dt_L \cdots + \cdots \end{aligned}$$

Taking the Fourier transform, we have

$$\begin{aligned} G^+(\mathbf{k},\omega) = G_0^+(\mathbf{k},\omega) &+ \left[G_0^+(\mathbf{k},\omega)\right]^2 V_{M_{kk}} + \left[G_0^+(\mathbf{k},\omega)\right]^2 V_{L_{kk}} + \\ &+ \left[G_0^+\right]^3 V_{M_{kk}}^2 + 2\left[G_0^+\right]^3 V_{M_{kk}} V_{L_{kk}} + \left[G_0^+\right]^3 V_{L_{kk}}^2 + \\ &+ \left[G_0^+\right]^4 V_{M_{kk}}^3 + \cdots \end{aligned} \tag{3.18}$$

We now pull the trick of partial summation here. We assume that the scattering with V_M is much more important than the scattering with V_L, then the Feynman diagram series can be approximated by:

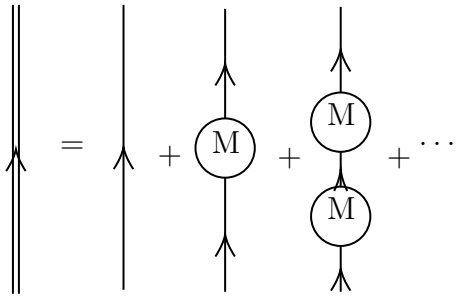


Figure 3.1: Partial Summation of Quantum Pinball Game

Convert this series to equation we have:

$$\begin{aligned} G^+(\mathbf{k},\omega) &\approx G_0^+(\mathbf{k},\omega) + [G_0^+(\mathbf{k},\omega)]^2 V_{M_{kk}} + [G_0^+]^3 V_{M_{kk}}^2 + \ldots \\ &= G_0^+(1 + G_0^+ V_M + (G_0^+ V_M)^2 + \ldots) \\ &= \frac{G_0^+(\mathbf{k},\omega)}{1 - G_0^+(\mathbf{k},\omega) V_{M_{kk}}} \end{aligned} \tag{3.19}$$

Of course we can reproduce this calculation by manipulating the Feynman diagram series:

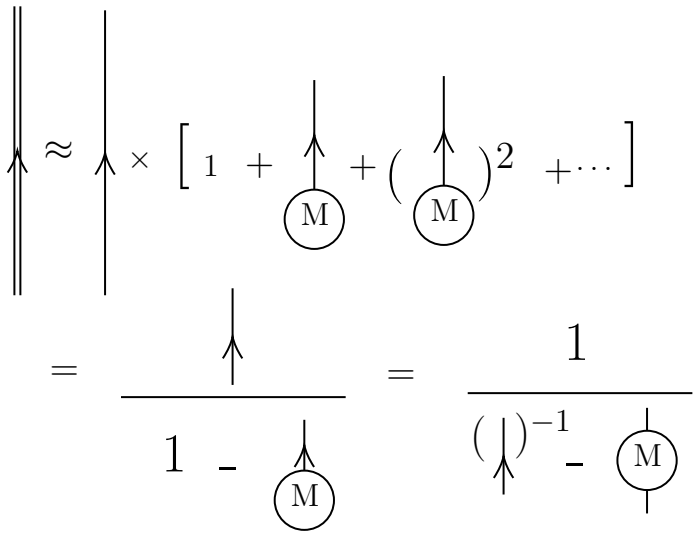
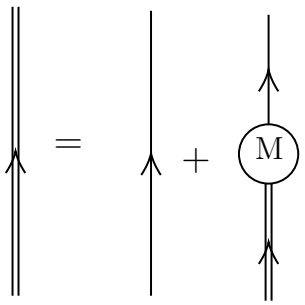


Figure 3.2: Diagram Calculation for the "M" Partial Summation

The diagram series above can also be rewritten in alternative form as:



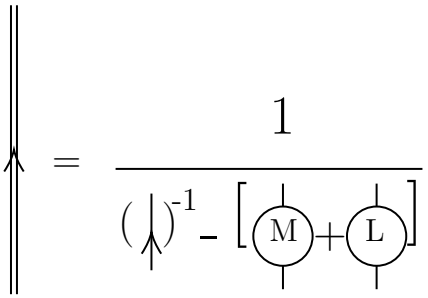
Finally, we substitute for G_0^+ and for V_M and obtain:

$$G^+(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_k + i\delta - V_{M_{kk}}} = \frac{1}{\omega - (\epsilon_k + Mk^2) + i\delta} \tag{3.20}$$

Comparing this with the quasi particle propagator we find

$$\begin{array}{l} \epsilon'_k = \epsilon_k + Mk^2 = \left(\frac{1}{2m} + M\right) k^2 \\ \tau_k = \frac{1}{\delta} = \infty \end{array} \tag{3.21}$$

If we consider V_L, we calculate the whole diagram series as



or, translating:

$$G^+(\mathbf{k},\omega) = \frac{1}{\left(G_0^+\right)^{-1} - \left(V_{M_{kk}} + V_{L_{kk}}\right)} = \frac{1}{\omega - \left(\frac{k^2}{2m} + Mk^2 + Lk^4\right) + i\delta} \tag{3.22}$$

3.2 Where the diagram expansion or the propagator really comes from

We will now show in a rough way how the diagram expansion of G^+ in this single-particle case can be gotten from the Schrodinger equation. 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

$$L\psi(\mathbf{x},t) = f(\mathbf{x},t) \tag{3.23}$$

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

$$LG\left(\mathbf{x}-\mathbf{x}',t-t'\right) = \delta\left(\mathbf{x}-\mathbf{x}'\right)\delta\left(t-t'\right) \tag{3.24}$$

Now the unperturbed Schrodinger equation may be written

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

Thus, the associated Green's function obeys

$$\left(+\frac{\nabla^2}{2m}+i\frac{\partial}{\partial t}\right)G\left(\mathbf{x}-\mathbf{x}',t-t'\right)=\delta\left(\mathbf{x}-\mathbf{x}'\right)\delta\left(t-t'\right) \tag{3.25}$$

Since

$$G\left(x-x',t-t'\right)=\int\frac{d^3k}{(2\pi)^3}e^{ik\cdot(x-x')}G\left(k,t-t'\right) \tag{3.26}$$

and using the Fourier transform of $\delta(x-x')$ we find that

$$\left(-\frac{k^2}{2m}+i\frac{\partial}{\partial t}\right)G\left(\mathbf{k},t-t'\right)=\delta\left(t-t'\right) \tag{3.27}$$

If we use the fact that

$$\frac{d\theta_x}{dx}=\delta(x),\quad f(x)\delta(x)=f(0)\delta(x) \tag{3.28}$$

and substitute $G_0^+(\mathbf{k},\omega)=-i\theta_{t-t'}e^{-i\epsilon_k(t=t')}$ into (3.27), we find the G_0^+ is satisfied.

In a similar way, the Shrodinger equation with a perturbing potential $V(\nabla)$

$$\left[+\frac{\nabla^2}{2m}+i\frac{\partial}{\partial t}-V(\nabla)\right]\psi(\mathbf{x},t)=0 \tag{3.29}$$

has associated Green's function as

$$\left[-\frac{k^2}{2m}+i\frac{\partial}{\partial t}-V(\mathbf{k})\right]G^+\left(\mathbf{k},t-t'\right)=\delta\left(t-t'\right) \tag{3.30}$$

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

$$\boldsymbol{G}^+\left(\mathbf{k},t-t'\right)=G_{\mathbf{0}}^+\left(\mathbf{k},t-t'\right)+\int_{-\infty}^{+\infty}dt^*G_0^+\left(\mathbf{k},t-t^*\right)V(\mathbf{k})G^+\left(\mathbf{k},t^*-t'\right) \tag{3.31}$$

This can be seen by substituting (3.31) into (3.30) and use (3.27) with $G=G_0^+$.Expanding the (3.31) we recover the series in spacetime.

3.3 Energy and lifetime of an electron In an Impure metal

We will now apply the propagator method to a more realistic problem, i.e., an electron in an impure metal. For simplicity, Jet 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, which are identical in a volume Ω. If we use $\mathbf{R}_i$ to represent ion coordinates, then the potential well for an impurity at the $\mathbf{R_i}$ has the form of $W(\mathbf{r}-\mathbf{R}_i)$. Recall that $\phi(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}$, we have the matrix element of transitioning amplitude from $\mathbf{k}$ to $\mathbf{l}$ at R_i as

$$-iV_{\mathbf{lk}}(\mathbf{R}_i) = \frac{-i}{\Omega}\int d^3\mathbf{r} e^{-i(\mathbf{l}-\mathbf{k})\cdot\mathbf{r}}\mathbf{W}(\mathbf{r}-\mathbf{R}_i) \tag{3.32}$$

Now using $\mathbf{r}' = \mathbf{r} - \mathbf{R}_i$, we have (3.32) becomes

$$-iV_{\mathbf{lk}} = \frac{(-i)}{\Omega} e^{-i(\mathbf{l}-\mathbf{k})\cdot\mathbf{R}_i}\mathbf{W}_{lk} \tag{3.33}$$

where

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

After eliminating the i 's and suppressing ω 's for brevity, (noting that it is necessary to sum over all values of the intermediate momentum, $\mathbf{l}$) we have:

$$\begin{aligned} G^+(\mathbf{k}_2,\mathbf{k}_1) =& G_0^+(\mathbf{k}_1)\delta_{k_1k_2} + G_0^+(\mathbf{k}_2)\sum_{t=1}^{N} V_{k_2k_1}(\mathbf{R}_i) G_0^+(\mathbf{k}_1) + \\ &+ G_0^+(\mathbf{k}_2)\left[\sum_l\sum_{i=1}^{N} V_{k_2l}(\mathbf{R}_i) G_0^+(\mathbf{l}) V_{lk_1}(\mathbf{R}_i)\right] G_0^+(\mathbf{k}_1) + \\ &+ G_0^+(\mathbf{k}_2)\left[\sum_l\sum_{j\neq 1} V_{k_2l}(\mathbf{R}_j) G_0^+(\mathbf{l})\sum_{i=1}^{N} V_{lk_1}(\mathbf{R}_l)\right] G_0^+(\mathbf{k}_1) + \cdots \end{aligned} \tag{3.34}$$

The above G^+ is for a particular set of $\mathbf{R}_i$'s, and for each different set of $\mathbf{R}_t'$'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 impurtity, $\mathbf{R_i}$, 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, in the limit $N\to\infty$ (with

$N/\Omega =$ constant), the ratio of the mean square fluctuation $\left(\langle G^{+2}\rangle - \langle G^{+}\rangle^2\right)$ 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))**. Hence our object here will be to calculate $\langle G^{+}\rangle$.

From 3.34, we have

$$\left\langle G_0^+(\mathbf{k}_2)\, G_0^+(\mathbf{k}_1) \sum_{i=1}^{N} V_{k_2 k_1}(\mathbf{R}_i) \right\rangle = G_0^+(\mathbf{k}_2)\, G_0^+(\mathbf{k}_1)\, \frac{W_{k_2 k_1}}{\Omega} \left\langle \sum_{i=1}^{N} e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot \mathbf{r}_i} \right\rangle \tag{3.35}$$

where

$$\left\langle \sum_{t=1}^{N} e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot \mathbf{R}_i} \right\rangle = \sum_{i=1}^{N} \langle e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot \mathbf{R}_i}\rangle = N \langle e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot \mathbf{R}_i}\rangle \tag{3.36}$$

Since the distribution of the ions is totally random, we have

$$\langle e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot \mathbf{R}_i}\rangle = \frac{1}{\Omega}\int d^3\mathbf{R}_i e^{-i(\mathbf{k}_2-\mathbf{k}_1)\cdot \mathbf{R}_i} = \frac{1}{\Omega} \times \Omega \delta_{\mathbf{k}_2 \mathbf{k}_1} \tag{3.37}$$

Box

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 (3.37) is just the three-dimensional version of this with $\Omega = L^3$. If $\mathbf{k}$ is continuous, the integral (3.37) yields $(2\pi)^3 \delta(\mathbf{k}_2 - \mathbf{k}_1)$, which is a Dirac δ -function.

Similarly, for successive scattering on the same ion, we have

$$\begin{aligned} \sum_l G_0^+(\mathbf{l}) \left\langle \sum_i V_{\mathrm{k}_2 l}(\mathrm{R}_i)\, V_{l k_1}(\mathrm{R}_i) \right\rangle &= \sum_{\mathbf{l}} G_0^+(\mathbf{l}) \frac{W_{\mathrm{k}_2 l} W_{\mathrm{l k}_1}}{\Omega^2} \left\langle \sum_{\mathrm{i}} e^{-i(k_2 - l + l - \mathrm{k}_1)\cdot R_i} \right\rangle \\ &= \frac{N}{\Omega^2} \sum_l G_0^+(\mathbf{l}) W_{\mathrm{k}_2 l} W_{l k_1} \delta_{\mathrm{k}_2 \mathrm{k}_1} \end{aligned} \tag{3.38}$$

It is usually more convenient to change from a sum over $\mathbf{l}$ to an integral by

$$\sum_l \to \frac{\Omega}{(2\pi)^3}\int d^3\mathbf{l} \tag{3.39}$$

The factor $\Omega/(2\pi)^3$ is the density of points in k -space. To see this, we note that in one dimension, $k = 2\pi n/L$ ($n =$ integer). 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.

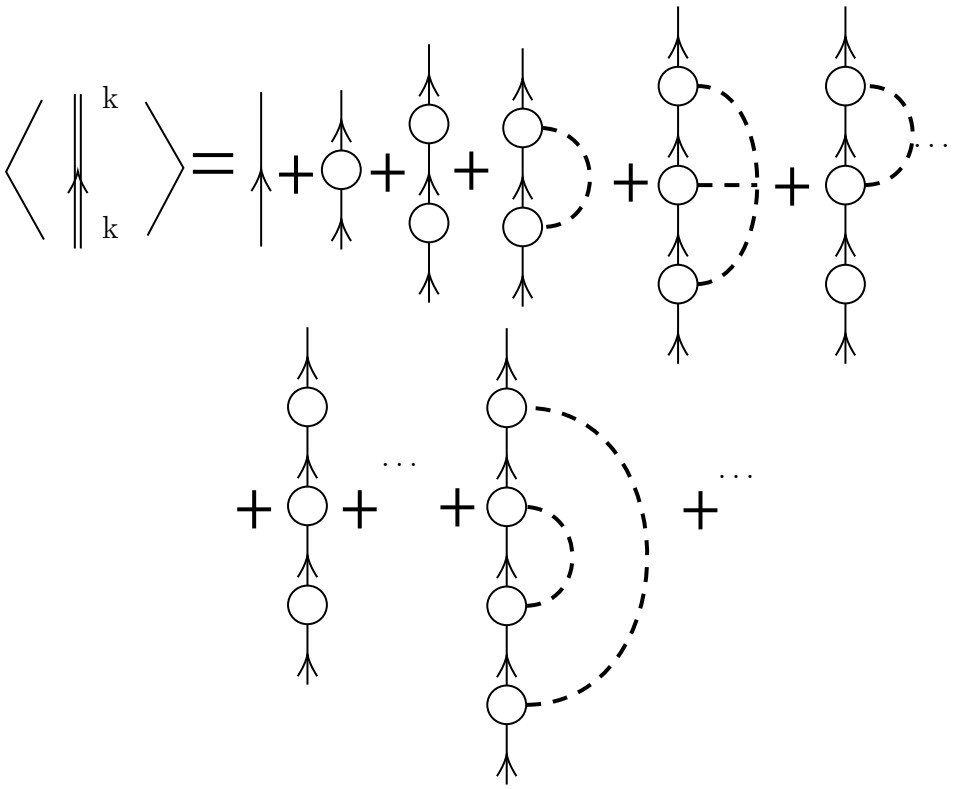
3.38 now becomes

$$= \frac{N}{\Omega}\int \frac{d^3\mathbf{l}}{(2\pi)^3} G_0^+(1) W_{k_2 l} W_{l k_1} \delta_{k_2 k_1}$$

The two successive scattering term from different ions contains the average

$$\begin{aligned}
&\textstyle\sum_l G_0^+(l)\left\langle \sum_{l,j\neq i} V_{k_2 l}\left(R_i\right) V_{l k_1}(R_i)\right\rangle \\
&= \textstyle\sum_l G_0^+(l)\frac{W_{k_2 l} W_{l k_1}}{\Omega^2}\left\langle \sum_{l,j\neq i} e^{-i(k_2-\mathbf{l})\cdot R_j} e^{-i(\mathbf{l}-k_1)\cdot R_i}\right\rangle \\
&= \textstyle\sum_l G_0^+(1)\frac{W_{k_2 l} W_{l k_1}}{\Omega^2} N(N-1)\int \frac{d^3\mathbf{R}_j}{\Omega}\int \frac{d^3\mathbf{R}_i}{\Omega} e^{-i(k_2-\mathbf{l})\cdot R_j} e^{-i(\mathbf{l}-k_1)\cdot R_i}) \\
&\approx \left(\tfrac{N}{\Omega}\right)^2 \textstyle\sum_l G_0^+(l) W_{k_2 l} W_{l k_1}\delta_{k_2 l}\delta_{l k_2} \\
&= \left(\tfrac{N}{\Omega}\right)^2 G_0^+\left(\mathbf{k}_1\right) W_{k_1 k_1}^2 \delta_{k_2 k_1}
\end{aligned}$$

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, we use just an empty circle to represent $V_{lk}(\mathbf{R}_i)$, for the transition probability amplitude W_{lk} 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:



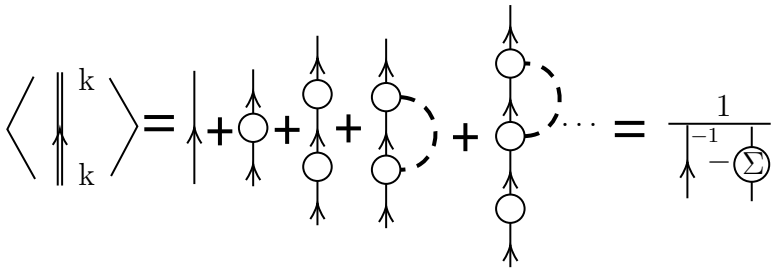
(3.40)

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

Table 3.1: Dictionary for electron propagating through a system of randomly distributed impurity ions

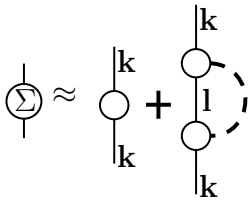
Diagram Element	Factor
	$i\langle G^+(\mathbf{k},\omega)\rangle$
	$-iW_{lk}$
	factor N/Ω
intermediate momentum, I	$\int \frac{d^3l}{(2\pi)^3}$
	$iG_0^+(\mathbf{k},\omega) = \frac{i}{\omega-\varepsilon_{\mathbf{k}}+i\delta}$

Let's evaluate 3.40 by 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 are neglected.The partial sum may easily be carried out and yields

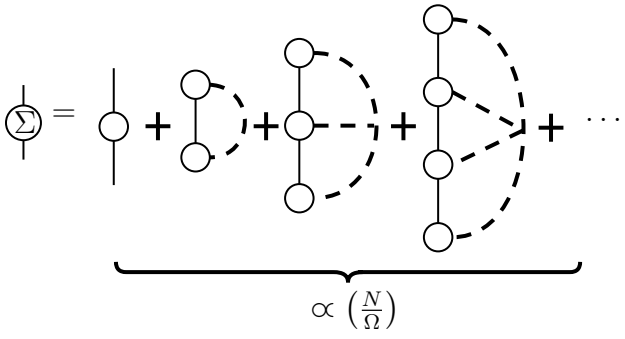


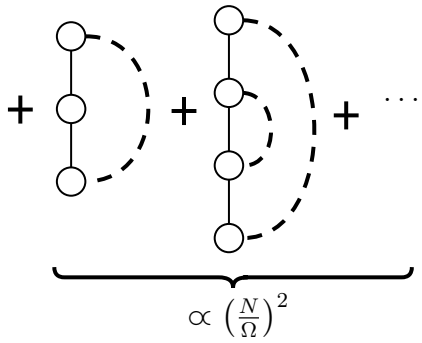
(3.41)

where



Note that the complete series for Σ is





For small N/Ω, we only consider the terms $\propto (N/\Omega)$, i.e., terms representing multiple scattering from a single impurity. Translating (3.41) into functions

$$\langle G(\mathbf{k},\omega)\rangle = 1/\left[\omega - \epsilon_k + i\delta - \Sigma(\mathbf{k},\omega)\right] \tag{3.42}$$

where

$$\Sigma(\mathbf{k},\omega) = \frac{N}{\Omega} W_{\mathbf{kk}} + \frac{N}{\Omega}\int \frac{d^3\mathbf{l}}{(\mathbf{2}\pi)^3} \frac{|W_{kl}|^2}{\omega - \epsilon_l + i\delta} \tag{3.43}$$

In order to find the new energy and lifetime of the electron, we need the complex pole of (3.42), that is:

$$\omega - \epsilon_k - \Sigma(\mathbf{k},\omega) + i\delta = 0 \tag{3.44}$$

Note: if in 3.42 we use the original sum over $\mathbf{l}$,$\Sigma_{\mathbf{l}}$ instead of $\int d^3\mathbf{l}$, we find that, the pole equation 3.43 will have real solutions. This can be seen at once by plotting $(N/\Omega)W_{\mathbf{kk}} + (N/\Omega)\sum_{\mathbf{t}} |W_{\mathbf{kl}}|^2 / (\omega - \epsilon_{\mathbf{l}} + i\delta)$ and $y(\mathbf{k},\omega) = \omega - \epsilon_{\mathbf{k}} \mathbf{v}s.\omega$ and noting that the poles occur at the intersection of $\Sigma(k,\omega)$ and $y(\mathbf{k},\omega)$.**The complex solution of 3.44** arise because we have gone from a sum to an integral.

If W is small so that Σ is small then the zeroth-order approximation to ω is $\omega = \epsilon_{\mathbf{k}}$. The first-order approximation may be obtained by setting $\omega = \epsilon_k$ into $\Sigma(\mathbf{k},\omega)$ and re-solving for ω. 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 Σ by $\omega - \epsilon_{\mathbf{l}} - i\delta$ we find for the real and imaginary parts of $\Sigma(\mathbf{k},\epsilon_k)$:

$$\begin{aligned} \mathrm{Re}\sum(\mathbf{k},\epsilon_k) &= \frac{N}{\Omega} W_{kk} + \lim_{\delta\to 0}\left(\frac{N}{\Omega}\right)\int \frac{d^3\mathbf{l}}{(2\pi)^3} \frac{|W_{lk}|^2 (\epsilon_k - \epsilon_l)}{(\epsilon_k - \epsilon_l)^2 + \delta^2} \\ &= \frac{N}{\Omega} W_{kk} + \left(\frac{N}{\Omega}\right) P\left(\int \frac{d^3\mathbf{l}}{(2\pi)^3} \frac{|W_{lk}|^2}{(\epsilon_k - \epsilon_l)}\right) \end{aligned} \tag{3.45}$$

$$\begin{aligned} \mathrm{Im}\sum(\mathbf{k},\epsilon_k) &= -\lim_{\delta\to 0}\left(\frac{N}{\Omega}\right)\int \frac{d^3\mathbf{l}}{(2\pi)^3} |W_{kl}|^2 \frac{\delta}{(\epsilon_k - \epsilon_l)^2 + \delta^2} \\ &= -\pi\left(\frac{N}{\Omega}\right)\int \frac{d^3\mathbf{l}}{(2\pi)^3} |W_{kl}|^2 \delta(\epsilon_k - \epsilon_l) \end{aligned} \tag{3.46}$$

Where P stands for "principal part". Using the usual definition, we have the following

example of "principal part":

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

or using the alternative definition:

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

$$\begin{aligned}\mathrm{Im}\sum(\mathbf{k},\epsilon_k)&=-\lim_{\delta\to 0}\left(\frac{N}{\Omega}\right)\int\frac{d^3\mathbf{l}}{(2\pi)^3}\left|W_{\mathbf{lk}}\right|^2\frac{\delta}{\left(\epsilon_{\mathbf{k}}-\epsilon_l\right)^2+\delta^2}\\&=-\pi\left(\frac{N}{\Omega}\right)\int\frac{d^3\mathbf{l}}{(2\pi)^3}\left|W_{\mathbf{lk}}\right|^2\delta\left(\epsilon_{\mathbf{k}}-\epsilon_l\right)\end{aligned}\tag{3.47}$$

In 3.46 we used the "squeezed Lorentzian" definition of δ-function. The results of 3.45 and 3.46 are usually obtained with the following theorem:

$$\frac{1}{x+i\delta}=P(\frac{1}{x})-i\pi\delta(x)\tag{3.48}$$

which is short for

$$\int\frac{dxf(x)}{x+i\delta}=P\int\frac{dxf(x)}{x}-i\pi\int dxf(x)\delta(x)\tag{3.49}$$

This can be applied in the present case by noting that the integral in $\Sigma(\mathbf{k},\omega)$ may be written in the general form:

$$\int d^3\mathbf{l}\frac{\boldsymbol{A}(\mathbf{l},\ldots)}{\boldsymbol{B}(\mathbf{l},\ldots)+i\boldsymbol{\delta}}=\int d\phi\int d\boldsymbol{\theta}\sin\theta\int dl\frac{l^2A(l,\boldsymbol{\theta},\phi,\ldots)}{B(l,\boldsymbol{\theta},\boldsymbol{\phi},\ldots)+i\delta}\tag{3.50}$$

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 using (3.49).($f(x)=l^2B'^{,-1}(x)A$). Transforming back to $\mathbf{l}$ again after this is done yields

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

Hence, using (3.45,3.46) we find

$$\epsilon_k'=\epsilon_k+\frac{N}{\Omega}W_{kk}+\left(\frac{N}{\Omega}\right)P\int\frac{d^3\mathbf{l}}{(2\pi)^3}\frac{\left|W_{lk}\right|^2}{\epsilon_k-\epsilon_l}\tag{3.51}$$

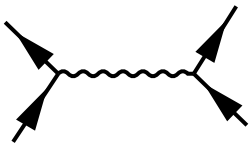
$$\tau_k^{-1}=\pi\left(\frac{N}{\Omega}\right)\int\frac{d^3\mathbf{l}}{(2\pi)^3}\left|W_{lk}\right|^2\delta\left(\epsilon_k-\epsilon_l\right)\tag{3.52}$$

4 Quantum Particle in Fermi System

4.1 Propagator method in many-body systems

In this chapter we will start with non-interacting Fermi-system problem. This is really a fake many-body problem,since as the problem is actually only a one-body problem. By doing this trivial problem, we will describe Fermi system 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,"occupation number formalism", or "second quantization". Finally, it shows us how to extend the definition of the propagator to the case where $t_2 < t_1$. 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.**

By introducing a tree-level two-body interaction



we again can represent the propagator for this case as an infinite series of diagrams, which may be evaluated approximately by partial summation.

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 approxiamation is good for low-density systems like nuclear matter. Only the Hartree and Hartree-Fock will be discussed in this chapter.

Table 4.1: Some important partial sum approx.

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

We first introduce the particle-hole nomenclature for describing Fermi systems. Suppose we have a single particle in a potential $U(\mathbf{r})$, with energy eigenstates $\phi_k(\mathbf{r})$. The energy levels may be represented as in Fig.4.1,where for simplicity the system is non-degenerate.

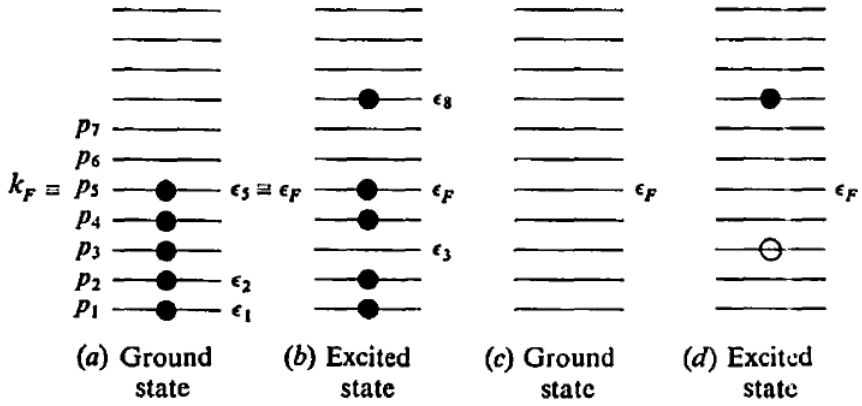


Figure 4.1: Non-interacting Fermi System

In the case where $U(\mathbf{r}) = 0$, the particles are free and $\mathbf{k}$ in 4.1(a) are momentum, or wavenumber. The ground state of the single particle has energy ϵ_F. If we now put N particles into the system, by Pauli principle the energy levels will be filled from the bottom as shown in 4.1(a) for $N = 5$. The highest filled energy level is the ***Fermi level***,ϵ_F. In ground state, the free particles fill a sphere in $\mathbf{k}-$space having radius $k_F = \sqrt{2m\epsilon_F}$,where k_F is called the **Fermi momentum**. The filled sphere is called Fermi sea. The surface of this sphere is **Fermi surface**.

In Fig 4.1(b) the excited states of the system are formed by removing a particle from a state below ϵ_F to a state above. The empty state here is called "hole". In "particle-hole description" we can omit the filled Fermi sea and only focus on excited particle and holes, yielding 4.1(c) and (d). **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**

$$\epsilon_k^{\text{hole}} = -\epsilon_k \tag{4.1}$$

The time-dependent wave function is thus

$$\psi_k(t)^{\text{hole}} = \phi_k e^{-i(-\epsilon_k)t}, \quad \epsilon_k < \epsilon_F \tag{4.2}$$

4.3 A primer of second quantization formalism

The total wave function for the ground and excited states of a system of non-interacting particles is the Slater determinant:

$$\Phi_{k_1,\ldots,k_N}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \frac{1}{\sqrt{(N!)}} \begin{vmatrix} \phi_{k_1}(\mathbf{r}_1)\ldots\phi_{k_1}(\mathbf{r}_N) \\ \vdots \quad \vdots \\ \phi_{k_N}(\mathbf{r}_1)\ldots\phi_{k_N}(\mathbf{r}_N) \end{vmatrix} \tag{4.3}$$

If the particles are allowed to interact with each other or external potential, then the exact wave function of the system is a linear combination of 4.3:

$$\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \sum_{k_1,\ldots,k_N} A_{k_1,\ldots,k_N}\Phi_{k_1,\ldots,k_N}(\mathbf{r}_1,\ldots,\mathbf{r}_N) \tag{4.4}$$

That is, the $\Phi_{k_1,k_2,\ldots}$ for the non-interacting system are the basis states used to describe the interacting system. Noting that all particles are indistinguishable, the essential information in 4.3 is just how many particles in each state, n. For short, we shall represent this as

$$\Phi_{k_1,k_2,\ldots} = |n_{p_1}, n_{p_2}, \ldots\rangle \tag{4.5}$$

meaning:n_{p_1} particles in state ϕ_{p_1}, n_{p_2} in ϕ_{p_3}, etc., where $n = 0$ or 1 by Pauli principle. This notation is called "occupation number notation". It is important to note that just as the original Slater determinant form a complete orthogonal set of basis functions, so do the states in occupation number notation and we have

$$\langle n'_1, \ldots n'_i \ldots | n_1, \ldots, n_i \ldots\rangle = \delta_{n'_1 n_1} \ldots \delta_{n'_i n_i} \ldots \tag{4.6}$$

The wave function for interacting system is now becoming:

$$\Psi = \sum_{n_1,\ldots,n_i,\ldots} A_{n_1,\ldots,n_i,\ldots} |n_1, \ldots, n_i, \ldots\rangle \tag{4.7}$$

In the particle-hole notation, it is necessary to introduce hole creation and destruction operators, $b_1^\dagger, b_1$, and similarly particle operators $a_1^\dagger, a_1$, as follows: if $k_i < k_F$, then c_i destroys a particle under the Fermi level, thus creating a hole. Hence

$$\begin{aligned} \text{for } k_l > k_F, & c_l = a_l \\ k_l < k_F, & c_l = b_l^\dagger \end{aligned} \tag{4.8}$$

and

$$\begin{aligned} \text{for } k_l > k_F, & c_l^\dagger = a_l^\dagger \\ k_l < k_F, & c_l^\dagger = b_l \end{aligned} \tag{4.9}$$

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

$$a_i^\dagger|0\rangle = |1_i^p\rangle\,, \quad a_i\,|1_l^p\rangle = \delta_{il}|0\rangle, \quad b_j^\dagger a_i^\dagger\,|1_m^\rho\rangle = \left|1_m^p, 1_i^p, 1_j^h\right\rangle$$

where the superscripts represent "particle" and "hole", respectively. The operator in the occupation number formalism, $\mathcal{O}^{occ}$ is:

$$\mathcal{O}^{occ} = \sum_{mn} \mathcal{O}_{mn} c_m^\dagger c_n \tag{4.10}$$

where

$$\begin{aligned} c_l &= \theta_{k_l - k_F} a_l + \theta_{k_{F-k_l}} b_l^\dagger \\ c_l^\dagger &= \theta_{k_1 - k_F} a_l^\dagger + \theta_{k_F - k_l} b_l \end{aligned} \tag{4.11}$$

and $\theta_x = 1$ for $x > 0$; $\quad \theta_x = 0$ for $x < 0$.

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:

$$H_{\text{Neand.}} = \underbrace{\sum_i \left[\frac{p_1^2}{2m} + U(\mathbf{r}_i) \right]}_{H_0} + \underbrace{\sum_i V(\mathbf{r}_i)}_{H_1(\text{ perturbation })} \tag{4.12}$$

The single-particle states ϕ_k satisfy:

$$\left[\frac{p^2}{2m} + U(\mathbf{r}) \right] \phi_k = \epsilon_k \phi_k \tag{4.13}$$

Then it is found that

$$H_0 = \sum_k \epsilon_k c_k^\dagger c_k = \sum_{k>k_F} \epsilon_k a_k^\dagger a_k + \sum_{k<k_F} \epsilon_k b_k b_k^\dagger \tag{4.14}$$

$$\begin{aligned} H_1 = &\sum_{m,n>k_F} V_{mn} a_m^\dagger a_n + \sum_{m>k_F, n<k_F} V_{mn} a_m^\dagger b_n^\dagger + \sum_{m<k_F, n>k_F} V_{mn} b_m a_n + \\ &+ \sum_{m,n<k_F} V_{mn} b_m b_n^\dagger \end{aligned} \tag{4.15}$$

For a system of mutually interacting particles with a Hamiltonian

$$H_{\text{old}} = \underbrace{\sum_l \frac{p_l^2}{2m}}_{H_0} + \underbrace{\frac{1}{2} \sum_{i,J} V(\mathbf{r}_i - \mathbf{r}_j)}_{H_1(\text{ perturbation })} \tag{4.16}$$

We also find that

$$H_0 = \sum_{k>k_F} \epsilon_k a_k^\dagger a_k + \sum_{k<k_F} \epsilon_k b_k b_k^\dagger \quad \epsilon_k = k^2/2m \tag{4.17}$$

$$\begin{aligned} H_1 = &\frac{1}{2} \sum_{k,l,m,n>k_F} V_{klmn} a_l^\dagger a_k^\dagger a_m a_n + \sum_{k,l,m>k_F; n<k_F} V_{klmn} a_l^\dagger a_k^\dagger a_m b_n^\dagger + \\ &+ \cdots + \frac{1}{2} \sum_{k,l,m,n<k_r} V_{klmn} b_l b_k b_m^\dagger b_n^\dagger \end{aligned} \tag{4.18}$$

We will define V_{klmn} later. It should be carefully remembered that **in the case of interacting system, the wave functions are given by the linear combination of 4.5.**

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

To treat the general situation of "holes", we extend the definition of propagator to times $t_2 < t_1$. This leads us to the definition:

$$iG(k_2, k_1, t_2 - t_1)_{t_2<t_1} \equiv iG^-(k_2, k_1, t_2 - t_1) \tag{4.19}$$

which is $-1\times$probability amplitude that if at time t_2 we remove a particle in state ϕ_{k_2} from (i.e., if we add a hole in ϕ_{k_2} to) the interacting system in its ground state, then at time t_1 the system will be in its ground state with a particle removed from (i.e., an added hole in $)\phi_{k_1}$.The factor of (-1) here compared with iG^+ comes because we have fermions. Note that G^- is called an "advanced" propagator or Green's function.

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

$$iG^-(k_2, k_1, t_2 - t_1)_{t_2>r_1} = 0 \tag{4.20}$$

In the case of a free hole, we have

$$G_0^-(k, t_2 - t_1) = \begin{cases} i\theta_{t_1-t_2} e^{-i\epsilon_k(t_2-t_1)} & t_2 \neq t1, \epsilon_k < \epsilon_F \\ i, \quad \text{for } t_2 = t_1 \end{cases} \tag{4.21}$$

with Fourier transform

$$G_0^-(k, \omega) = \frac{1}{\omega - \epsilon_k - i\delta}, \quad \epsilon_k < \epsilon_F \tag{4.22}$$

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

$$V_{kl} = \int d^3\mathbf{r}\phi_k^*(\mathbf{r})V(\mathbf{r}, \mathbf{p})\phi_l(\mathbf{r}) \tag{4.23}$$

There are four possibilities of V_{kl} shown in the table below. They mean:(a) scattering of a particle in particle-hole formalism 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 $\phi_k, \epsilon_k > \epsilon_F$, thus simultaneously creating a particle

in ϕ_k and a hole in $\phi_l, (c)$, etc. Note that these four possibilities correspond to the four interaction terms in the particle-hole Hamiltonian for this case (4.16).

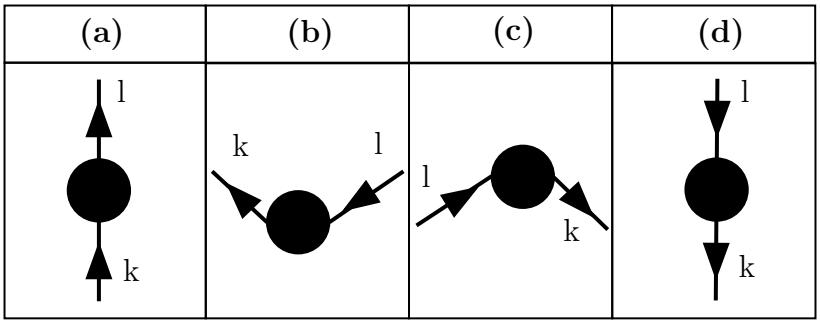
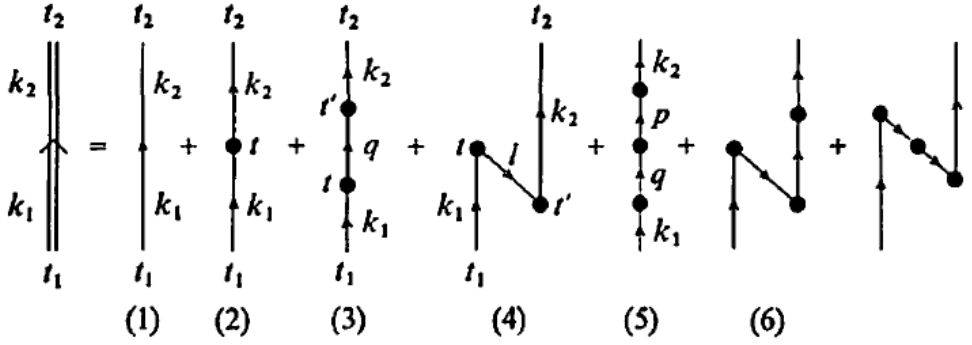


Figure 4.2: Kinds of iV_{kl}

With the aid of the table above, the diagrammatic series for G^+ may be drawn as the sum of all possible diagrams which can be built up out of sequences of interaction dots connected by particle and hole lines:



$+\ldots$ (4.24)

The first diagram disappear if $k_2 \neq k_1$. Look 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 explained later. It's included

here mainly to make the math correct. Translate the diagram (4) into equations, we have:

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

$$a_{k_1}|0\rangle = |1_{k_1}\rangle$$

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

$$V_{k_2 l}, a^{\dagger}_{k_2} b^{\dagger}_{l} \left|1^{p}_{k_1}\right\rangle = V_{k_2 l} \left|1^{p}_{k_1}, 1^{h}_{l}, 1^{p}_{k_2}\right\rangle$$

(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 the particle out:

$$a_{k_2}[V_{k_2 l} V_{lk_1} |1^{P}_{k_2}\rangle] = V_{k_2 l} V_{lk_1} |0\rangle$$

The above diagram series may be written out in words in (k,t) space:

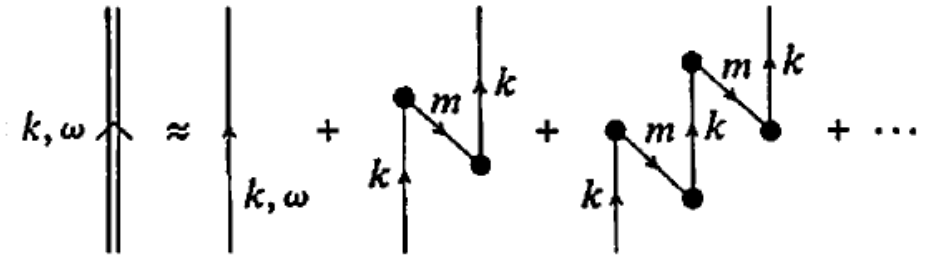
$$\begin{aligned} G^{+}(k_2, k_1, t_2 - t_1) = G^{+}_{0}(k_1, t_2 - t_1)\,\delta_{k_1 k_2} \\ + \int_{-\infty}^{+\infty} dt G^{+}_{0}(k_2, t_2 - t)\, V_{k_2 k_1} G^{+}_{0}(k_1, t - t_1) + \\ + \sum_{q > k_F} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \cdots + \cdots \end{aligned} \tag{4.25}$$

In (k, ω) space:

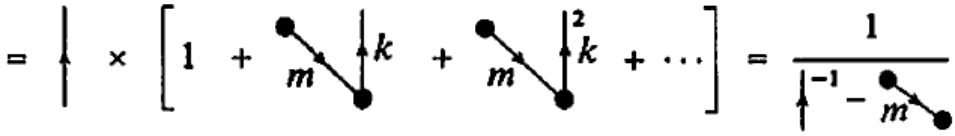
$$\begin{aligned} G^{+}(k_2, k_1) = \delta_{k_1 k_2} \quad & G^{+}_{0}(k_1) + G^{+}_{0}(k_1)\, V_{k_2 k_1} G^{+}_{0}(k_2) \\ & + \textstyle\sum_{q > k_F} G^{+}_{0}(k_1)\, V_{q k_1} G^{+}_{0}(q) V_{k_2 q} G^{+}_{0}(k_2) + \\ & + \textstyle\sum_{l < k_F} G^{+}_{0}(k_1)\, V_{l k_1} G^{-}_{0}(l) V_{k_2 l}, G^{+}_{0}(k_2) + \cdots \end{aligned} \tag{4.26}$$

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_{mk} and $V_{km}(\epsilon_m < \epsilon_F)$ are large, and all the other V's are small. Then the propagator in 4.26 may be approximated by the sum

of the following diagrams:



(4.27)



Thus

$$
\begin{aligned}
G^{+}(k,\omega) &= \frac{1}{\left[G_0^{+}(k,\omega)\right]^{-1} - V_{km}V_{mk}G_0^{-}(m,\omega)} \\
&= \frac{1}{(\omega-\epsilon_k+i\delta) - \frac{|V_{km}|^2}{(\omega-\epsilon_m-i\delta)}}
\end{aligned}
\tag{4.28}
$$

Dropping the $i\delta$'s(they have no significance in this simple calculation) yields

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

$$
\begin{aligned}
\omega = \epsilon_k' &= \frac{\epsilon_k+\epsilon_m}{2} + \frac{1}{2}\sqrt{\left\{(\epsilon_k-\epsilon_m)^2 + 4\,|V_{km}|^2\right\}} \\
= \epsilon_m' &= \frac{\epsilon_k+\epsilon_m}{2} - \frac{1}{2}\sqrt{\{(\epsilon_k-\epsilon_m)^2 + 4|V_{km}|^2\}}
\end{aligned}
$$

Note that the summation must go to infinite order to get quasi-particle energies. Any finite order will still lead to the unperturbed energies.

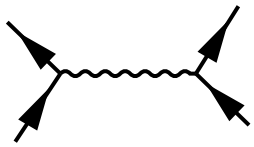
4.5 Interacting Fermi system

Imagine now we have a system consisting of N fermions interacting by means of two-body forces $V(|\mathbf{r}_i - \mathbf{r}_j|)$. Assume there is no external fields, so that the single particle states are just $\phi_k = \Omega^{-1/2}\exp(i\mathbf{k}\cdot\mathbf{r})$ with $\epsilon_k = k^2/2m$. The object of this section is to construct diagramatically the perturbation expansion of the propagator for this system, evaluate it by partial summation and examine the result for quasi particle behavior.

The first thing is to find 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}, this is just the matrix element

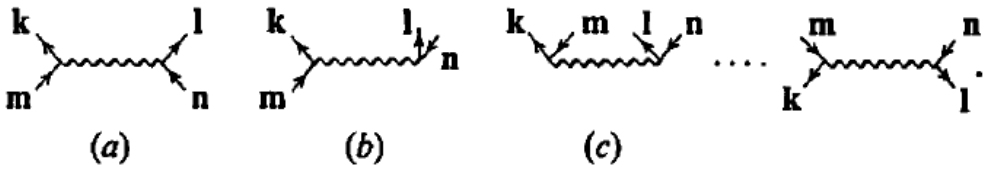
$$V_{klmn} = \int d^3\mathbf{r} \int d^3\mathbf{r}' \phi_k^*(\mathbf{r}) \phi_l^*(\mathbf{r}') V(|\mathbf{r} - \mathbf{r}'|) \phi_m(\mathbf{r}) \phi_n(\mathbf{r}') = V_{iknm} \tag{4.29}$$

Such interaction may be represented diagrammatically by a wiggly line:



$\equiv (-i)\frac{1}{2} V_{klmn}$

Using the particle-hole formalism, this may be drawn in more detail, thus:



(4.30)

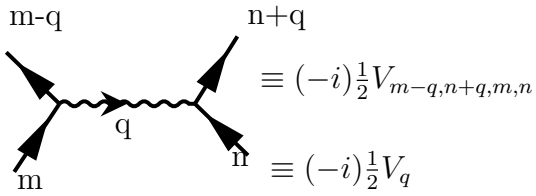
Diagram (a) pictures scattering of two particles at state ϕ_m and ϕ_n into ϕ_k and ϕ_l. In (b) a particle at state ϕ_m interacts with another particle below the Fermi surface in state ϕ_n to create a hole in ϕ_n and a particle in ϕ_l. At the same time the original particle undergoes a transition to state ϕ_k. Note that the diagrams in 4.30 correspond precisely to the interaction terms in the Hamiltonian of 4.16.

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 $V(|\mathbf{r} - \mathbf{r}'|)$ only depends on the distance between the particles so it conserves linear and spin momentum. Thus

$$\mathbf{k} + \mathbf{l} = \mathbf{m} + \mathbf{n}; \quad \boldsymbol{\sigma}_k + \boldsymbol{\sigma}_l = \boldsymbol{\sigma}_m + \boldsymbol{\sigma}_n$$

We can incorporate this conservation law into our diagrams by labelling the "momentum flow" shown below:

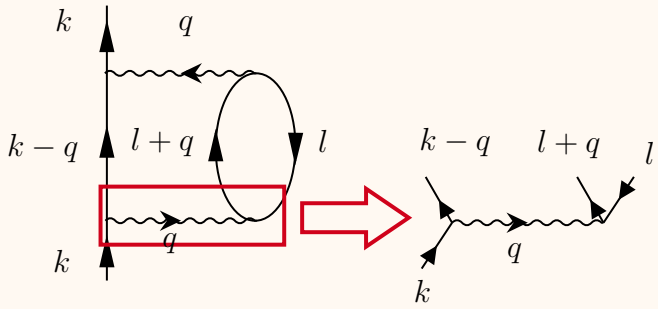


$$\equiv (-i)\tfrac{1}{2}V_{m-q,n+q,m,n}$$

$$\equiv (-i)\tfrac{1}{2}V_q \tag{4.31}$$

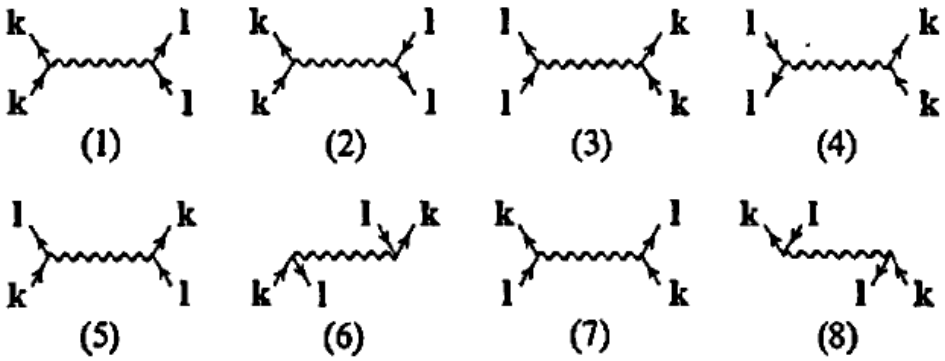
By changing the dummy indices in 4.29 we have $V_{klmn} = V_{lknm}$, so $V_q = V_{-q}$. V_{-q} corresponds to the diagram in 4.31 twisted through 180^o, has momentum transfer $\mathbf{q}' = \mathbf{n} - \mathbf{l}$.

It is important to note that although the collisions conserves momentum, they do not conserve energy. For example, at the lower interaction of the diagram shown below we see the energy flow into the interaction (in the unit 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 with virtual particles during the interactions.



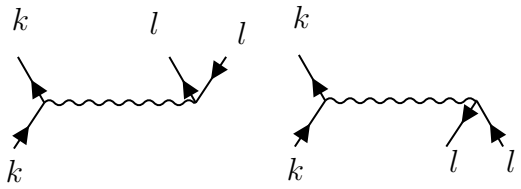
The diagram in the box above depicts a particle in $\mathbf{k}$ being scattered into $\mathbf{k} - \mathbf{q}$ and simultaneously knocking a particle out of $\mathbf{l}$ into $\mathbf{l} + \mathbf{q}$ (i.e., creating a particle in $\mathbf{l} + \mathbf{q}$ and a hole in $\mathbf{l}$. At later time, the particle in $\mathbf{k} - \mathbf{q}$ knocks the particle in $\mathbf{l} + \mathbf{q}$ back into the hole state $\mathbf{l}$ (thus annihilating the particle-hole pair) and is itself scattered into state $\mathbf{k}$. **This is a second-order process, because it involves two interactions.**

The possibilities of first-order interactions are shown below



(4.32)

The diagrams such as



are not allowed since they have a particle and a hole in the same state **l**. It can be shown that diagrams (1),(3),(5) and (7) above do not occur either. The term in disturbed Hamiltonian that corresponds to (1) is

$$V_{klkl} a_k^\dagger a_l^\dagger a_k a_l \tag{4.33}$$

when this acts on the state with one incoming particle in ϕ_k, we find

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

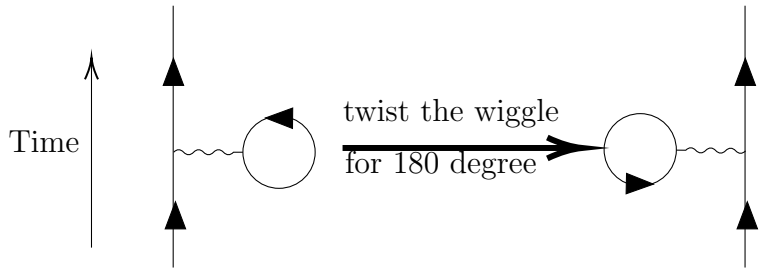
Diagrams (3),(5), and (7) are similarly eliminated. Note that the term in H_1 corresponding to diagram (2) is (following the rule of left-out,right-out, left-in,right-in):

$$V_{klkl} a_k^\dagger b_l a_k b_l^\dagger \tag{4.34}$$

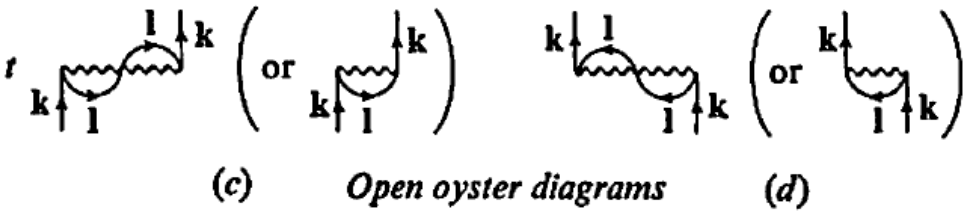
and

$$V_{klkl} a_k^\dagger b_l a_k b_l^\dagger \, |1_k^p\rangle = V_{klkl} \, |1_k^p\rangle \neq 0 \tag{4.35}$$

The possible first-order processes may then be drawn using (2),(4),(6),(8). **This can only be done in one way, e.g., by in each case attaching the outgoing l line to the incoming one. Thus we find:**



(4.36)



(4.37)

The bubble processes can be physically interpreted as follows: a particle enters in $\mathbf{k} > k_F$, knocks a particle out of state $\mathbf{l} < k_F$ at time t, then knocks the particle instantaneously back into $\mathbf{l}$ at time t, then continues freely in state $\mathbf{k}$.

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 $\mathbf{l}, (b)$ creates an instantaneous hole in $\mathbf{l}$ and (c) is exchanged for the particle in $\mathbf{l}$. Diagrams 4.37) 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.

We now see how to evaluate these diagrams. Consider 4.36(a), we have

$$G^+(\mathbf{k}, t_2 - t_1) = (-1) \sum_{l<k_F} \int_{-\infty}^{+\infty} dt \left[iG_0^+(\mathbf{k}, t - t_1)\right] \times \left[-\tfrac{i}{2} V_{klkl}\right] \times \\ \times \left[iG_0^-(l, t - t)\right] \times \left[iG_0^+(\mathbf{k}, t_2 - t)\right] \tag{4.38}$$

The extra factor of (-1) in front comes from the fact that the diagram contains one **"fermion loop"**. Note that an additional factor of (-1) appears because the propagator line for the

bubble is:

$$iG_0^-(1,t-t) = i \times ie^{-i\epsilon_l \times 0} = -1 \tag{4.39}$$

The Fourier transform is then

$$G^+(\mathbf{k},\omega) = (-1)\left[iG_0^+(\mathbf{k},\omega)\right]^2 \sum_{i<k_r}\left[-\frac{i}{2}V_{klkl}\right](-1) \tag{4.40}$$

In a similar fashion, 4.36(b) is

$$(-1)\left[iG^+(\mathbf{k},\omega) = G_0(\mathbf{k},\omega)\right]^2 \sum_{l<k_r}\left(-\frac{i}{2}\right)V_{lklk}(-1) \tag{4.41}$$

Since $V_{klkl} = V_{lklk}$ these diagrams are equivalent. From here, we have the following rule:

> 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 a correct factor in front.

In a manner similar to the bubble diagram calculation, the open oyser gives

$$G^+(\mathbf{k},\omega) = [iG_0^+(\mathbf{k},\omega)]^2 \sum_{l<k_F}(-i)V_{lkkl}(-1) \tag{4.42}$$

where the factor of 2 is included, and (-1) comes from $G_0^-(\mathbf{k},t-t)$. Observe that the frequency, ω, associated with the propagator line coming out of the interaction is the same as that entering. This is an illustration of "**conservation of frequency**", and it is a result from the fact that the Hamiltonian is time-dependent.

We now summarize the dictionary for the expansion series The diagrams may also be interpreted physically from a particular time t_0:

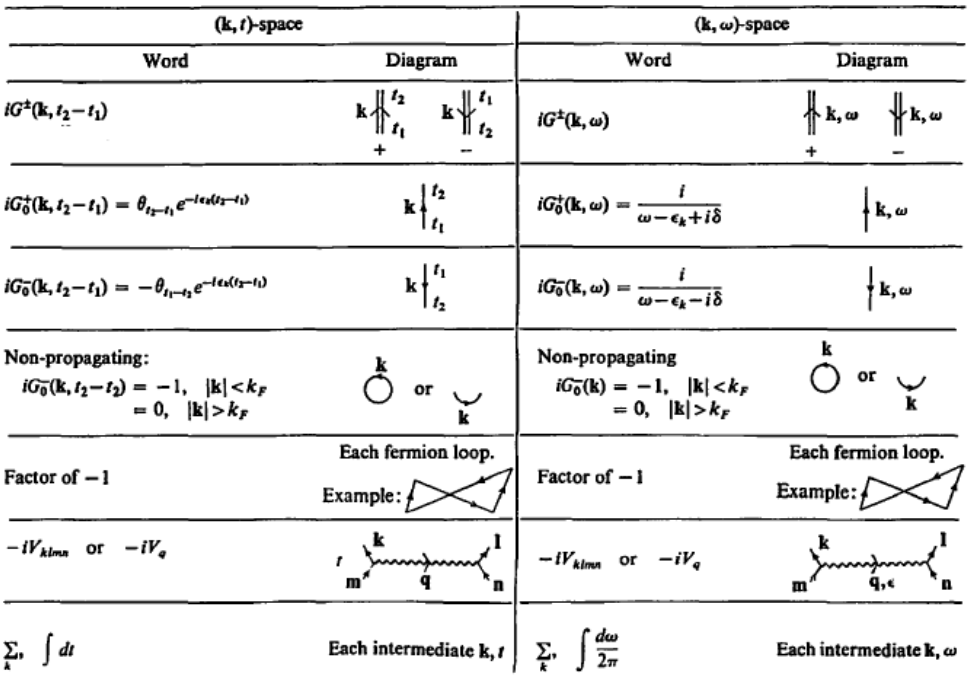
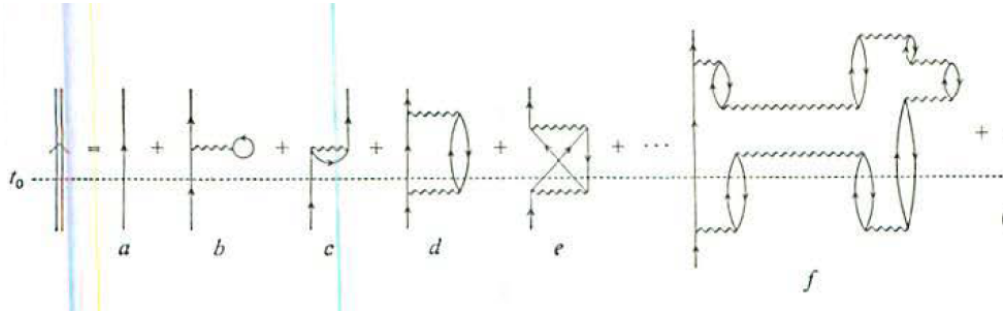


Figure 4.3: Diagram dictionary for interacting many-fermion system with no external potential (Goldstone method)

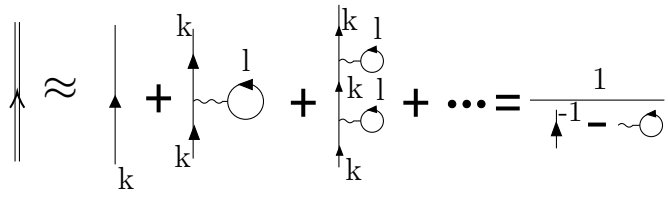


At t_0 we see that besides the bare particle, there may exist in the many-body system two "virtual' particles plus one hole created by second-order process d or two particles and a hole created by second-order sequence e, and so on, with the particle plus three particle-hole pairs created during the 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.**

4.6 Hartree and Hartree- Fock quasi particles

Imagine we have a hypothetical system with no external potential and with an interaction between particles which is dominated by **forward-scattering processes**(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 most important interaction diagrams are the forward-scattering ones. The diagrams which dominate the series will be those in which every interaction is of the forward-scattering type. The only diagrams of this sort are



(4.43)

Translate into equations, the series becomes:

$$iG^{+}(\mathbf{k},\omega)=\frac{1}{\left[iG_{0}^{+}(\mathbf{k},\omega)\right]^{-1}-(-1)\sum_{l<k_{F}}(-iV_{klkl})(-1)} \tag{4.44}$$

or

$$G^{+}(\mathbf{k},\omega)=\frac{1}{\omega-\epsilon_{k}-\sum_{l<k_{F}}V_{klkl}+i\delta} \tag{4.45}$$

Thus the dispersion law and lifetime of the quasi-particle are:

$$\epsilon_{k}'=\epsilon_{k}+\sum_{l<k_{F}}V_{klkl};\quad \tau_{k}=1/\delta=\infty \tag{4.46}$$

where $\sum_{l<k_F}V_{klkl}$ is the "self-energy" of the particle. If spin is included there is a factor 2 multiplying V_{klkl}.

This result has a simple physical meaning. First we note that 4.43 has the exactly same form as the diagram series for a single particle moving through an external cation potential. Thus,$\sum_{i<k_F}(-i)V_{klkl}$ can be interpreted as a transition probability for $\phi_k \rightarrow \phi_k$ scattering caused by an "effective external potential", ν_{eff}. We can find ν_{eff} by writing out $\sum_{i<k_F}V_{klkl}$

in detail, using (4.29):

$$\sum_{i<k_F} V_{klkl} = \int d^3\mathbf{r}\phi_k^*(\mathbf{r})\{\underbrace{\sum_{l\leq k_F}\int |\phi_l(\mathbf{r}')|^2 V(\mathbf{r}-\mathbf{r}')\, d^3\mathbf{r}'}_{\nu_{\text{eff}}}\}\phi_k(\mathbf{r}) \tag{4.47}$$

$|\phi_1(\mathbf{r}')|^2$ is the density at point $\mathbf{r}'$ of a particle in ϕ_1, ν_{eqf} 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_t are plane waves, ν_{eff} is independent of $\mathbf{r}$.) If we write a Schrodinger equation with energy eigenvalues ϵ_k' by using ν_{eff} as external potential, we end up with Hartree equation:

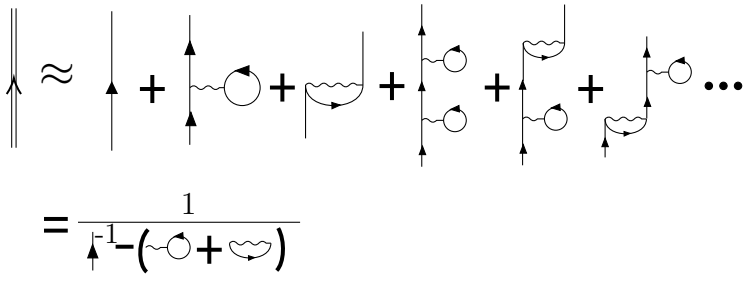
$$\left[\frac{p^2}{2m} + \nu_{\text{eff}}(\mathrm{r})\right]\phi_k(\mathrm{r}) = \epsilon_k'\phi_k(\mathrm{r}) \tag{4.48}$$

If the eigenfunctions are to be solved for in (4.48), we must calculate ϕ_k **self-consistently**:

Box

put an assumed ϕ_k in ν_{eff} , find a new ϕ_k from (4.48) put the new ϕ_k in ν_{eff} calculate a newer ϕ_k, etc., until ϕ_k stops changing appreciably.

From here, we take another step to the quasi-particle in Hartree-Fock (HF) approximation by assuming the exchange scattering (open oyster diagrams) is also an important forward scattering.



(4.49)

Translating by means of propagator dictionary yields

$$G^+(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_k - \sum_{i<k_F}(V_{klkl} - V_{lkkl}) + i\delta} \tag{4.50}$$

The dispersion law and the lifetime are therefore

$$\begin{array}{l}\epsilon_k' = \epsilon_k + \sum_{k<k_F}(V_{klkl} - V_{lkkl}) \\ r_k = \infty\end{array} \tag{4.51}$$

where V_{lkkl} is the well-known "exchange term". Analogous to what was done in the Hartreen approximation, we can here construct another Schrodinger equation including the effective external "exchange" potential. This turns out to be the **Hartree-Fock** equation. Note that the lifetime here is infinite because of the crudeness of the HF approximation. Better approximations produce finite lifetimes.

4.7 Hartree-Fock quasi particles in nuclear matter

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 a hypothetical matter based on the "liquid drop" model of the nucleus. For nuclear interaction potential, we assume it has the form of a simple Yukawa potential ($V_0 < 0$):

$$V = +aV_0 \frac{e^{-|r-r'|/a}}{|\mathbf{r}-\mathbf{r}'|} \tag{4.52}$$

If we convert the sum in k-space to an integral using

$$\sum_l \to \Omega \int \frac{d^3\mathbf{l}}{(2\pi)^3} \tag{4.53}$$

we have the energy of HF quasi particle is

$$\epsilon'_k = \frac{k^2}{2m} + \Omega \int_{|\mathbf{l}|<k_r} \frac{d^3\mathbf{l}}{(2\pi)^3} \left(V_{klkl} - V_{lkkl}\right) \tag{4.54}$$

The transition matrix element V_{klmn} is

$$V_{klmn} = +\frac{V_0}{\Omega^2} \iint d^3\mathbf{r} d^3\mathbf{r}' e^{-i(\mathbf{k}\cdot\mathbf{r}+1\cdot\mathbf{r}'-\mathbf{m}\cdot\mathbf{r}-\mathbf{n}\cdot\mathbf{r}')} \frac{e^{-|r-r'|/a}}{|\mathbf{r}-\mathbf{r}'|/a} \tag{4.55}$$

If we substitute $\mathbf{r}'' + \mathbf{r}' = \mathbf{r}$, and integrate over $\mathbf{r}'$, we find:

$$V_{klmn} = \frac{1}{\Omega} \frac{4\pi V_0 a^3 \delta_{k+l,m+n}}{[1+(\mathbf{k}-\mathbf{m})^2 a^2]} = \frac{1}{\Omega} \frac{4\pi V_0 a^3 \delta_{k+l,m+n}}{[1+(k^2+m^2-2km\cos\theta)\, a^2]} \tag{4.56}$$

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

$$V_{klkl} = +\frac{4\pi V_0 a^3}{\Omega}, \quad V_{lkkl} = +\frac{1}{\Omega} \frac{4\pi V_0 a^3}{[1+(l^2+k^2-2k/\cos\theta)\, a^2]} \tag{4.57}$$

Substituting these expressions in (4.54) 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

$$\epsilon_k' = \frac{k^2}{2m} + \frac{2V_0a^3k_F^3}{3\pi} - \frac{V_0}{2\pi}\left[F\left(ka+k_Fa\right) - F\left(ka-k_Fa\right)\right] \tag{4.58}$$

where

$$F(z) = \frac{1}{2ka}\left[1+z^2\right]\left[\ln\left(1+z^2\right)-1\right] - \left[z\ln\left(1+z^2\right) - 2z + 2\tan^{-1}z\right] \tag{4.59}$$

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 $\left[F\left(ka+k_Fa\right) - F\left(ka-k_Fa\right)\right]$, 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:

$$\epsilon_k' \approx \frac{2V_0a^5k_F^3}{5\pi} + \left[\frac{1}{2m} + \frac{2V_0a^5k_F^3}{3\pi}\right]k^2 \tag{4.60}$$

from which we see that the effective mass in $k^2/2m^*$ is

$$m^* = \frac{m}{1+\frac{4mV_0a^5k_F^3}{3\pi}} \tag{4.61}$$

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

If the electrons in metal is assumed to interact by purely Coulomb forces, and the ions are motionless, we call this system as "electron gas".

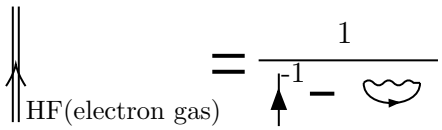
Using the HF approximation, the Coulomb interaction and its transition matrix element are just the Yukawa interaction with $V_0 > 0$ and its matrix element (4.56) with $V_0a = e^2$,i.e.:

(a) $V\left(\mathbf{r},\mathbf{r}'\right) = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$

(b) $V_{klmn} = \frac{4\pi e^2}{|\mathbf{k}-\mathbf{m}|^2}$

where spins are left out for simplicity, and we take $\Omega = 1\text{cm}^3$.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 (4.52) being the 'shielding factor'.**

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 is cancelled by the positive charge background**:



The expression for the quasi particle energy turns out to be

$$\epsilon'_k = \frac{k^2}{2m} - \frac{e^2 k_F}{2\pi}\left[2 + \frac{(k_F^2 - k^2)}{kk_F}\ln\left|\frac{k+k_F}{k-k_F}\right|\right] \tag{4.62}$$

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 :

$$\epsilon'_k = \epsilon'_{k_F} + \left(\frac{\partial \epsilon'_k}{\partial k}\right)_{k_F}(k - k_F) + \cdots \tag{4.63}$$

where $k = |\mathbf{K}|$. For the non-interacting system

$$\boldsymbol{\epsilon}_k = \frac{k_F^2}{2m} + \frac{k_F}{m}(k - k_F) + \cdots \tag{4.64}$$

comparing (4.63) with (4.64), we may regard the effective mass as given by

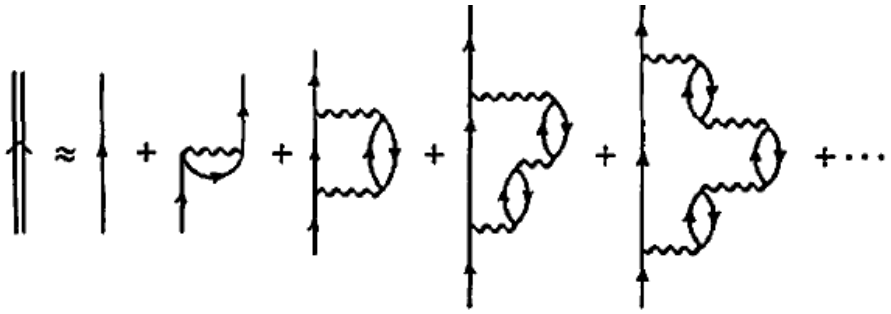
$$\frac{k_F}{m^*} = \left(\frac{\partial \epsilon'_k}{\partial k}\right)_{k_F} \qquad \text{or} \qquad m^* = k_F \Big/ \left(\frac{\partial \epsilon'_k}{\partial k}\right)_{k_F} \tag{4.65}$$

For ϵ'_k as in (4.62) we find that $m^*_{\text{HF(electron gas)}} = 0$! 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. **The HF approximation is not adequate to handle such singular interactions.**

Box

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 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.**

It turns out that in the limit of a high density electron gas, the most important diagrams are those occurring in the following approximation for G (Random Phase Approximation):



(4.66)

5 Ground State Energy and Vacuum Amplitude

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. The diagrammatic methods in this chapter provide a neat way of handling 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

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

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:**vacuum amplitude expansion.**

The vacuum amplitude, $R(t)$, is defined as follows: Let Φ_0 be the ground state of the unperturbed system (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'**. $R(t)$ can also be called **"no-particle propagator"**.

If there is no interaction, then the wave function at time t will simply be $\Phi_0 e^{-iW_0 t}$ where W_0 is the ground state energy. If the interaction is now switched on at time $t = 0$, the system will start to make transition from Φ_0 to all possible N-particle states. Let the state after time t be $\Psi(t)$, **this must be obtainable fro m the ground state Φ_0, by some**

sort of operation. Thus:

$$\Psi(t) = U(t)\Phi_0 \tag{5.2}$$

which may be regarded as the equation defining the **"time development operator"**,$U(t)$. The probability amplitude $R(t)$ is thus:

$$\begin{aligned} R(t) &= \left(\Phi_0 e^{-iW_0 t}, \Psi(t)\right) = \int \Phi_0^* e^{+iW_0 t} U(t)\Phi_0 d\mathbf{r}_1 \dots d\mathbf{r}_N \\ &\equiv \langle \Phi_0 | U(t) | \Phi_0 \rangle \, e^{+iW_0 t} = \text{ vacuum amplitude.} \end{aligned} \tag{5.3}$$

The importance of the vacuum amplitude lies in the fact that the ground state energy, E_0, may be obtained from it with the aid of the theorem

$$E_0 = W_0 + \lim_{t\to\infty(1-i\eta)} i\frac{d}{dt} \ln R(t) \tag{5.4}$$

where η is an infinitesimal. Thus, if we can get a diagrammatic expansion of $R(t)$, then the diagram series for E_0 follows from 5.4.

Box

The diagrammatic perturbation expansion of $R(t)$ is considerably more complicated because of the **"unlinked" diagrams (i.e. not all vertices are connected).** Lukily, the Logarithm of R turns out to be the sume over just **"linked diagrams"**. This is the famous **"linked cluster theorem"**.

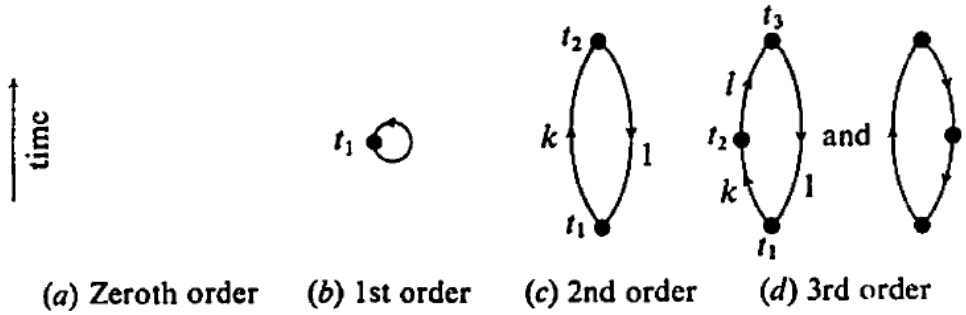
5.2 Quantum vacuum amplitude for one-particle system

Consider the simplest situation first: a Fermi system consisting of one particle in an external potential, with non-degenerate energy levels-for example, an electron in a one-dimensional harmonic oscillator potential. Let the unperturbed Hamiltonian be

$$H_0 = \frac{p^2}{2m} + U(r)$$

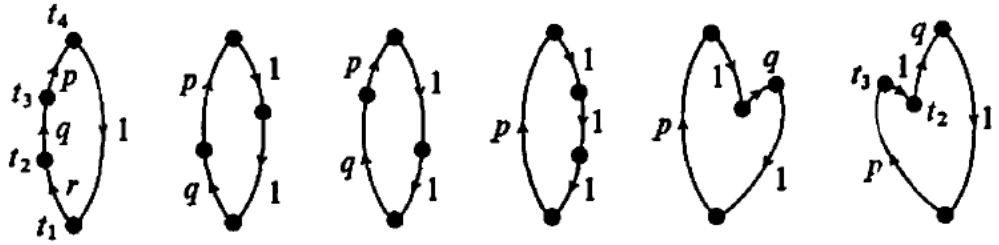
with eigensolutions ϕ_k,ϵ_k. The grpund state of the system consist of one particle in ϕ_1 and no particles in any higher states; in occupation number formalism this is $\Phi_0 = |1_1, 0_2, 0_3, \ldots\rangle$. The corresponding ground state is just $W_0 = \epsilon_1$. A typical excited state is one particle in ϕ_k and no particle in any other state: $\Phi_{\text{excited}} = |0_1, 0_2, \ldots, 1_k, \ldots\rangle$. In particle-hole notation, the ground state is $\Phi_0 = |0\rangle$, while a typical excited state consists of a hole in ϕ_1 and a particle in ϕ_k : $\Phi_{\text{exe}} = \left|1_1^h, 1_k^p\right\rangle$. Note that in this one-particle system, there is only one possible hole state, e.g., ϕ_1.

Suppose now a perturbation $V(\mathbf{r})$ is added to H_0. The vacuum amplitude in that case is the probability amplitude that if the system starts in its ground state Φ_0 at $t = 0$, and is acted upon zero or more times by V(r), then it will be in $\Phi_0 e^{-iW_0 t}$ at time t. By analogy with the pinball case, $R(t)$ will be the sum of the probability amplitudes for all the different ways the system can start out in Φ_0, interact with $V(\mathbf{r})$ arbitrary times and return to Φ_0. **In the zeroth-order process, nothing at all happens as illustrated below:**



(5.5)

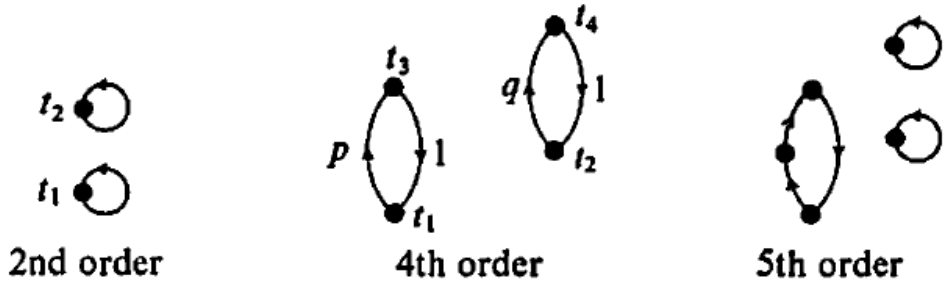
In second order, at t_1, $V(\mathbf{t})$ can scatter the particle up into the state ϕ_k, thus simultaneously creating a hole in ϕ_1 and a particle in ϕ_k, and at t_2 scatter the particle back into ϕ_1. The fourth-order ones are



(5.6)

Note that in the last two diagrams of (5.6) there are two particle lines and two hole lines between t_2 and t_3, whereas our one-particle system can have at most one particle and one

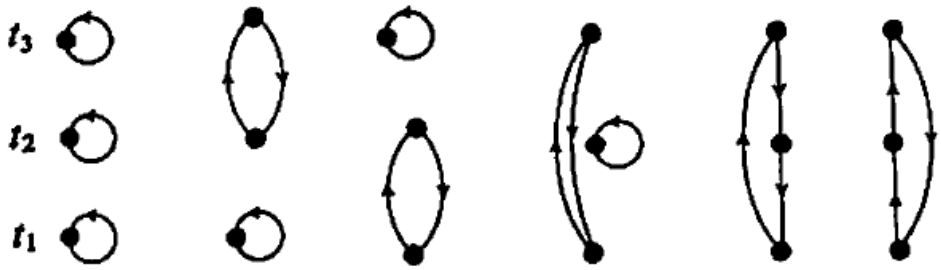
hole. However, it is easily shown that **these diagrams are exactly cancelled by unlinked diagrams of the sort in (5.7) below**.



(5.7)

For example, because of **the (-1) from the extra fermion loop**, the last diagram in (5.6) is cancelled by the fourth-order diagram in (5.7). Nevertheless, it is necessary to retain such diagrams which violate conservation of particle number, in order to prove the linked cluster theorem. The same argument holds for diagrams which violate the Pauli exclusion principle.

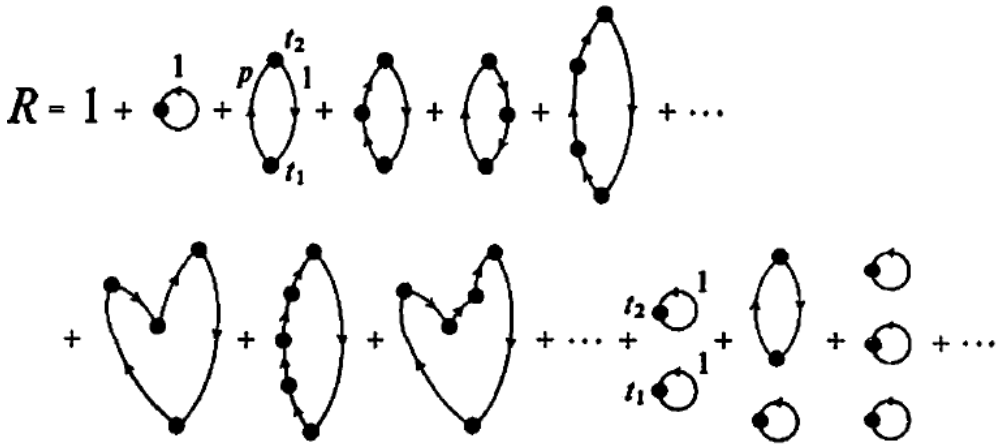
In order to draw all diagrams in n th order, draw n dots in a vertical row, label them $t_1, t_2, \ldots, t_n$ and connect them up in all possible **'topologically distinct'** (see below) ways with one line entering and one leaving each dot. For example in third order we find the six diagrams



Two diagrams are ' **topologically equivalent**' if one can be distorted into the other without changing the vertical ordering of the dots; otherwise they are distinct. This is illustrated by the fourth-order diagrams (**note significance of the direction of the arrows**).

Finally, the diagrammatic expansion for the vacuum amplitude will just be the sum of

all diagrams such as the above:



(5.8)

where the 1 expresses the fact that in the unperturbed case, the probability amplitude for the system staying in its ground state is 1. Translate the series into equation we have

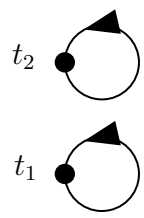
$$\begin{aligned} R(t) = 1 - & V_{11}\int_0^t dt_1 G_0\left(1, t_1 - t_1\right) - \\ & - \sum_{p>1} V_{1p}V_{p1}\int_0^t dt_1 \int_0^t \underset{t_2>t_1}{dt_2}\, G_0^+\left(p, t_2 - t_1\right) G_0^-\left(1, t_1 - t_2\right) + \cdots \\ & + V_{11}V_{11}\int_0^t dt_1 \int_0^t \underset{t_2>t_1}{dt_2} \quad G_0^-\left(1, t_1 - t_1\right)\sigma_0\left(1, t_2 - t_2\right) + \cdots \end{aligned} \tag{5.9}$$

5.3 Linked cluster theorem for one-particle system

The theorem states that

$$lnR(t) = \Sigma \text{ all linked graphs} \tag{5.10}$$

The proof is based on the fact that **the contribution from a unlinked diagram is proportional to the product of the contribution of its various parts.** Consider for example the $V_{11}V_{11}$ term:

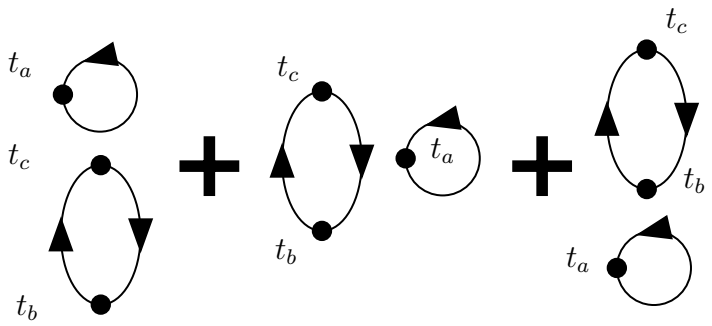


Translating it into equation we have

$$
\begin{aligned}
&V_{11}V_{11}\int_0^t dt_1 \int_0^t \underset{t_2>t_1}{dt_2}\, G_0^- G_0^- = V_{11}^2 G_0^{-2} \int_0^t dt_1 \int_0^t \underset{t_2>t_1}{dt_2} \\
&= V_{11}^2 G_0^{-2} \int_0^t dt_1 \int_0^t dt_2 \times \frac{1}{2} \quad (\text{where } t_2 > \text{ or } < t_1) \\
&= \frac{1}{2}\left[V_{11}\int_0^1 dt_1 G_0^-\left(1, t_1 - t_1\right)\right] \times \left[V_{11}\int_0^t dt_2 G_0^-\left(1, t_2 - t_2\right)\right] \\
&= \frac{1}{2!} \times
\end{aligned}
$$

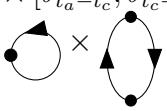
In general, it turns out that the value of an unlinked diagram with n identical links L, is just $(1/n!) \times L^n$.

A similar factorization occurs for non-identical links if we first sum over all possible time orders. For example, the following three graphs can be summed over:



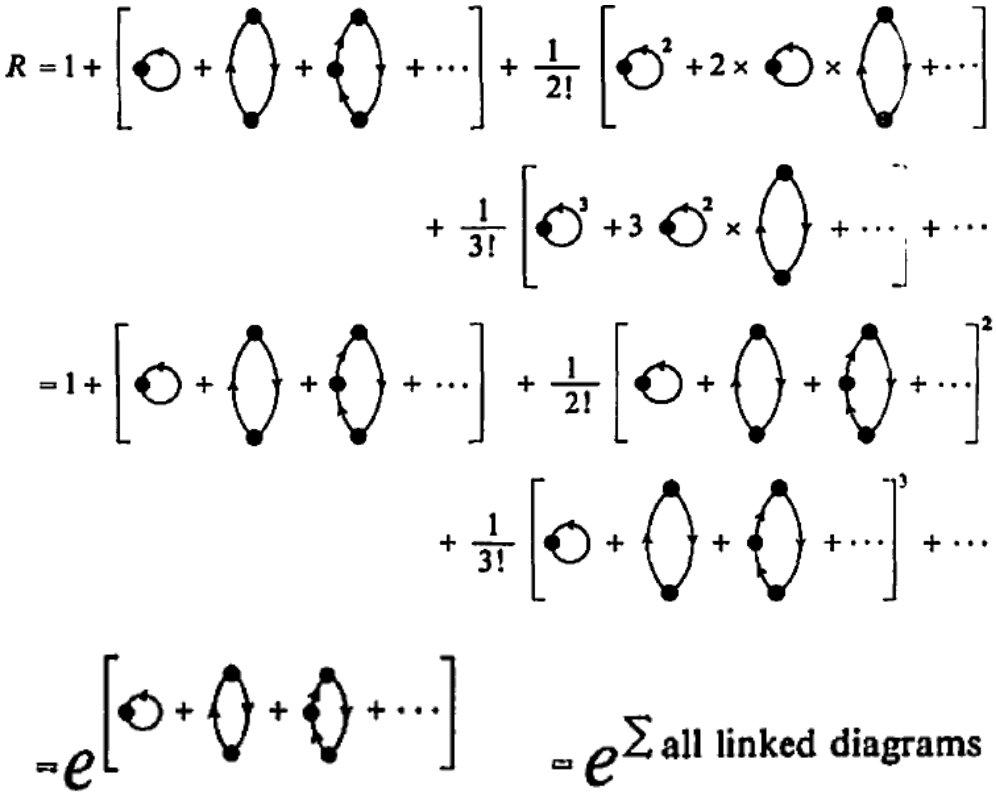
Translate into equations we have

$$
\begin{aligned}
&\textstyle\sum_k V_{k1}V_{1k}V_{11} \iiint dt_a dt_b dt_c \times \\
&\quad \times G_0^+\left(k, t_c - t_b\right) G_0^-\left(1, t_b - t_c\right) G_0^-\left(1, t_a - t_a\right) \times \\
&\quad \times \left[\theta_{t_a - t_c}, \theta_{t_c - t_b} + \theta_{t_c - t_a}\theta_{t_a - t_b} + \theta_{t_c - t_b}\theta_{t_b - t_c}\right] \\
&= \quad \times
\end{aligned}
\tag{5.11}
$$



The $\theta' s$ are used as a convenient way of writing the time order in the three diagrams. For $t_c > t_b$, some concentration shows that the term in brackets $= 1$ regardless of where t_a lies. This means the integral over t_a is independent of that over t_b and t_c, so the triple integral factorizes into two parts producing the result shown.

Combining these results, one finds that R may be written



(5.12)

In the many-body case, there is a deeper reason for the importance of the linked cluster theorem, e.g., if we do not use it, we find that the perturbation series for the energy appears to diverge badly as the number of particles $N \to \infty$.

5.4 Finding the ground state energy in one-particle system

Because the ground state energy depends only on the logarithm of R:

$$E_0 = \epsilon_1 + \lim_{t\to\infty(1-i\eta)} i\frac{d}{dt}\ln R(t)$$

it is now possible to obtain the expression for the ground state energy by translating the above diagrams into the following equations(remember the (-1) factor in front of the "limit"

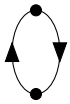
is for the "fermion loop"):

$$E_0 = \epsilon_1 - \lim_{n\to\infty(1-i\eta)} i\frac{d}{dt}\left\{(-i)V_{11}\int_0^t dt_1 iG_0^-(1,t_1-t_1) + \right.$$
$$\left. + \sum_{p\neq 1}(-i)^2 V_{1p}V_{p1}\int_0^t dt_1\int_0^t \underset{t_2>t_1}{dt_2}\, iG_0^+(p,t_2-t_1)\, iG_0^-(1,t_1-t_2) + \cdots \right\} \tag{5.13}$$

Thus,

$$E_0^{(1)} = \lim_{t\to\infty(1-i\eta)} i\frac{d}{dt}$$  $$= V_{11}$$

and the second term produces

 $$= (-1)^2(-i)^2\sum_{p\neq 1} V_{1p}V_{p1}\int_0^1 dt_1\int_0^t dt_2\theta_{t_2-t_1}e^{-i(\epsilon_p-\epsilon_1)(t_2-t_1)}$$

$$= (-1)^2(-i)^2\sum_{p\neq 1} V_{1p}V_{p1}\int_0^t dt_1\int_0^{t-t_1} d(t_2-t_1)\, e^{-i(\epsilon_p-\epsilon_1)(t_2-t_1)}$$

Thus

$$\lim_{t\to\infty(1-i\eta)} i\frac{d}{dt}$$  $$= -i\sum_{p\neq 1} V_{1p}V_{p1}\left[-\frac{e^{-i(\epsilon_p-\epsilon_1)\omega(1-i\eta)}}{i(\epsilon_p-\epsilon_1)} + \frac{1}{i(\epsilon_p-\epsilon_1)}\right]$$

or

$$E_0^{(2)} = \sum_{p\neq 1}\frac{V_{1p}V_{p1}}{\epsilon_1-\epsilon_p} \tag{5.14}$$

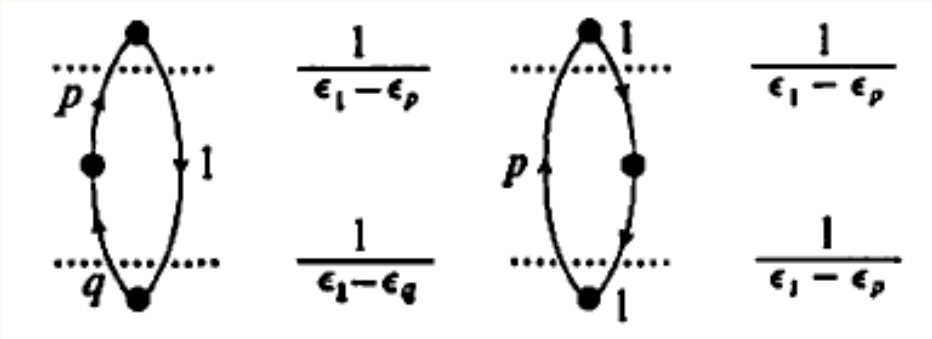
where **the oscillating exponential is killed because** $(\epsilon_1-\epsilon_p)$ **and the infinitesimal** η **are both positive. (Note that** η **is chosen such that** $\eta\times\infty = \infty$.) Proceeding in this way yields the third-and fourth-order terms:

$$E_0^{(3)} = \sum_{p,q\neq 1}\frac{V_{1p}V_{pq}V_{q1}}{(\epsilon_1-\epsilon_p)(\epsilon_1-\epsilon_q)} - \sum_{p\neq 1}\frac{V_{1p}V_{p1}V_{11}}{(\epsilon_1-\epsilon_p)^2} \tag{5.15}$$

$$E_0^{(4)} = \sum_{p,q,r\neq 1}\frac{V_{1p}V_{pq}V_{qr}V_{r1}}{(\epsilon_1-\epsilon_p)(\epsilon_1-\epsilon_q)(\epsilon_1-\epsilon_r)} - \sum_{p,q\neq 1}\frac{V_{1p}V_{pq}V_{q1}V_{11}}{(\epsilon_1-\epsilon_p)^2(\epsilon_1-\epsilon_q)} -$$
$$- \sum_{p,q\neq 1}\frac{V_{1p}V_{pq}V_{q1}V_{11}}{(\epsilon_1-\epsilon_p)(\epsilon_1-\epsilon_q)^2} + \sum_{p\neq 1}\frac{V_{1p}V_{p1}V_{11}V_{11}}{(\epsilon_1-\epsilon_p)^3} - \tag{5.16}$$
$$- \sum_{p,q\neq 1}\frac{V_{1p}V_{p1}V_{1q}V_{q1}}{(\epsilon_1-\epsilon_p)^2(\epsilon_1-\epsilon_q)}$$

This is the well-known Rayleigh-Schrodinger perturbation series carried out to fourth order. Now we use diagrammatic method to carry out the calculation to infinite order by **providing a systematic method for writing out the** $nth-$**order term in the expansion of** E_0**.**

To get the numerator of each term in (5.15-5.16), the product of V_{kl} factors associated with the interaction dots will do. To get the denominator, draw light dotted horizontal lines between successive (in time) pairs of vertices, thus



and associated a factor of

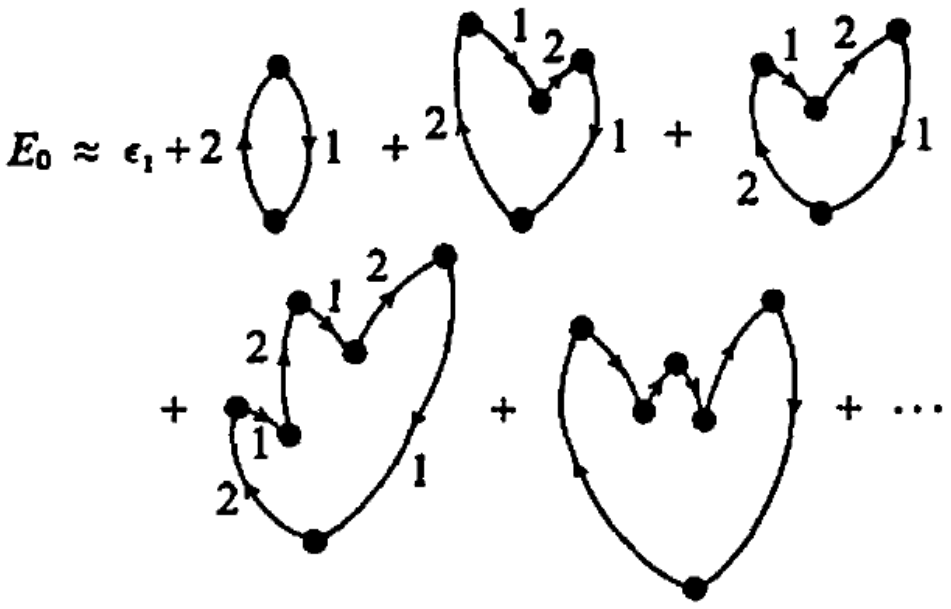
$$\frac{1}{\underset{\text{all hole lines intersected by dotted line}}{\Sigma\epsilon_1} - \underset{\text{all particle lines intersected by dotted line}}{\Sigma\epsilon_p}} \tag{5.17}$$

The proper sign is obtained by multiplying by the factor $(-1)^{h+1}$ where h=number of hole lines in the diagram. The final rule is to sum over all particle indices.

Applying these rules (which can be rigorously proved from the vacuum amplitude expansion) yields both of the third-order terms and they also produce the correct result in the other orders. (Note that in fourth order, the last term in (5.16) is obtained by summing the two "mitten" diagrams of (5.6).)

Imagine that the perturbing potential is so large that it is impossible to get a decent result by using the usual method of cutting off the series after the first few orders. But suppose, for example, that the potential happens to have big matrix elements only between the ground and first excited states, i.e.,that V_{12} and V_{21} are large but all others are small. Then the perturbation series may be approximated by a partial sum over just those special diagrams in which all vertices connect '1' lines and '2' lines. This means that E_0 reduces to

a sum over just the following diagrams



(5.18)

Note that the odd-order diagrams do not occur. And each term representing a graph type is multiplied with a degeneracy factor. Using the rules this series yields

$$\begin{aligned} E_0 \approx \epsilon_1 &+ \frac{|V_{12}|^2}{\epsilon_1 - \epsilon_2} - \frac{|V_{12}|^4}{(\epsilon_1 - \epsilon_2) \times 2\,(\epsilon_1 - \epsilon_2) \times (\epsilon_1 - \epsilon_2)} \times 2 \\ &+ \frac{|V_{12}|^6}{(\epsilon_1 - \epsilon_2) \times 2\,(\epsilon_1 - \epsilon_2) \times (\epsilon_1 - \epsilon_2) \times 2\,(\epsilon_1 - \epsilon_2) \times (\epsilon_1 - \epsilon_2)} \times 4 \\ &+ \frac{|V_{12}|^6}{(\epsilon_1 - \epsilon_2) \times 2\,(\epsilon_1 - \epsilon_2) \times 3\,(\epsilon_1 - \epsilon_2) \times 2\,(\epsilon_1 - \epsilon_2) \times (\epsilon_1 - \epsilon_2)} \times 12 \\ &+ \cdots \\ &= \epsilon_1 + \frac{|V_{12}|^2}{\epsilon_1 - \epsilon_2} - \frac{|V_{12}|^4}{(\epsilon_1 - \epsilon_2)^3} + \frac{2\,|V_{12}|^6}{(\epsilon_1 - \epsilon_2)^5} + \cdots \end{aligned} \tag{5.19}$$

Note that the term $2(\epsilon_1 - \epsilon_2)$ comes from the fact that the vertical line intersects with 2 hole lines and 2 particle liens. By adding and subtracting $\epsilon_1/2$ and factoring out $\frac{1}{2}(\epsilon_1 - \epsilon_2)$ yielding

$$E_0 = \frac{\epsilon_1 + \epsilon_2}{2} + \frac{(\epsilon_1 - \epsilon_2)}{2}\left[1 + \frac{2\,|V_{12}|^2}{(\epsilon_1 - \epsilon_2)^2} - \frac{2\,|V_{12}|^4}{(\epsilon_1 - \epsilon_2)^4} + \frac{4\,|V_{12}|^6}{(\epsilon_1 - \epsilon_2)^6} + \cdots\right] \tag{5.20}$$

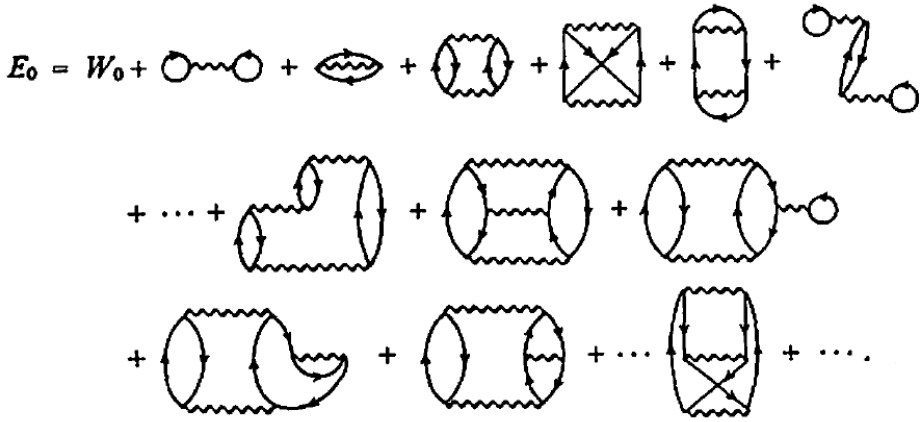
The bracketed term is seen to be just the infinite series for the square root, giving us the

final result

$$E_0 \approx \frac{\epsilon_1 + \epsilon_2}{2} + \frac{(\epsilon_1 - \epsilon_2)}{2}\sqrt{\left\{1 + \frac{4\left|V_{12}\right|^2}{(\epsilon_1 - \epsilon_2)^2}\right\}} \tag{5.21}$$

5.5 The many-body case

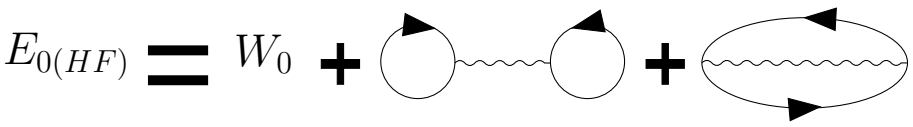
The vacuum amplitude may then be built up as the sum of all possible sequences of interactions beginning and ending in the many-body ground state, or vacuum. The ground state energy again involves just the sum over linked diagrams and may be written as follows:



(5.22)

Here we will content ourselves with briefly mentioning a few popular approximations for the ground state energy which can be made with (5.22).

The simplest approximation is the **Hartree-Fock (HF), which is just the sum of the double-bubble and oyster diagrams**:



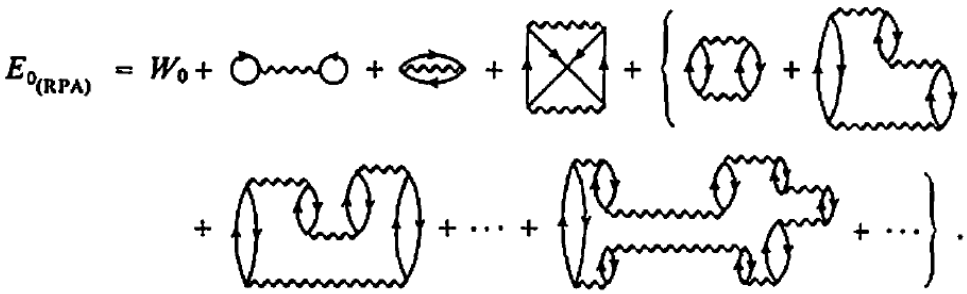
(5.23)

These diagrams involve only three simple rules, so we will evaluate them bere. The rules are: (1) V_{klmn} for each interaction,(2) factor (-1) for each hole line and each fermion loop, and (3) a factor of $\frac{1}{2}$ because the graphs are symmetric. Remembering that all lines are hole

lines here, we find

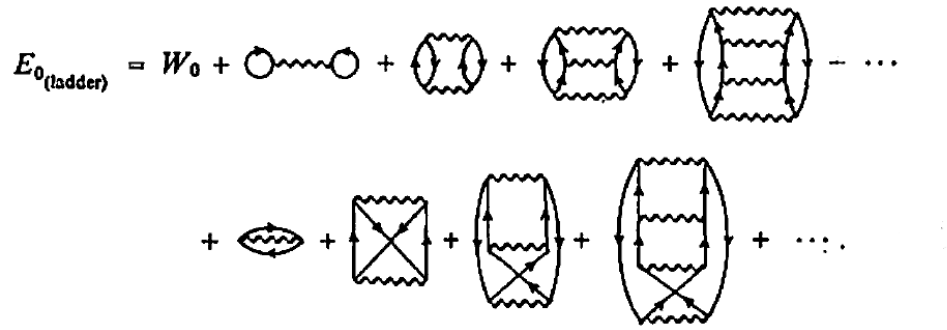
$$E_{0(HF)} = \sum_{k<k_F} \epsilon_k + \frac{1}{2} \sum_{k,l<k_F} V_{klkl} - \frac{1}{2} \sum_{k,l<k_F} V_{lkkl}$$

The approximation which is good for the high density electron gas (random phase approximation, or 'RPA') involves a partial sum over all 'ring' diagrams in second and higher order:



(5.24)

In the case of nuclear matter, we have the 'ladder approximation' involving a partial sum over all ladders:



(5.25)

6 Bird's-Eye View of Diagram Methods in the Many-Body Problem

Field theoretic ingredient	Significance in many-body theory
(1)Occupation number notation	Expresses arbitrary state of manybody system
(2)Creation and destruction operators	Primitive operators out of which all many-body operators are built
(3)Single particle propagator (Green's function)	Yields quasi particle energies, particle momentum distribution, particle density, ground energy
(4)Vacuum amplitude	Gives ground state energy
(5)Two-particle Green's function propagator	Yields energies of collective excitations, electrical conductivity, other non-equilibrium properties
(6)Finite temperature vacuum amplitude	Gives equilibrium thermodynamic properties of system
(7)Finite temperature propagator	Yields temperature dependence of properties in (3)

7 Occupation Number Formalism (Second Quantization)

7.1 Advantages of occupation number formalism

Since simple things can sometimes get to look pretty formidable in second quantization it is a good idea to understand why many-body physicists all use it. The first reason is that it enables us to deal with systems containing a **variable number of particles**.It turns out to give an enormous flexibility in the formalism if **N is allowed to vary in intermediate stages of a calculation and becomes fixed only at the end.** For example, we can put in and remove test particles at will, as in the case of the propagator. Or we can introduce the particle-hole formalism in which the number of particles and holes is variable.

The second reason for the occupation number formalism has to do with the symmetry properties of Fermi and Boss system. Doing things the old way, we always have to worry about the complicated business of keeping the wave function properly symmetrized. But it turns out that in second quantization, the **creation and destruction operators obey certain commutation rules which have built into them all the symmetry properties of the system**. By just using these rules we are automatically free from symmetrization headaches.

7.2 Many-body wave function in occupation number formalism

Imagine that we are given a system of N identical fermions, which are in general interacting with each other and with an external potential. We have seen that such a system may be described in terms of a set of basis states, $|n_1, ..., n_l, ...\rangle$ in which the n_l meant n_l particles in the unperturbed single-particle energy eigenstate, ϕ_l. Actually, the single-particle states used can be any orthonormal set. This means that in general, $|n_1, ..., n_l, ...\rangle$ are not

energy eigenstates of either the interacting or the non-interacting system of particles and their choice is determined by convenience. Foe the moment, we will use the ϕ's which satisfy the Schrodinger equation:

$$\begin{gathered} H\phi_{k\sigma}(\mathbf{r},\gamma) = \epsilon_{ko}\phi_{ko}(\mathbf{r},\gamma) \\ H = \frac{p^2}{2m} + U(\mathbf{r}) = -\frac{1}{2m}\nabla^2 + U(\mathbf{r}) \\ (\hbar = 1) \end{gathered} \tag{7.1}$$

and γ, σ are the spin co-ordinate and quantum number respectively. In the case $U(\mathbf{r}) = 0$, this has the solutions:

$$\begin{aligned} \phi_{k\sigma}(\mathbf{r},\gamma) &= \frac{1}{\sqrt{\Omega}} e^{+i\mathbf{k}\cdot\mathbf{r}} \eta_\sigma(\gamma) \\ \epsilon_k &= \frac{k^2}{2m} (\hbar = 1) \end{aligned} \tag{7.2}$$

where η is the spin eigenfunction. In general, σ, γ will be suppressed for brevity, and $\mathbf{k}$ will be short for $\mathbf{k}, \sigma$, and $\mathbf{r} \equiv \mathbf{r}, \gamma$.

If there are now N identical non-interacting fermions, the Hamiltonian and Schrodinger equation become

$$\begin{gathered} H_0 = \textstyle\sum_{l=1}^{N} H_l, \quad H_0\Phi\left(\mathrm{r}_1, \ldots, \mathrm{r}_N\right) = E\Phi\left(\mathrm{r}_1, \ldots, \mathrm{r}_N\right) \\ H_i = \frac{p^2}{2m} + U\left(\mathrm{r}_i\right); \quad H_i\phi_{k_i} = \epsilon_{k_i}\phi_{k_i} \end{gathered} \tag{7.3}$$

since the system consists of identical fermions, the wave function must be antisymmetric, i.e., change sign when any two particle co-ordinates are interchanged. This is accomplished by forming a Φ given by the Slater determinant.

$$\Phi_{k_1 \ldots\ldots k_N}\left(\mathrm{r}_1, \ldots, \mathrm{r}_N\right) = \frac{1}{(N!)^{\frac{1}{2}}} \sum_P \gamma_P P\left[\phi_{k_1}\left(\mathrm{r}_1\right)\phi_{k_2}\left(\mathrm{r}_2\right)\ldots\phi_{k_N}\left(\mathrm{r}_N\right)\right] \tag{7.4}$$

or

$$\Phi_{k_1,\ldots,k_N}\left(\mathbf{r}_1, \ldots, \mathbf{r}_N\right) = \frac{1}{(N!)^{\frac{1}{2}}} \begin{vmatrix} \phi_{k_1}\left(\mathbf{r}_1\right)\phi_{k_1}\left(\mathbf{r}_2\right)\ldots\phi_{k_1}\left(\mathbf{r}_N\right) \\ \vdots \\ \phi_{k_N}\left(\mathbf{r}_1\right)\phi_{k_N}\left(\mathbf{r}_2\right)\ldots\phi_{k_N}\left(\mathbf{r}_N\right) \end{vmatrix} \tag{7.5}$$

In the first form, P is the permutation operator which interchanges the $\mathbf{r}_i$'s in all possible ways (starting from some standard order), and $\gamma_P = -1$ for an odd number of interchanges, and $+1$ for an even number. The fact that $\Phi = 0$ when any two k_i 's are equal means that there can't be more than one particle in any state.

A tricky thing about (7.5) is its sign. For example, in a two-particle system with one particle in state ϕ_1, and the other in ϕ_3, the wave function is $\Phi_{k_1=1,k_2=3} \equiv \Phi_{13}$ or $\Phi_{k_1=3,k_2=1} \equiv \Phi_{31}$. Since the particles are identical, these represent the same state, but by (7.5) they differ by a minus sign. To remove this ambiguity, we always write Φ with the k's in standard order given by:

$$\Phi_{k_1<k_2<\ldots<k_N} \tag{7.6}$$

A compact way of writing Φ is

$$\begin{aligned} \Phi_{k_1,k_2,\ldots,k_N}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) &= \Phi_{n_1,\ldots,n_i,\ldots}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) \\ &= \langle \mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N | n_1,\ldots,n_i,\ldots\rangle \end{aligned} \tag{7.7}$$

It is important to remember that the $|n_1,\ldots,n_1,\ldots\rangle$ are orthogonal and normal because the $\Phi_{k_1,\ldots,k_N}$ are, and we may write this in the various equivalent ways

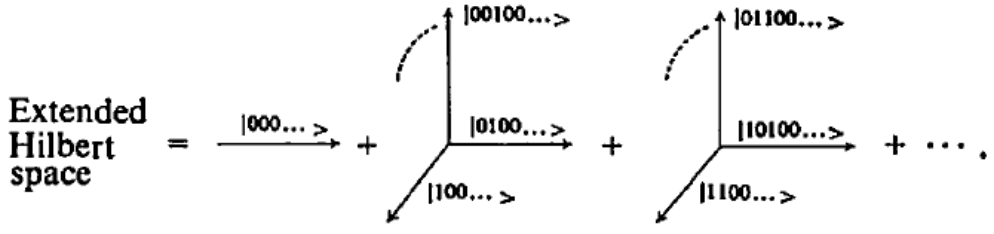
$$\begin{aligned} &\langle n_1',n_2',\ldots,n_1',\ldots|n_1,n_2,\ldots,n_1,\ldots\rangle \\ &\equiv \left(\Phi_{n_1',n_2'\ldots,n_l',\ldots},\Phi_{n_1,n_2,\ldots,n_l,\ldots}\right) \\ &\equiv \int d^3\mathbf{r}_1\ldots d^3\mathbf{r}_N \Phi'_{n_1',n_2},\ldots.(\mathbf{r}_1,\ldots,\mathbf{r}_N)\,\Phi_{n_1,n_2,\ldots}(\mathbf{r}_1,\ldots,\mathbf{r}_N) \\ &= \delta_{n_1',n_1}\delta_{n_2',n_2}\ldots\delta_{n_l',n_l}\cdots. \end{aligned} \tag{7.8}$$

Now we take the step to allow N to be variable, running from 0 to ∞. Thus generates the set of basis functions in the following table:

Table 7.1: Complete set of basis functions used in second quantization

N	$\Phi_{k_1,k_2,\ldots k_N}$	$= \lvert n_1,n_2,\ldots,n_i,\ldots\rangle$
0	Φ_0	$\lvert 000\ldots\rangle$
1	$\Phi_1,\Phi_2,\Phi_3,\ldots$	$\lvert 100\ldots\rangle, \lvert 0100\ldots\rangle, \lvert 00100\ldots\rangle\ldots$
2	$\Phi_{12},\Phi_{13},\Phi_{23},\ldots$	$\lvert 1100\ldots\rangle, \lvert 101000\ldots\rangle, \lvert 01100\ldots\rangle,\ldots$
$\vdots$	$\vdots$	$\vdots$

This Hilbert space may be pictured as follows:



(7.9)

This set is often called 'occupation number basis', and the whole formalism is sometimes referred to as 'occupation number representation'. Note carefully that we did not get this new basis by unitary transformation (like, for example, is done in going from position to momentum basis).

Only systems of independent fermions without perturbing interactions of any sort have been considered thus far. In the presence of such interactions, the $|n_1, \ldots, n_t, \ldots)$ are no longer eigenstates of the total Hamiltonian for the system and the correct eigenstates must be obtained as the linear combination

$$\begin{aligned} \Psi' &= \Phi_0 + \sum_{k_1} A_{k_1} \Phi_{k_1} + \sum_{k_1 < k_2} A_{k_1,k_2} \Phi_{k_1,k_2} + \cdots \\ &= \sum_{n_1,\ldots,n_i,\ldots} A_{n_1,\ldots,n_i,\ldots} \, |n_1, \ldots, n_i, \ldots\rangle \end{aligned} \tag{7.10}$$

7.3 Operators in occupation number formalism

It was pointed out in Chapter 4 that all operators in this new formalism may be expressed in terms of the creation and destruction operator $c_i^\dagger$,c_i. The definition of these operators must include a factor of (± 1) because of antisymmetry. Thus, if $c_i^\dagger$,c_i act in such a sequence on the wave function that their net efferct is to exchange two particles, then the wave function must change its sign. Some thought shows that the proper definition is

$$\begin{aligned} c_1^\dagger \, |n_1, \ldots, n_1, \ldots\rangle &= (-1)^{\Sigma_i} \, (1 - n_i) \, |n_1, \ldots, n_i + 1, \ldots\rangle \\ c_1 \, |n_1, \ldots, n_1, \ldots\rangle &= (-1)^{\Sigma_i} n_i \, |n_1, \ldots, n_i - 1, \ldots\rangle \end{aligned} \tag{7.11}$$

where $\Sigma_i = n_1 + n_2 + \ldots n_{i-1}$. That is, we get a factor of (-1) for each particle (i.e., each occupied state) standing to the left of the state i in the wave function.

One of the nice properties of the $c_1^\dagger$ operators is that by applying them repeatedly to the "true vacuum" state (state with no particles in it), it is possible to generate all other states, thus:

$$\begin{aligned} \Phi_{k_1,k_2,\ldots,k_N} &= c_{k_1}^\dagger c_{k_2}^\dagger \ldots c_{k_n}^\dagger |000\ldots\rangle \\ |n_1, n_2, \ldots\rangle &= (c_1)^{n_1} \, (c_2)^{n_2} \ldots |0000\ldots\rangle \end{aligned} \tag{7.12}$$

Another important property of the $c_1^\dagger, c_l$ operators is that they are **'hermitian adjoints'** of each other. This can be seen by constructing matrices for them, using the $|n_1 n_2, \ldots, n_1, \ldots\rangle$'s as basis states

$$\langle n_1, n_2, \ldots, n_l', \ldots | c_l | n_1, n_2, \ldots, n_l, \ldots \rangle = (-1)^{\Sigma_l} \times \begin{array}{c|cc} & \ldots 0_l \ldots & \ldots 1_l \ldots \\ \hline \langle \ldots 0_l \ldots | & 0 & 1 \\ \langle \ldots 1_l \ldots | & 0 & 0 \end{array} \tag{7.13}$$

$$\langle n_1, n_2, \ldots, n_l', \ldots | c_l^\dagger | n_1, n_2, \ldots, n_l, \ldots \rangle = (-1)^{\Sigma_l} \times \begin{array}{c|cc} & \ldots 0_l \ldots & \ldots 1_l \ldots \\ \hline \langle \ldots 0_l \ldots | & 0 & 0 \\ \langle \ldots 1_l \ldots | & 1 & 0 \end{array}$$

so that

$$c_i^\dagger = (c_i)^\dagger \tag{7.14}$$

where † means hermitian adjoint. This further shows that $c_h^\dagger c_l$ are nonhermitian and are therefore not observables. (otherwise, we should have $c_i = c_i^\dagger$). Using the matrices above we can show that:

$$\left(c_i^\dagger c_i\right)^\dagger = c_i^\dagger c_i \tag{7.15}$$

so that $c_i^\dagger c_i$ is hermitian. This combination is the famous "**number operator**":

$$\hat{n}_l = c_l^\dagger c_l; \quad \left(\hat{N} = \sum_l c_l^\dagger c_l\right) \tag{7.16}$$

For example

$$c_i^\dagger c_i \, |n_1, \ldots, n_i, \ldots\rangle = n_i \, |n_1, \ldots, n_i, \ldots\rangle$$

The $c_1^\dagger, c_1$ operators obey the following important 'fermion commutation rules':

$$\begin{aligned} &(1)\ \left[c_l, c_k^\dagger\right]_+ = c_l c_k^\dagger + c_k^\dagger c_l = \delta_{lk} \\ &(2)\ \left[c_l, c_k\right]_+ = 0 \\ &(3)\ \left[c_l^\dagger, c_k^\dagger\right]_+ = 0 \end{aligned} \tag{7.17}$$

These can be easily proved from the definitions:

$$\begin{aligned} c_1 c_k \left|n_1, \ldots, n_1, \ldots, n_k, \ldots\right\rangle &= (-1)^{\Sigma_x} n_k c_l \left|n_1, \ldots, n_l, \ldots, n_k - 1, \ldots\right\rangle \\ &= (-1)^{\sum_k + \Sigma_l} n_k n_l \left|n_1, \ldots, n_l - 1, \ldots, n_k - 1, \ldots\right\rangle \end{aligned}$$

$$\begin{aligned} c_k c_l \left|n_1, \ldots, n_l, \ldots, n_k, \ldots\right\rangle &= (-1)^{\Sigma_l} n_l c_k \left|n_1, \ldots, n_l - 1, \ldots, n_k, \ldots\right\rangle \\ &= (-1)(-1)^{\Sigma_k + \Sigma_l} n_k n_l \left|n_1, \ldots, n_l - 1, \ldots, n_k - 1, \ldots\right\rangle \end{aligned}$$

where the extra (-1) on line four comes from the fact that there is one less particle to the left of state k. Adding the two equations yields the second rule in (7.17).

The importance of the above sets of' anti-commutation' relations lies in the fact that all the antisymmetry properties are built into them. Therefore, by using them in the right places, we don't have to worry either about the symmetry of the wave functions themselves.

Let us now consider how to express the usual quantum operators in terms of $c_i^\dagger$,c_i. We require equality between the matrix elements of the operator as computed in occupation number formalism and in the old cave-man formalism. For example, in a one-particle system, the operator $\mathcal{O}(\mathbf{r}, \mathbf{p})$ with matrix elements:

$$O_{ij} = \langle \phi_1 | \mathcal{O} | \phi_j \rangle = \int \phi_i^*(\mathbf{r}) \mathcal{O}(\mathbf{r}, \mathbf{p}) \phi_j(\mathbf{r}) d^3\mathbf{r} \tag{7.18}$$

has the occupation number form

$$\mathcal{O}^{\text{occ}} = \sum_{\boldsymbol{k},l} \mathcal{O}_{kl} c_k^\dagger c_l \tag{7.19}$$

This is easily checked as

$$\begin{aligned}\langle 00\ldots 1_i\ldots|\theta^{occ}|\,00\ldots 1_j\ldots\rangle &= \sum_{k,l}\mathcal{O}_{kl}\left\langle 00\ldots 1_i\ldots\left|c_k^\dagger c_l\right|\,00\ldots 1_j\ldots\right\rangle \\ &= \sum_{k,l}\mathcal{O}_{kl}\delta_{lj}\delta_{ik} \\ &= \mathcal{O}_{ij}\end{aligned} \tag{7.20}$$

Suppose we have an operator

$$\mathcal{O} = \sum_{i=1}^{N}\mathcal{O}\left(\mathbf{r}_i,\mathbf{p}_i\right) \tag{7.21}$$

like for example the external potential:

$$V\left(\mathbf{r}_1,\ldots,\mathbf{r}_N\right) = \sum_{i=1}^{N}V\left(\mathbf{r}_i\right) \tag{7.22}$$

Such operators are called "one-body" operators sicne they are a sum of operators each of which acts separately on one particle. Thus we have the valuable result that **in occupation number formalism, the single-particle operators have a form independent of N.**

In a similar way, it can be shown that the "two-body" operator

$$\mathcal{O} = \frac{1}{2}\sum_{\substack{i,j=1\\(i\neq j)}}^{N}\mathcal{O}\left(\mathbf{r}_l,\mathbf{p}_i,\mathbf{r}_j,\mathbf{p}_j\right) \tag{7.23}$$

For instance the interaction potential

$$V\left(\mathbf{r}_1,\ldots,\mathbf{r}_N\right) = \frac{1}{2}\sum_{\substack{i,j=1\\(i\neq j)}}V\left(\mathbf{r}_i-\mathbf{r}_j\right) \tag{7.24}$$

becomes

$$\mathcal{O}^{\text{occ}} = \frac{1}{2}\sum_{klmn}\mathcal{O}_{k\,\text{lm}\,n}c_l^\dagger c_k^\dagger c_m c_n \tag{7.25}$$

where

$$\mathcal{O}_{klmn} = \int d^3\mathbf{r}\int d^3\mathbf{r}'\phi_k^*(\mathbf{r})\phi_i^*\left(\mathbf{r}'\right)\mathcal{O}\left(\mathbf{r},\mathbf{r}';\mathbf{p},\mathbf{p}'\right)\phi_m(\mathbf{r})\phi_n\left(\mathbf{r}'\right) \tag{7.26}$$

We remark here that the results also hold true in the case of bosons.**If by now you are still confused by the subscript sequence in $c_l^\dagger c_k^\dagger c_m c_n$, please check Appendix A.**

7.4 Hamiltonian and Schrodinger equation In occupation number formalism

Assume that the particles interact by means of a two-body force of form (7.24), and that there is in addition an external perturbing potential $V(\mathbf{r})$. In the stone-age notation this is

$$H = \sum_i \underbrace{\left[\frac{p_i^2}{2m} + U(\mathbf{r}_i)\right]}_{H_0} + \underbrace{\frac{1}{2}\sum_{ij} V(\mathbf{r}_i - \mathbf{r}_j)}_{H_1} + \underbrace{\sum_i V(\mathbf{r}_i, \mathbf{p}_i)}_{H_2} \tag{7.27}$$

The first term has the form of the one-body operator, $\mathcal{O}$ in (7.19). Hence,

$$H_0 = \sum_{k,l} \left\langle \phi_k \left| \frac{p^2}{2m} + U(\mathbf{r}) \right| \phi_l \right\rangle c_k^\dagger c_l \tag{7.28}$$

If ϕ_k are chosen to be eigenstates of $p^2/2m + U(\mathbf{r})$, with eigenvalues ϵ_k, then this becomes:

$$H_0 = \sum_{k,l} \epsilon_k \delta_{kl} c_k^\dagger c_l = \sum_k \epsilon_k c_k^\dagger c_k \tag{7.29}$$

Similarly, H_1 is translated into

$$H_1 = \frac{1}{2} \sum_{k,l,m,n} V_{klmn} c_l^\dagger c_k^\dagger c_m c_n \tag{7.30}$$

and H_2 becomes

$$H_2 = \sum_{k,l} V_{kl} c_k^\dagger c_l; \quad V_{kl} = \int d^3 r \phi_k^*(r) V(r,p) \phi_l(\mathbf{r}) \tag{7.31}$$

Hence in the occupation number formalism H is:

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \tfrac{1}{2} \sum_{k,l,m,n} \begin{array}{l} V_{klmn} c_l^\dagger c_k^\dagger c_m c_n \\ + \sum_{k,l} V_{kl} c_k^\dagger c_l \end{array} \tag{7.32}$$

For practice, let us solve the Schrodinger equaion, $H\Phi = E\Phi$, in occupation number formalism in some trivial cases. Suppose that both one-body and two-body interactions are ignored. Then we have

$$H|\Psi\rangle = \sum_k \epsilon_k c_k^\dagger c_k |\Psi\rangle = E|\Psi\rangle \tag{7.33}$$

It is easy to see that the solution is

$$|\Psi\rangle = |n_1, n_2, \ldots, n_i, \ldots\rangle$$

The energy eigenvalues are evidently

$$E = \Sigma_k \epsilon_k n_k$$

which is the sum of the individual particle energies.

Another example is for a one-particle system subjected to an external perturbing potential $V(\mathbf{r})$. The Schrodinger equation is

$$H\Phi = (H_0 + V)\Phi = E\Phi$$

with

$$H_0\phi_k = \epsilon\phi_k$$

which **yields the secular equation for the energy**:

$$det[(\epsilon_i - E)\delta_{ij} + V_{ij}] = 0$$

In the ultra-simple case where all $V_{ij} = 0$ except V_{pq} and V_{qp}, this becomes

$$(\epsilon_1 - E)(\epsilon_2 - E)\ldots \begin{vmatrix} \epsilon_p - E & V_{pq} \\ V_{qp} & \epsilon_q - E \end{vmatrix} \ldots = 0$$

which has the solutions

$$E = \epsilon_i \quad (i \neq p, q)$$

othewise,

$$E = \frac{\epsilon_p + \epsilon_q}{2} \pm \frac{1}{2}\sqrt{\{(\epsilon_p - \epsilon_q)^2 + 4\,|V_{pq}|^2\}}$$

In the occupation number formalism, we have

$$H|\Psi\rangle = \left[\sum_k \epsilon_k c_k^\dagger c_k + \sum_k V_{kl} c_k^\dagger c_l\right]|\Psi\rangle = E|\Psi\rangle \tag{7.34}$$

Since there is only one particle

$$|\Psi\rangle = \sum_j A_j |00\ldots 1_j, \ldots\rangle$$

Putting this in(7.34) and multiplying one the left by $\langle 00\ldots 1_i \ldots|$ gives

$$\Sigma A_j\,[H_{ij} - E\delta_{ij}] = 0$$

where

$$H_{ij} = \langle 00\ldots 1_i \ldots |H| \ldots 1_j \ldots \rangle$$
$$= \sum_k \epsilon_k \left\langle \ldots 1_i \ldots \left| c_k^\dagger c_k \right| \ldots 1_j \ldots \right\rangle + \sum_{k,l} V_{kl} \left\langle \ldots 1_i \ldots \left| c_k^\dagger c_l \right| \ldots 1_j \ldots \right\rangle$$

The real many-body case we shall deal with most often is one in which the external potential is zero and the interaction potential depends only on the distance between pairs of particles. In this case, $V_{kl} = 0$. Let's now work out the form of V_{klmn} in this case. Remembering $\mathbf{k} \equiv \mathbf{k}, \sigma$, and summing over spin variables yields

$$V_{k\sigma_1,l\sigma_2,m\sigma_3,n\sigma_4} = \frac{\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}}{\Omega^2} \int d^3\mathbf{r} \int d^3\mathbf{r}' V(\mathbf{r}-\mathbf{r}')\, e^{-i((\mathbf{k}-\mathbf{m})\cdot r + (\mathbf{l}-\mathbf{n})\cdot r']}$$
$$= \frac{\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}}{\Omega^2} \int d^3\rho V(\rho) e^{-i(\mathbf{k}-\mathbf{m})\cdot\rho} \int d^3\mathbf{r}' e^{-i(\mathbf{k}-\mathbf{m}+\mathbf{l}-\mathbf{n})\cdot\mathbf{r}'} \tag{7.35}$$
$$\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\Omega^{-2} V_{k-m}\Omega\delta_{k+l,m+n}$$

where

$$V_{k-m} = \int d^3\rho e^{-i(k-m)\cdot\rho} V(\rho) \tag{7.36}$$

and

$$V(\rho) = \frac{1}{(2\pi)^3} \int d^3\mathbf{k} e^{+i(\mathbf{k}-\mathbf{m})\cdot\rho} V_{k-m} \tag{7.37}$$

Since

$$I = \int d^3\mathbf{r} e^{-i(p-q)\cdot r} = \Omega\delta_{pq}$$

Equation (7.35) may be written

$$V_{m+q,\sigma_1,n-q,\sigma_2:m\sigma_3,n\sigma_4} = \Omega^{-1}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} V_q$$

The δ -functions express conservation of spin angular momentum (since V does not involve spin) and linear momentum (since V depends only on $\mathbf{r}-\mathbf{r}'$ and therefore cannot move the centre of mass).

Box

The Coulomb case where $V(\mathbf{r}-\mathbf{r}') = e^2/|\mathbf{r}'-\mathbf{r}|$ yields

$$V_{ko_1,\ldots,no_4} = \frac{\delta_{o_1\sigma_3}\delta_{\sigma_2\sigma_4}}{\Omega}\frac{4\pi e^2}{|\mathbf{k}-\mathbf{m}|^2}\delta_{k+l,m+n}$$

or

$$V_{q\sigma_1 o_2\sigma_3 o_4} = \delta_{\sigma_1\sigma_3}\delta_{o_2\sigma_4}\frac{4\pi e^2}{q^2}\times\frac{1}{\Omega} \tag{7.38}$$

7.5 Particle-hole formalism

A few comments about particle-hole formalism will be added here.

First of all, since particles in the particle-hole formalism exist only above the Fermi level $\mathbf{k}_F$ and holes exist only below, we may write:

$$\mathbf{k}_{\text{holo}} \neq \mathbf{k}_{\text{particle}} \tag{7.39}$$

Second, we can enlarge the commutation rules for the $c_i^\dagger, c_i$ to take care of holes. Using the definition of the a's and b's in Chapter 4, one can write out a complete set of rules for all these operators:

$$\begin{gathered}\left[a_k, a_l^\dagger\right]_+ = \delta_{kl}, \quad [a_k, a_l]_+ = \left[a_k^\dagger, a_l^\dagger\right]_+ = 0 \\ \left[b_m, b_p^\dagger\right]_+ = \delta_{mp}, \quad [b_m, b_p]_+ = \left[b_m^\dagger, b_p^\dagger\right]_+ = 0 \\ [a_k, b_m]_+ = \left[a_k, b_m^\dagger\right]_+ = \left[a_k^\dagger, b_m\right]_+ = \left[a_k, b_m^\dagger\right]_+ = 0\end{gathered} \tag{7.40}$$

Rewriting the many-body Hamiltonian in particle-hole scheme is straightforward. Making use of the definition and rules for the b's yields

$$H_0 = \sum_{k<k_F}\epsilon_k - \sum_{k<k_F}\epsilon_k b_k^\dagger b_k + \sum_{k>k_r}\epsilon_k a_k^\dagger a_k \tag{7.41}$$

Similarly

$$H_1 = \tfrac{1}{2}\sum_{k,l,m,n>k_F} V_{klmn} a_1^\dagger a_k^\dagger a_m a_n + \tfrac{1}{2}\sum_{\substack{k,l,m>k_F \\ n<k_F}} V_{klmn} a_l^\dagger a_k^\dagger a_m b_n^\dagger \\ + \cdots \tfrac{1}{2}\sum_{k,l,m,n<k_F} V_{klmn} b_l b_k b_m^\dagger b_n^\dagger \tag{7.42}$$

and

$$H_2 = \sum_{m,n>k_F} V_{mn} a_m^\dagger a_n + \sum_{\substack{m>k_F \\ n<k_F}} V_{mn} a_m^\dagger b_n^\dagger \\ + \sum_{m<k_F n<k_F} V_{mn} b_m a_n + \sum_{m,n<k_F} V_{mn} b_m b_n^\dagger \tag{7.43}$$

With the aid of (7.41), we can deduce an equation for the hole wave function. Suppose we have a system of N non-interacting particles filling the Fermi sea up to ϵ_F and remove N_h of them, thus creating N_h holes but not particles. Then (7.41) becomes

$$H_0^{\text{bole}} = W_0 - \sum_{k<k_F} \epsilon_k b_k^\dagger b_k$$

where

$$W_0 = \sum_{k<k_F} \epsilon_k \text{ and } \sum_k b_k^\dagger b_k = N_h$$

Hence we can reason backwards and conclude that H_0^{hole} in ordinary notation must be

$$H_0^{hole} = W_0 + \sum_{i=1}^{N_\text{h}} \left[\frac{-p_i^2}{2m} - U\left(\mathrm{r}_i\right)\right] \tag{7.44}$$

The corresponding wave equation for the single hole is

$$\left[\frac{p_i^2}{2m} + U(\mathbf{r})\right] \phi_k(\mathbf{r}) = -\epsilon_k \phi_k(\mathbf{r}) \tag{7.45}$$

Finally, it may be remarked that for the same reason that the hole energy is negative we find

hole momentum $= -\mathbf{k}$(for $U = 0$)

hole spin $= -\sigma$

hole charge $=-$ particle charge

7.6 Occupation number formalism based on single-particle position eigentates

The treatment up to now has been based on single-particle states which are eigenstates of the single-particle Hamiltonian, i.e., the energy operator. However,there is no law against using any convenient set of single-particle states. For example, eigenstates of the single-particle momentum or position operator. Because of its utility, we will discuss the case of a scheme based on the position operator $\hat{\mathbf{r}}$.

The single-particle position operator has the eigenvalue equation

$$\hat{\mathbf{f}}\delta(\mathbf{r}-\mathbf{R}) = \mathbf{R}\delta(\mathbf{r}-\mathbf{R}) \tag{7.46}$$

where the eigenvalue $\mathbf{R}$ is at any point in space. In a similar way, we have here the total position (i.e., center of mass) operator for N particles

$$\hat{R} = \sum_{i=1}^{N} \hat{r}_i \tag{7.47}$$

with eigenfunction

$$\Phi_{R_1,R_2,\ldots,R_N}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \frac{1}{(N!)^{\frac{1}{2}}} \begin{vmatrix} \delta(\mathbf{r}_1-\mathbf{R}_1)\ldots\delta(\mathbf{r}_N-\mathbf{R}_1) \\ \vdots \\ \delta(\mathbf{r}_1-\mathbf{R}_N)\ldots\delta(\mathbf{r}_N-\mathbf{R}_N) \end{vmatrix} \tag{7.48}$$

This is of caurse not an eigenstate of H_0. The transition to occupation number scheme is made by:

$$\begin{aligned} \Phi_{R_1,R_2,\ldots,R_N} &= \Phi_{n_{x_1},n_{x_2},\ldots,n_{x_i}} \\ &\equiv |n_{x_1},n_{x_2},\ldots,n_{x_i}\ldots\rangle \end{aligned} \tag{7.49}$$

where n_{x_i} is the particle number at the point $\mathbf{x}_i$. Thus, $|n_{x_1},n_{x_2},\ldots,n_{x_i}\ldots\rangle$ **describes the distribution of particles in space.**

Similarly, the creation and destruction operators here are: $c^{\dagger}_{x_1}, c_{x_1}$ which respectively create and destroy a particle at the point x_i. These operators are usually written in an form which makes them look as though they were ordinary wave functions:

$$\begin{aligned} \psi^{\dagger}(\mathbf{x}_i) &\equiv c^{\dagger}_{x_i} : \text{ creates particle at point } \mathbf{x}_i \\ \psi(\mathbf{x}_i) &\equiv c_{x_i} : \text{ destroys particle at point } \mathbf{x}_i \end{aligned} \tag{7.50}$$

The $\psi^\dagger(\mathbf{x}), \psi(\mathbf{x})$ are the basic field operators of quantum field theory. The combination

$$p(\mathbf{x}) = \psi^\dagger(\mathbf{x})\psi(\mathbf{x}) \tag{7.51}$$

is the number operator for this case, and has eigenfunctions. Since its eigenvalues are the number of particles ar the point $\mathbf{x}$, it is evidently just a **density operator**.

It is easy to show that the $\psi^\dagger(\mathbf{x}_i), \psi(\mathbf{x}_i)$, are related to the $c_i^\dagger, c_i$ the same transformation which connects the eigenfunctions $\delta(\mathbf{r}-\mathbf{R})$ to the $\phi_k(\mathbf{r})$. Thus, we have

$$\delta(\mathbf{r}-\mathbf{x}_i) = \sum_k A_{lk}\phi_k(\mathbf{r})$$

or

$$|00\ldots 1_{x_i} 00\ldots\rangle = \sum_k A_{ik}\,|00\ldots 1_k 00\ldots\rangle$$

or

$$c_{x_1}^\dagger|000\ldots\rangle = \sum_k A_{lk}c_k^\dagger|000\ldots\rangle$$

whence

$$\begin{array}{l}\psi^\dagger(x_i) = \sum_k A_{ik}c_k^\dagger \\ \psi(x_i) = \sum_k A_{ik}^* c_k\end{array} \tag{7.52}$$

where

$$A_{ik} = \int d^3r\phi_k^*(r)\delta(r-x_i) = \phi_k^*(x_i) \tag{7.53}$$

By using this transformation, it can be shown that the Hamiltonian may be written in terms of the field operators like this:

$$\begin{aligned}H = &\int d^3\mathbf{x}\psi^\dagger(\mathbf{x})\left[-\frac{1}{2m}\nabla_x^2 + U(\mathbf{x})\right]\psi(\mathbf{x}) + \\ &+\frac{1}{2}\iint d^3\mathbf{x}d^3\mathbf{x}'\psi^\dagger(\mathbf{x})\psi^\dagger(\mathbf{x}')\,V(\mathbf{x}-\mathbf{x}')\,\psi(\mathbf{x}')\,\psi(\mathbf{x})\end{aligned}$$

Substituting (7.52) into the first term of H with $\mathbf{x}\equiv\mathbf{x}_i$:

$$H_0 = \int d^3\mathbf{x_i}\sum_{k,l} A_{lk}c_k^\dagger\left[-\frac{1}{2m}\nabla_{x_i}^2 + U(x_i)\right]A_{il}^* c_l$$

Using (7.53), we find

$$\begin{aligned} H_0 &= \sum_{k,l} c_k^\dagger c_l \int d^3\mathbf{x}_i \phi_k\left(\mathbf{x}_i\right) \epsilon_l \phi_l^*\left(\mathbf{x}_i\right) \\ &= \sum_k \epsilon_k c_k^\dagger c_k \end{aligned}$$

The transformation (7.52) allows us to break $\psi^\dagger$,ψ up into "particle" and "hole" parts, thus:

$$\begin{aligned} \psi^\dagger\left(\mathbf{x}_i\right) &= \sum_{k>k_F} A_{ik} a_k^\dagger + \sum_{k<k_F} A_{ik} b_k \\ &= \psi_{part}^\dagger\left(\mathbf{x}_i\right) + \psi_{hole}\left(\mathbf{x}_i\right) \end{aligned} \tag{7.54}$$

$$\psi\left(x_i\right) = \psi_{\text{hole}}^\dagger\ \left(x_i\right) + \psi_{\text{part}}\ \left(x_i\right) \tag{7.55}$$

7.7 Bosons

The occupation number story can easily be re-written with the boson as protagonist. We find:

(1) The wavefunction becomes replaced by the symmetrized

$$\begin{aligned} \Phi_{k_1,k_2\ldots k_N}\left(\mathbf{r}_1,\ldots,\mathbf{r}_N\right) &= \sqrt{\left(\frac{n_1!n_2!\ldots}{N!}\right)\sum_P (+1)P\left[\phi_{k_1}\left(\mathbf{r}_1\right)\ldots\phi_{k_N}\left(\mathbf{r}_N\right)\right]} \\ &= \Phi_{n_1,\ldots,n_1,\ldots}\left(\mathbf{r}_1,\ldots,\mathbf{r}_N\right) \equiv \left\langle \mathbf{r}_1,\ldots,\mathbf{r}_N | n_1,\ldots,n_i,\ldots\right\rangle \end{aligned} \tag{7.56}$$

where: $n_i = 0,1,2,3,\ldots$

(2)The $c_i^\dagger, c_i$ operators are re-defined by

$$\begin{aligned} c_i^\dagger\left|n_1\ldots n_i\ldots\right\rangle &= \sqrt{\left(n_i+1\right)}\left|n_1,\ldots,n_i+1,\ldots\right\rangle \\ c_i\left|n_1\ldots n_i\ldots\right\rangle &= \sqrt{n_i}\left|n_1,\ldots,n_i-1,\ldots\right\rangle \end{aligned} \tag{7.57}$$

(3) The commutation relations are replaced by

$$\begin{aligned} \left[c_l, c_k^\dagger\right]_- &= c_l c_k^\dagger - c_k^\dagger c_l = \delta_{lk} \\ \left[c_l, c_k\right]_- &= 0 \\ \left[c_l^\dagger, c_k^\dagger\right]_- &= 0 \end{aligned} \tag{7.58}$$

(4) There are no holes in the boson case, hence no particle-hole formalism.

(5) The one- and two-body operators are the same as in the fermion case, hence also the expression for the Hamiltonian. (**This is not true for phonons, where the interaction terms may involve the product of any number of creation and destruction operators**)

8 More about Quasi Particles

8.1 A soluble fermion system: The pure Hartree model

Imagine that we have an N-fermion system with no external potential, and with a pure forward-scattering interaction between particles of the form

$$V_{klmn} = V_{klkl}\delta_{mk}\delta_{nl}$$

Placing this in the general Hamiltonian yields

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \frac{1}{2}\sum_{ki} V_{klkl} c_l^\dagger c_k^\dagger c_k c_l \tag{8.1}$$

This model H will be called the 'pure Hartree' Hamiltonian, since, as we shall show, the only terms in it are those giving rise to the 'Hartree effective field'. Our object here is to get a solution to the problem in the form of

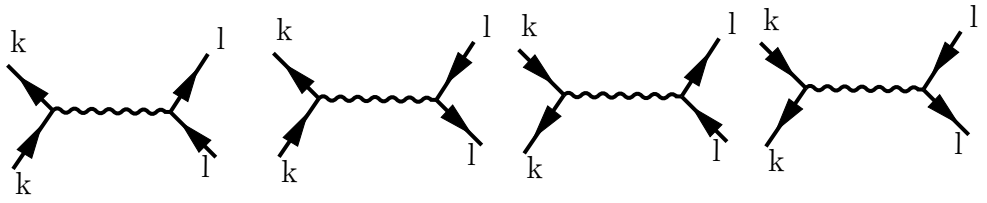
$$H' = E_0 + \sum_q \epsilon_q' A_q^\dagger A_q + \underbrace{f\left(\ldots, A_q, \ldots, A_q^\dagger, \ldots\right)}_{\text{small}} \tag{8.2}$$

from

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \frac{1}{2}\sum_{k,l,m,n} V_{klmn} c_l^\dagger c_k^\dagger c_m c_n \tag{8.3}$$

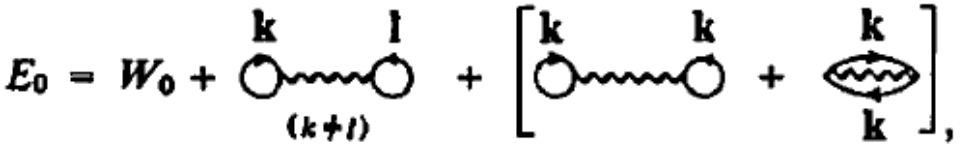
, i.e., the ground state energy plus a set of approximately independent elementary excitations above the ground state. We do this by the straightforward diagrammatic method.

The interaction (8.1) has only the simple forms



(8.4)

Hence the only graphs occurring in the series for the ground state energy are



(8.5)

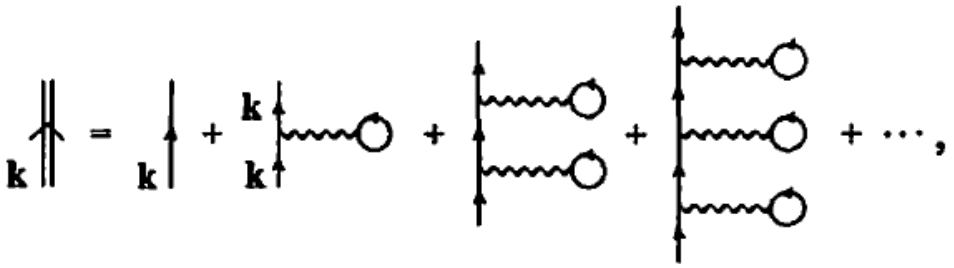
Note that **the propagator lines in these diagrams are all hole lines. Also the diagrams in brackets violate the exclusion principle since there are simultaneously two hole lines in state k**.

$$E_0 = \sum_{k<k=7} \epsilon_k + \frac{1}{2} {\sum_{k,l<k_F}}' V_{klkl} \tag{8.6}$$

$\mathbf{k}\neq\mathbf{l}$

The $\mathbf{k} = \mathbf{l}$ graphs cancel because of the fermion loop in bubble diagram.

Now let us get the quasi particle energies, ϵ'_k, from the poles of the Green's function. In this case, the propagator is given exactly by the sum over just the bubble graphs:

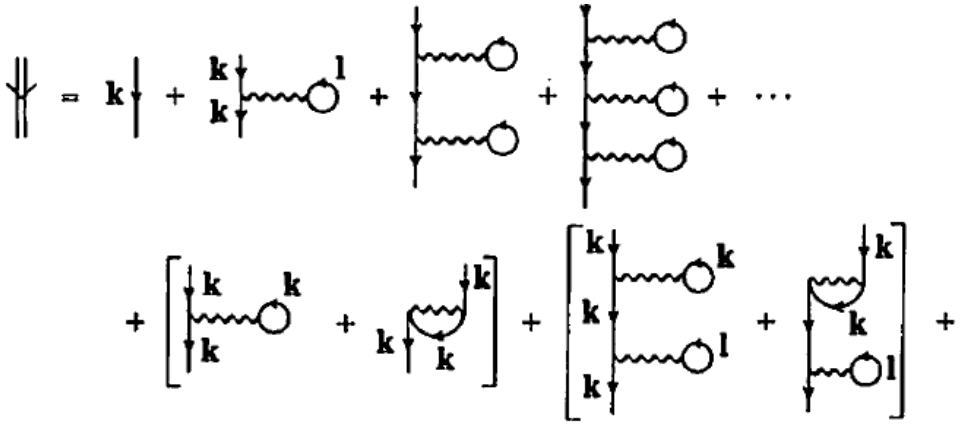


(8.7)

Series (8.7) was summed and gives the result for quasi particle energy, as shown in chapter 4,

$$\begin{array}{l} \epsilon'_k = \epsilon_k + \sum_{l<k_F} V_{klkl}, \quad k > k_F \\ \tau_k = \infty \end{array} \tag{8.8}$$

In the case of quasi holes we just sum

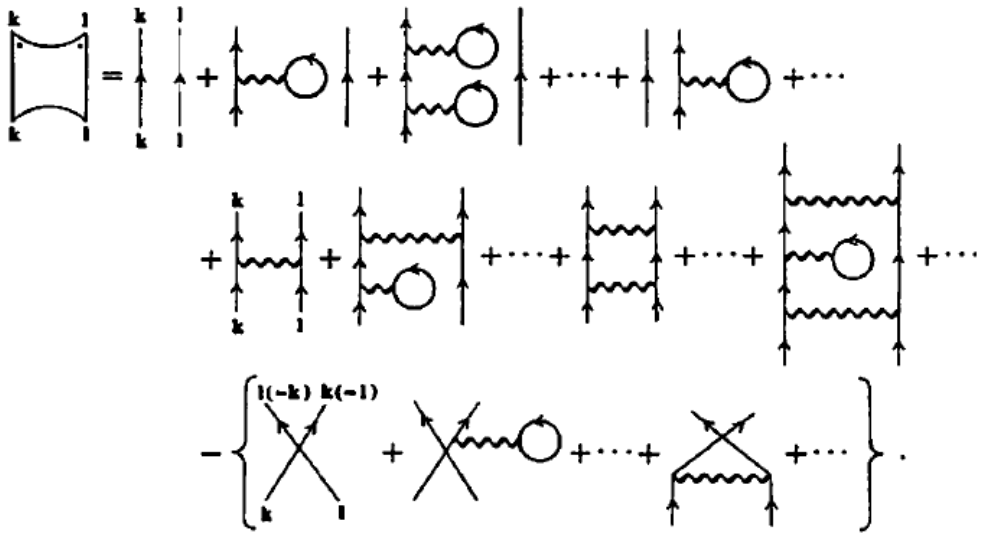


(8.9)

The bracketed diagrams cancel because of the fermion loop and we get the result:

$$\begin{array}{l} \epsilon'_k = \epsilon_k + {\sum_{l<k_F}}' V_{klkl}, \quad k < k_F \\ \tau_k = \infty \end{array} \tag{8.10}$$

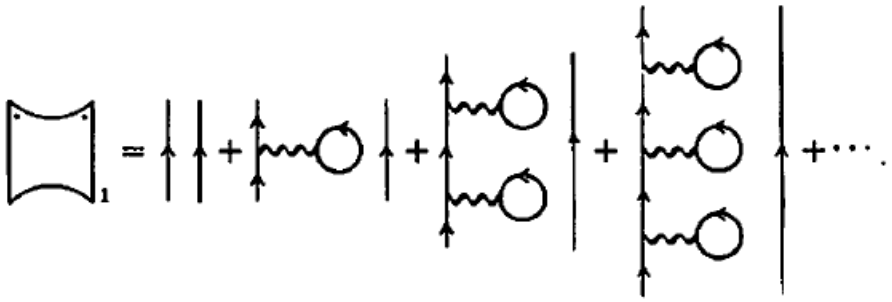
Finally, we need the interaction between quasi particles (f-term in (8.1)).This can be obtained from the various two-particle propagators. Consider the particle-particle propagator first. In the present case, this is given by the sum:



(8.11)

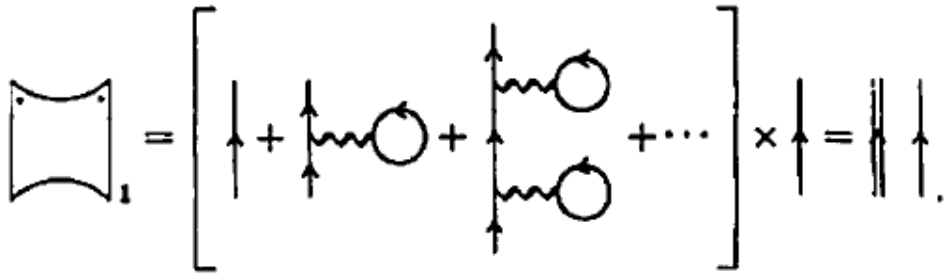
The crossed "exchange" diagrams in the brackets in (8.11) contribute only when $\mathbf{k} = \mathbf{l}$. because the labels on the incoming and outgoing lines in each diagram must match those of G_2 on the left. **Since these diagrams are negative, they cancel all the uncrossed diagrams when $\mathbf{k} = \mathbf{l}$, so $G_2 = 0$ for $\mathbf{k} = \mathbf{l}$.**

We can greatly simplify (8.11) in the following way: Consider the diagram subset consisting of more and more bubbles inserted into the first propagator,i.e.,:



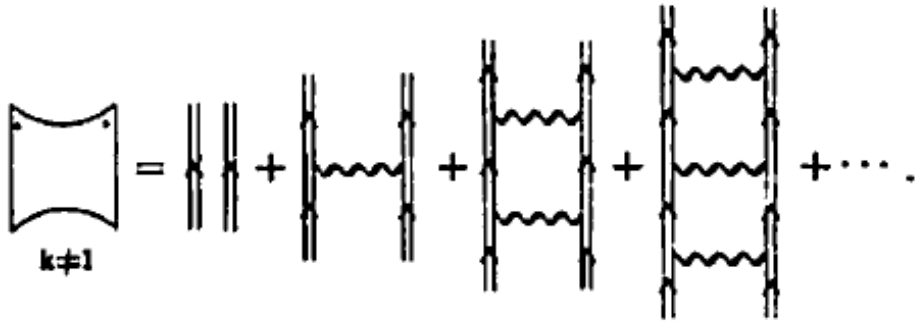
(8.12)

This can be summed as:



(8.13)

Similarly, we sum over all bubble insertions in all bare propagators, leading to a sum in which all propagators are clothed,i.e., in which all propagators are the quasi particle propagators:



(8.14)

In this form, we can see that the quasi particle interaction is:$V = V_{klkl}(l \neq k), V = 0(l = k)$. Similar arguments applied to the particle-hole and hole-hole propagators yield this same interaction.

We can now combine these results into a Hamiltonian of form (8.1). The expressions for E_0 and ϵ'_q are in (8.6),(8.8), and (8.10). The interaction term f in (8.1) will have the form

$$H_1 = \frac{1}{2} \sum_{k,l,m,n} V_{klmn} c^\dagger, c_k^\dagger c_m c_n$$

since the quasi particles here are fermions.

Letting $A_k^\dagger, A_k, B_k^\dagger, B_k$, be the quasi particle and quasi hole operators we find

$$\begin{aligned} H' = [\sum_{k<k_F} \epsilon_k + \frac{1}{2} {\sum_{k,l<k_F}}' V_{klkl}]+ \\ + \sum_{k<k_F} \left(\epsilon_k + \sum_{l<k_p} V_{klkl} \right) A_k^\dagger A_k - \sum_{k<k_F} \left(\epsilon_k + {\sum_{l<k_F}}' V_{klkl} \right) B_k^\dagger B_k + \\ + \frac{1}{2} {\sum_{l,k>k_F}}' V_{klkl} A_l^\dagger A_k^\dagger A_k A_l - \sum_{\substack{k>k_F \\ l<k_F}} V_{klkl} B_l^\dagger A_k^\dagger A_k B_l + \\ + \frac{1}{2} {\sum_{\substack{k<k_F \\ l<k_F}}}' V_{klkl} B_l^\dagger B_k^\dagger B_k B_l \end{aligned} \tag{8.15}$$

Observe that in the particle-particle and hole-hole interaction terms, **it is necessary to put in a factor $\frac{1}{2}$ to avoid counting interactions twice when we sum freely over k and l.** Note that the $(-)$ sign in the $B_k^1 B_k$ term is put in because the hole energies (and therefore the quasi hole energies) are negative. The (-) in the $B_l^t A_k^1 A_k B_l$ term occurs for the following reason: The energy of a quasi particle in, say, state $k_1 > k_F$, includes interactions with all particles in the filled Fermi sea. But if there is a hole in, say, state $l_1 < k_F$, then the corresponding energy,$V_{k_1 l_1 k_1 l_1}$ does not exist, and should be subtracted from the quasi particle energy. The term $-V_{k_1 l_1 k_1 l_1} B_{l_1}^\dagger A_{k_1}^\dagger A_{k_1} B_{l_1}$ takes care of this substraction.

8.2 Crude calculation of quasi particle lifetime

We mentioned that the quasi particle picture breaks down if the energy is two far away from the Fermi energy. In a Fermi system, since one deals with particle-like excitation above ϵ_F' (the Fermi energy of the interacting system), and hole-like ones below, the criterion is taken relative to the Fermi energy, i.e.:

$$\frac{1}{\tau_k} \ll \epsilon_k' - \epsilon_F' \tag{8.16}$$

In the pure Hartree model,$\tau_k = \infty$, so this is satisfied for any k. But this is not true in general. In fact, we are now going to show that in most Fermi systems the quasi particle

lifetime obeys

$$\frac{1}{\tau_k} \propto (\epsilon'_k - \epsilon'_F)^2 \tag{8.17}$$

Here we will give a crude quasi-proof of (8.17).

The lifetime of a quasi particle in momentum state **k** will be the **inverse of the transition probability per second that the quasi particle will be scattered out of state k by collisions with other quasi particles**. Let us pretend that quasi particle collisions are like those between real particles (they are not, actually, since quasi particles can have a 'retarded', i.e., time-dependent, interaction even when the bare particles interact instantaneously) and calculate the transition probability out of state $\mathbf{k}_1$ for a particle in state $\mathbf{k}_1$, where $|\mathbf{k}_1| \geq k_F$. In a typical interaction, the particle will collide with a particle in state $|\mathbf{k}_2| \leq k_F$ and final state will be a particle in $\mathbf{k}_3$ and $\mathbf{k}_4$, where

$$\mathbf{k}_4 = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 \tag{8.18}$$

The transition probability is

$$W_{k_1} \propto \int d^3k_2 \int d^3k_3 \, |V_{k_3,k_1+k_2-k_3,k_1,k_2}|^2 \tag{8.19}$$

To evaluate (8.19) we note that by the Pauli principle all states under k_F are occupied so that

$$|\mathbf{k}_3| \geqslant k_F, \quad |\mathbf{k}_4| \geqslant k_F \tag{8.20}$$

by conservation of energy,

$$k_1^2 + k_2^2 = k_3^2 + k_4^2 \tag{8.21}$$

The equations above imply that

$$k_1^2 + k_2^2 \geqslant 2k_F^2 \tag{8.22}$$

Consider first the limiting case when $|\mathbf{k}_1| = k_F$. Then by (8.22), $k_2^2 \geqslant k_F^2$. But since $|\mathbf{k}_2| \leqslant k_F$, this implies $|\mathbf{k}_2| = k_F$. Similarly, $|\mathbf{k}_3| = |\mathbf{k}_4| = k_F$. **That is, all momenta lie on the Fermi sphere.** Suppose now that $|\mathbf{k}_1| = k_F + \delta$ where $k_F \gg \delta > 0$. Then by (8.22) , $|\mathbf{k}_2| \geqslant k_F - \delta$. Similarly, since $|\mathbf{k}_2| \leqslant k_F$, we have that in order to satisfy (8.21), $|\mathbf{k_3}|$, $|\mathbf{k}_4|$ must be less than $k_F + \delta$. Hence all momenta lie in a shell of thickness $\delta = |\mathbf{k}_1| - k_F$ around the Fermi sphere.

Assuming there's nothing peculiar about the behaviour of V, the integral over the $\mathbf{k}_2$ -shell gives a factor $\propto 4\pi k_F^2 \left(|\mathbf{k}_1| - k_F\right)$, and the same for the $\mathbf{k}_3$ -shell, so

$$W_{k_1} \propto \left(|\mathbf{k}_1| - k_F\right)^2 \tag{8.23}$$

But

$$\begin{aligned} \epsilon_{k_1} - \epsilon_p \propto \left(k_1^2 - k_F^2\right) &= \left(|\mathbf{k}_1| - k_P\right)\left(|\mathbf{k}_1| + k_F\right) \\ &\approx 2k_F \left(|\mathbf{k}_1| - k_F\right) \end{aligned} \tag{8.24}$$

Whence

$$\frac{1}{\tau_k} = W_k \propto \left(\epsilon_k - \epsilon_F\right)^2 \tag{8.25}$$

8.3 General form of quasi particle propagator

We have learned that the single-particle propagator or "Green's function" is defined as

$$G\left(k_2, k_1, t_2 - t_1\right) = G^+\left(k_2, k_1, t_2 - t_1\right)_{t_2 > t_1} + G^-\left(k_2, k_1, t_2 - t_1\right)_{t_2 \leq t_1} \tag{8.26}$$

where $iG^+(k_2, k_1, t_2 - t1)$ is probability amplitude that if at time t_1 we add a particle in ϕ_{k_1} to the interacting system in its ground state, then at time t_2 the system will be in its ground state with an added particle in ϕ_{k_2}, and $-iG^-(k_2, k_1, t_2 - t1)$ is probability amplitude that if at time t_2 we add a hole in ϕ_{z_2} to the interacting system in its ground state, then at time t_1 the system will be in its ground state with an added hole in ϕ_{k_1}. (**The "-" sign on G^- is for fermions; bosons have a $+iG^-$ instead.**) These results may be written in a compact way by introducing the functions

$$\theta_x \begin{cases} = 1, & \text{for } x > 1 \\ = 0, & \text{for } x < 1 \end{cases}; \quad \delta_k \begin{cases} = +\delta, & \epsilon_k > \epsilon_F \\ = -\delta, & \epsilon_k < \epsilon_F \end{cases} \tag{8.27}$$

Letting $t = t_2 - t_1$, this c=gives

$$\begin{aligned} G_0(k,t) &= -i\left[\theta_t \theta_{\epsilon_k - \epsilon_F} e^{-i\epsilon_k t} - \theta_{-t}\theta_{\epsilon_F - \epsilon_k} e^{-i\epsilon_k t}\right], \quad t \neq 0 \\ &= +i\theta_{t_{p-t_2}}, \quad t = 0 \end{aligned} \tag{8.28}$$

and

$$G_0(k,\omega) = \frac{1}{\omega - \epsilon_k + i\delta_k} \tag{8.29}$$

Now in Chapter 3 we argue that in systems describable by quasi particles, G will look like G_0 except for replacing $\epsilon_{\mathbf{k}}$ by $\epsilon'_{\mathbf{k}}$, introducing a lifetime τ_k, and an amplitude factor, Z_k as in (3.11,3.12). However, this is not quite right, because it neglects the fact that when the bare particle is first put into the system, it will take some finite time, say t_c, for it to become 'clothed' so it will not act like a quasi particle until $t_2 - t_1 > t_c$. Further, it can be shown that the quasi particle expression for the propagator is no longer valid when $t_2 - t_1 \gg \tau_k$ where τ_k is the lifetime. For this reason **it is necessary to write the propagator as the sum of a pure quasi particle part plus a correction term which will be important for $t < t_e$ and $t > \tau_k$.** This consideration yields (setting $t = t_2 - t_1$ and $t \neq 0$):

$$\begin{aligned} G_{\substack{quasi \\ particle}}(k,t) = &- iZ_k \Big[\theta_t \theta_{\epsilon'_k - \epsilon'_F} e^{-i\left(\epsilon'_k - i\tau_k^{-1}\right)t} - \\ &-\theta_{-t}\theta_{\epsilon'_F - \epsilon'_k} e^{-i\left(\epsilon'_k + i\tau_k{}^{-1}\right)t}\Big] + F(k,t) \end{aligned} \tag{8.30}$$

where $0 < Z_k \leqslant 1$ (Z_k independent of t). Don't be scared by the term of $\epsilon'_k \pm i\tau_k^{-1}$. For G_0 we have $\epsilon_k \pm i\delta$. Since δ is infinitesimally small, so we have instead ϵ_k in the exponential of G_0. So they are the same thing with different lifetime.(finite vs. infinite)

Taking the Fourier transform :

$$G_{\substack{quasi \\ particle}}(k,\omega) = \frac{Z_k}{\omega - \epsilon'_k + i\left[2\theta_{\epsilon'_k - \epsilon'_F} - 1\right]\tau_k^{-1}} + F(k,\omega) \tag{8.31}$$

It must be remembered that these are bona fide quasi particles only if

$$\frac{1}{\tau_k} \ll \epsilon'_k - \epsilon'_F \tag{8.32}$$

9 The Single-Particle Propagator Re-Visited

9.1 Mathematical expression for the single-particle Green's function propagator

The closed mathematical expression for the propagator,G, appears usually in one of two forms:

$$\begin{aligned} G\left(k_2,k_1,t_2-t_1\right) &= -i\left\langle \Psi_0 \left| T\left\{ c_{k_2}\left(t_2\right) c_{k_1}^{\dagger}\left(t_1\right)\right\}\right| \Psi_0\right\rangle \\ G\left(\mathrm{r}_2,\mathrm{r}_1,t_2-t_1\right) &= -i\left\langle \Psi_0 \left| T\left\{ \psi\left(\mathrm{r}_2,t_2\right)\psi^{\dagger}\left(\mathrm{r}_1,t_1\right)\right\}\right| \Psi_0\right\rangle \end{aligned} \tag{9.1}$$

We shall only consider the first form-the second may be analysed in a similar way. First, Ψ_0 is the exact normalized wave function of the ground state of the interacting N -particle system. The operators $c_k(t), c_k^{\dagger}(t)$ respectively, destroy and create a particle in state k at time t. More precisely, they are the ordinary $c_k, c_k^{\dagger}$ transformed to 'Heisenberg picture', defined by

$$\begin{aligned} c_{k_1}^{\dagger}\left(t_1\right) &= e^{+iHt_1} c_{k_1} e^{-iHt_1} \\ c_{k_2}\left(t_2\right) &= e^{+iHt_2} c_{k_2} e^{-iHt_2} \end{aligned} \tag{9.2}$$

Finally the Wick time-ordering operator, T, is defined by

$$\begin{aligned} T\left\{A\left(t_1\right)B\left(t_2\right)\ldots\right\} =& (-1)^P \times \text{operators rearranged so that time} \\ & \text{decreases from left to right, assuming} \\ & \text{no two times are equal,} \\ =& (-1)^P \times \text{operators rearranged so all } c^{\dagger}\text{'s (or} \\ & a^{\dagger}\text{' s or } b\text{'s) stand to the left of } c\text{'s (or} \\ & a\text{'s or } \boldsymbol{b}^{\dagger}\text{ 's) for the case of equal} \\ & \text{times)} \end{aligned} \tag{9.3}$$

where P is the number of interchanges of operators required to get the operators in the proper time order, starting with the order given in the brackets.

Thus,

$$\begin{aligned} T\left\{c_{k_2}\left(t_2\right) c_{k_1}\left(t_1\right)\right\} &= c_{k_2}\left(t_2\right) c_{k_1}^{\dagger}\left(t_1\right) \text{ for } t_2 > t_1 \\ &= -c_{k_1}^{\dagger}\left(t_1\right) c_{k_2}\left(t_2\right) \text{ for } t_2 \leqslant t_1 \end{aligned} \tag{9.4}$$

and

$$\begin{aligned} G = G^{+}\left(k_2, k_1, t_2 - t_1\right) &= -i\left\langle \Psi_0 \left| c_{k_2}\left(t_2\right) c_{k_1}^{\dagger}\left(t_1\right) \right| \Psi_0 \right\rangle, \quad t_2 > t_1 \\ = G^{-}\left(k_2, k_1, t_2 - t_1\right) &= +i\left\langle \Psi_0 \left| c_{k_1}^{\dagger}\left(t_1\right) c_{k_2}\left(t_2\right) \right| \Psi_0 \right\rangle, \quad t_2 \leqslant t_1 \end{aligned} \tag{9.5}$$

Consider the $t_2 > t_1$ case first, we have

$$G^{+} = -\underbrace{I\left\langle \Psi_0 \right| e^{iHt_2} c_{k_2}}_{B^{\dagger}} \underbrace{e^{-iH(t_2-t_1)} c_{k_1}^{\dagger} e^{-iHt_1} \left| \Psi_0 \right\rangle}_{A} \tag{9.6}$$

Now $exp(-iHt)$ is the time development operator, so that $exp(-iHt_1)|\Psi_0\rangle$ is the ground state at time t_1, and $c_{k_1}^{\dagger} exp(-iHt_1)|\Psi_0\rangle$ is the state with one particle in ϕ_{k_1} added to the ground state at time t_1. Hence **A** is the state of the system at time t_2 when a particle ϕ_{k_1} was added at t_1. The $B^{\dagger}$ is

$$B^{\dagger} = \overline{c_{k_2}^{\dagger} e^{-iHt_2} |\Psi_0\rangle} \tag{9.7}$$

This is the complex conjugate of the state with one particle in ϕ_{k_2} added to the ground state at time t_2. Hence we obtain

$$\begin{aligned} G^{+} = B^{\dagger} A &= \text{component of B along A} \\ &= \text{probability amplitude that the state of the system} \\ &\quad \text{at } t_2\text{, when a particle in } \phi_{k_1} \text{ was added to the} \\ &\quad \text{ground state at } t_1\text{, is the state with one particle in} \\ &\quad \phi_{k_2} \text{ added to the ground state at time } t_2 \end{aligned} \tag{9.8}$$

It is a good brain-building exercise to show how (9.1) boils down to the expression for the free propagator (8.28), in the non-interacting case. The non-interacting Hamiltonian and ground state are given by

$$H_0 = \sum_p \epsilon_p c_p^{\dagger} c_p, \quad H_0 \left|\Phi_0\right\rangle = \sum_{p<k_F} \epsilon_p \left|\Phi_0\right\rangle, \quad \left|\Phi_0\right\rangle = \left|111\ldots1_F 000\ldots\right\rangle \tag{9.9}$$

Let us calculate just G_0^{+} setting $t_1 = 0, t_2 = t$:

$$G_0^{+}(k,t) = -i\left\langle \Phi_0 \left| e^{+iH_0 t} c_k e^{-iH_0 t} c_k^{\dagger} \right| \Phi_0 \right\rangle \theta_t \tag{9.10}$$

In an obvious notation,

$$c_k^\dagger \left|\Phi_0\right\rangle = (-1)^N \left|\Phi_0, 1_k\right\rangle \theta_{\epsilon_k - \epsilon_F} \tag{9.11}$$

Thus k must be greater than k_F. Now

$$H_0 \left|\Phi_0, 1_k\right\rangle = \sum_p \epsilon_p c_p^\dagger c_p \left|\Phi_0, 1_k\right\rangle = \left[\sum_{p<k_F} \epsilon_p + \epsilon_k\right] \left|\Phi_0 1_k\right\rangle \tag{9.12}$$

Thus

$$c_k e^{-iH_0 t} \left|\Phi_0, 1_k\right\rangle = (-1)^N \left|\Phi_0\right\rangle \exp\left\{-i\left[\sum_{p<k_F} \epsilon_p + \epsilon_k\right] t\right\} \tag{9.13}$$

Finally we have

$$G_0^+(k,t) = -i\theta_{\epsilon_k - \epsilon_F} \theta_t e^{-i\epsilon_k t} \tag{9.14}$$

confirming (8.28). It is now easy to obtain the ground state expectation value of any single-particle operator in terms of the propagator (7.19), thus

$$\left\langle \Psi_0 \left| \mathcal{O}^{occ} \right| \Psi_0 \right\rangle = -i \sum_{kl} \mathcal{O}_{kl} \lim_{t \to 0^-} G(l,k;t) \tag{9.15}$$

9.2 Spectral density function

The spectral density function is indispensable for analysing the mathematical properties of propagators, especially their analytic properties. Secondly, it is extremely convenient to use in many-body calculations which **involve diagrams containing 'dressed' or 'renormalized' propagators**. Here we provide a brief introduction to the subject here. More details can be found in Appendix.

The idea is similar to the spectral decomposition of a time-dependent function $f(t)$ into the sum of its components at various frequencies:

$$f(t) = \int_{-\infty}^{+\infty} F(\omega) e^{i\omega t} d\omega \tag{9.16}$$

where $F(\omega)$ gives the spectrum of $f(t)$. The corresponding expression for the propagator is, for a system with no external potential:

$$\begin{aligned} G(\mathbf{k},t) &= -i\int_0^\infty d\omega A^+(\mathbf{k},\omega)e^{-i(\omega+\mu)t}, \quad t>0 \\ &= +i\int_0^\infty d\omega A^-(\mathbf{k},\omega)e^{+i(\omega-\mu)t}, \quad t\leqslant 0 \end{aligned} \tag{9.17}$$

where μ is the chemical potential:

$$\mu = \begin{bmatrix}\text{ground state energy}\\ \text{of interacting } N\\ \text{particle system}\end{bmatrix} - \begin{bmatrix}\text{ground state energy}\\ \text{of interacting } N-1\\ \text{particle system}\end{bmatrix} = E_0^N - E_0^{N-1} \tag{9.18}$$

The $\mathbf{A}^\pm(\mathbf{k},\omega)$ is the "spectral density function". The Fourier transform of (9.17) yields

$$G(\mathbf{k},\omega) = \int_0^\infty d\omega' \left\{ \frac{A^+(\mathbf{k},\omega')}{\omega-\omega'-\mu+i\delta} + \frac{A^-(\mathbf{k},\omega')}{\omega'+\omega-\mu-i\delta}\right\} \tag{9.19}$$

which is the so-called 'Lehmann representation' of the propagator, especially useful for discussing analytic properties. The spectral density has the important properties that

$$\begin{aligned} A^\pm(\mathbf{k},\omega) &\gtrless 0, \quad \text{real} \\ \textstyle\int_0^\infty \left[A^+(\mathbf{k},\omega)+A^-(\mathbf{k},\omega)\right] d\omega &= 1 \quad (^*\text{ "sum rule"}) \end{aligned} \tag{9.20}$$

For free particles the spectral density is a $\delta-$function:

$$A_0^\pm(\mathbf{k},\omega) = \delta\left(\pm\omega - \epsilon_k + \mu\right) \tag{9.21}$$

For quasi particles, the $\delta-$function gets broadened out and we find the Lorentz form

$$A^\pm_{\text{quasi}}(\mathbf{k},\omega) = \frac{1}{\pi}\frac{(1/\tau_k)\,Z_k}{\left[\omega \mp (\epsilon_k' - \mu)\right]^2 + (1/\tau_k)^2} + D(\mathbf{k},\omega) \tag{9.22}$$

where $D(\mathbf{k},\omega)$ is a correction required so that the sum rule is satisfied. Finally, we note that if (3.48) is applied to (9.19) we obtain the following to calculate $\mathbf{A}^\pm$:

$$\begin{aligned} A^+(\mathbf{k},\omega-\mu) &= -\tfrac{1}{\pi}\,\mathrm{Im}\,G(\mathbf{k},\omega), \quad \omega>\mu \\ A^-(\mathbf{k},\mu-\omega) &= +\tfrac{1}{\pi}\,\mathrm{Im}\,G(\mathbf{k},\omega), \quad \omega<\mu \end{aligned} \tag{9.23}$$

9.3 Topology of diagrams

In order to develop general methods for working with diagrams, we need a systematic way of drawing all graphs in nth order. This will be discussed now.

The method of drawing the diagrams may be greatly simplified if we associate the full propagator, $G = G^- + G^+$ with directed lines instead of just G^+ or G^-. This is called the "**Feynman method**". Then in the integrals over intermediate times we automatically get $G_0(t'-t) = G_0^+$ when $t' > t$ and $G_0(t'-t) = G_0^-$ when $t' \leqslant t$. Thus it is no longer necessary to draw any hole lines since a directed line is a particle line for $t' > t$ and a hole line for $t' < t$. Thus the time order of the dots is no longer important.

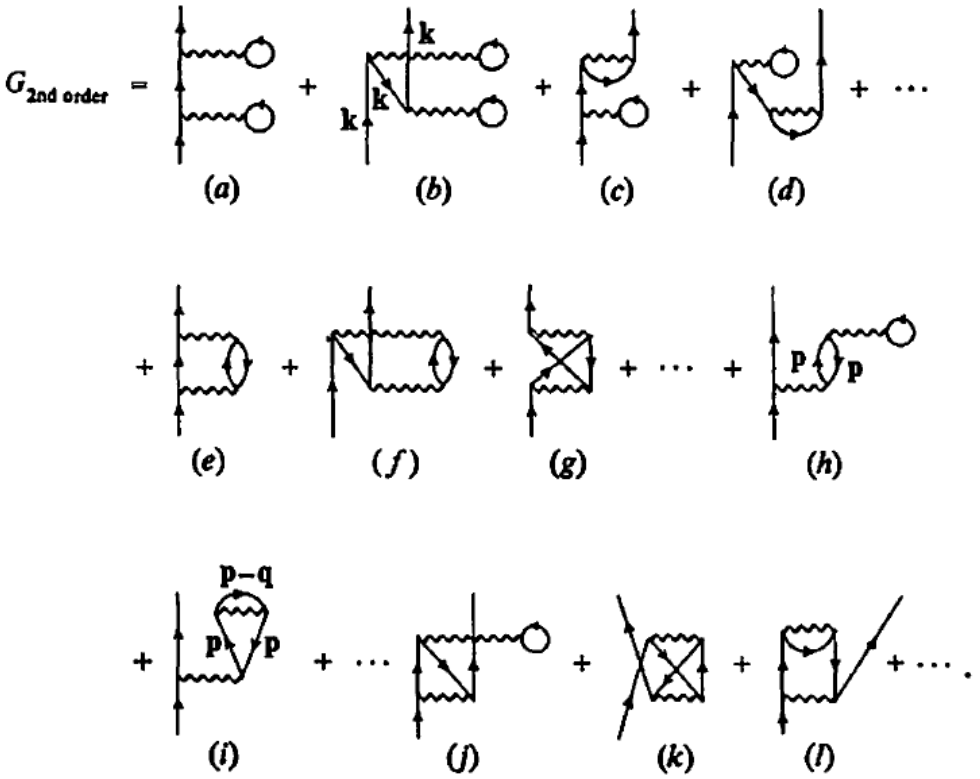
Drawing diagrams in the case of mutually interacting fermions with no external potential is considerably more difficult. To get all nth-order Goldstone diagrams, drawn wiggly lines each with vertex dots at both ends, and two fixed points, thus (note that the wiggles may have any vertical position relative to the fixed points). Join all points to each other with directed lines in all linked topologically distinct (in the Goldstone sense) ways such that one line enters and one leaves each vertex point, and a line enters one external point and leaves the other.

To illustrate, a few typical 2nd-order ones are shown in (9.24). Many of the diagrams in (9.24) can be eliminated. First because of conservation of momentum, graphs (b),(d),(h),(i),(j),(l) have a particle and a hole both in the same momentum state. But this is impossible in particle-hole formalism.

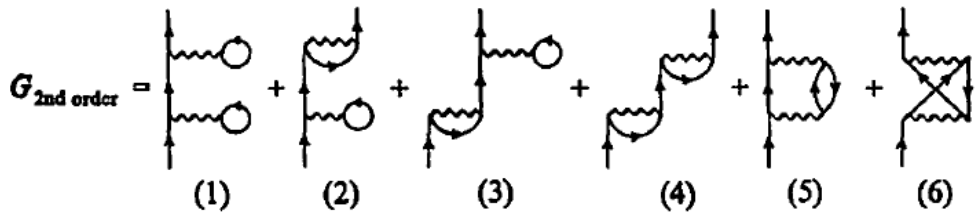
Box

Such graphs are called 'anomalous' or 'momentum non-conserving'. They do give a contribution when the system is non-isotropic, e.g. external field present, or at finite temperatures.

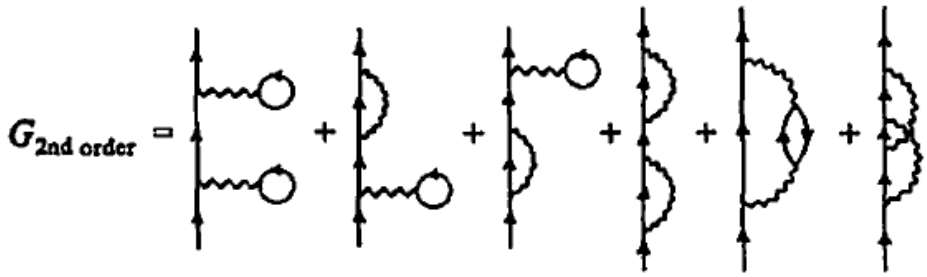
Second, it we agree to use the Feynman convention in which the full G is associated with each line and time order has no significance, then $(f) \equiv (e), (g) \equiv (k)$. Hence the only survivors are (9.25) or (9.26), where (9.26) is another conventional way of drawing the diagrams (obtained by making the diagrams out of rubber bands and pulling at top and bottom until the main line is straight). Equations (9.25) and (9.26) are topologically equivalent in the Feynman sense.



(9.24)

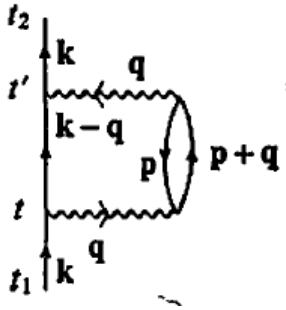


(9.25)



(9.26)

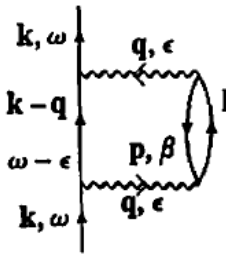
Let us evaluate a typical second-order diagram using the Feynman method.



$$= (-1)\sum_{q,p} \int_{-\infty(1-i\eta)}^{+\infty(1-i\eta)} dt\, dt' [iG_0(\mathbf{k}, t-t_1)][-iV_q] \times$$
$$\times [iG_0(\mathbf{k}-\mathbf{q}, t'-t)][iG_0(\mathbf{p}, t-t')] \times$$
$$\times [iG_0(\mathbf{p}+\mathbf{q}, t'-t)][-iV_q][iG_0(\mathbf{k}, t_2-t')].$$

(9.27)

Note that the order of the times in G is always: time at end of directed line minus time at beginning. The Fourier transform of (9.27) is

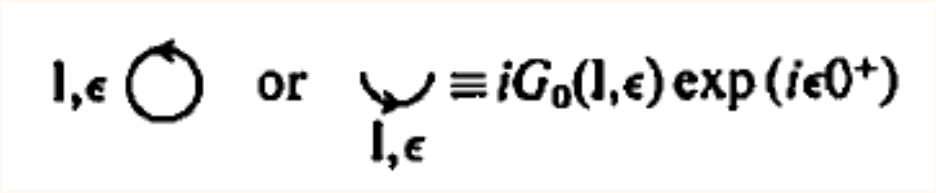


$$= (-1)[iG_0(\mathbf{k}, \omega)]^2 \sum_{p,q} \int \frac{d\epsilon}{2\pi} \frac{d\beta}{2\pi} [iG_0(\mathbf{k}-\mathbf{q}, \omega-\epsilon)] \times$$
$$\times [iG_0(\mathbf{p}, \beta)][iG_0(\mathbf{p}+\mathbf{q}, \beta+\epsilon)][-iV_q]^2.$$

(9.28)

It is seen that the frequencies, ω, ϵ, β, etc., are conserved at the vertices, just like the momentum. This comes about because of the appearance of δ -functions similar to the $2\pi\delta(\omega' - \omega)$ when the transform is carried out. **The "2π" in $\frac{d\epsilon}{2\pi}$ comes from Fourier transformation too.**

One more thing, We can avoid treating the 'non-propagating' lines as a special case by including a convergence factor $exp(i\omega 0^+)$ when translating these lines into functions, where 0^+ is a positive infinitesimal such that $0^+ \times \infty = \infty$, thus



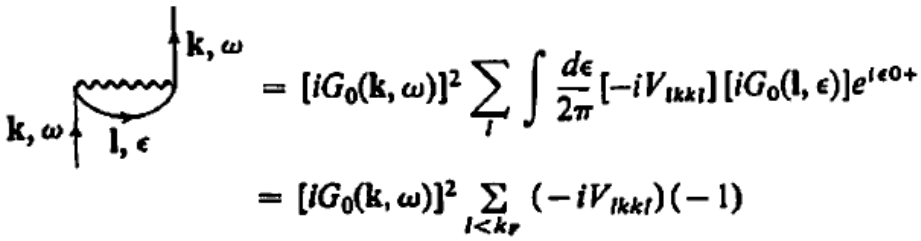
(9.29)

Hence the integral over the intermediate frequency ϵ gives:

$$\int_{-\infty}^{+\infty} \frac{d\epsilon}{2\pi} \frac{ie^{i\epsilon 0^+}}{\epsilon - \epsilon_l + i\delta_l} = \begin{matrix} -1 \text{ for} & l < k_F \\ 0 \text{ for} & l > k_F \end{matrix} \tag{9.30}$$

where $\delta_l = -\delta$ when $l < k_F$. The integral is done by contour residues theorem. The contour is closed in the upper half-complex-plane where the convergence factor makes the arc integral vanish.

Thus, for example



9.4 Diagram rules for single-particle propagator

We have now reached the point where we can present in summary form the rules for drawing and evaluating the type of graphs which will be used in the next two chapters. These are the diagrams describing a system of mutually interacting fermions with no external field and they will always be drawn in $(\mathbf{k}, \omega)$-space, using the Feynman method. The rules are:

1. In nth order, drawn wiggly lines with vertex dots and two external points

2. Join all vertex dots and external points to each other with directed lines in all linked

topologically distinct (in the Feynman sense) ways, with one line entering and one leaving each vertex dot and a line entering one external point and leaving the other. Two diagrams are topologically distinct if they are visualized as made of rubber bands, and one cannot be deformed into the other.

3. Label each line and wiggle with a momentum, k (short for $\mathbf{k}, \sigma$, where $\boldsymbol{\sigma}$ = spin), and frequency ω, such that the sum of momenta (and frequencies) entering each vertex = sum of those leaving. Eliminate all 'anomalous' or 'momentum-non-conserving' diagrams, i.e., which have a hole and a particle in the same state.

4. Evaluate graphs by means of the dictionary in the following table

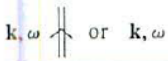
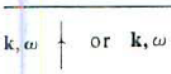
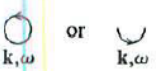
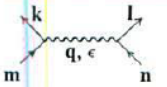
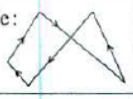
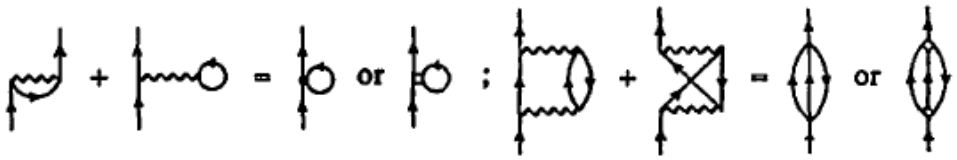
Diagram element	Factor
	$iG(\mathbf{k}, \omega)$
	$iG_0(\mathbf{k}, \omega) = \dfrac{i}{\omega - \epsilon_k + i\delta_k}, \quad \delta_{k>k_F} = +\delta \quad \delta_{k<k_F} = -\delta$
	$iG(\mathbf{k}, \omega)\exp(i\omega 0^+)$ $(0^+ \times \infty = \infty)$
	$iG_0(\mathbf{k}, \omega)\exp(i\omega 0^+)$ $\left(\text{so that: } \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} iG_0(\mathbf{k}, \omega) \times \right.$ $\left. \times \exp(i\omega 0^+) = -\theta_{k_F - k}\right)$
	$-iV_{klmn}$ or $-iV_q$ (use $V_{klmn}(\epsilon)$ or $V_q(\epsilon)$ for time-dependent interaction)
Each fermion loop Example: 	(-1)
Each intermediate frequency ω	$\int \dfrac{d\omega}{2\pi}$
Each intermediate momentum, k	$\sum_{\mathbf{k}}$ or $\int \dfrac{d^3\mathbf{k}}{(2\pi)^3}$ (for $\Omega = 1$) (include sum over spins)

Table 9.1: Diagram dictionary for interacting many-fermion system with no external potential (Feynman method)

Some physicists use abbreviated diagram in which the interaction wiggles are compressed to points or little squares. Thus, for example



(9.31)

Those drawn with points are called "Hugenholtz diagrams", while those with squares are "Abrikosov diagrams".

9.5 Modified propagator formallsm using chemical potential,μ

The formalism just described can be somewhat inconvenient in actual calculations because, unless special precautions are taken, it may produce approximations for G which yield the wrong total number of particles for the system.

In order to understand this, let us first derive the relation between the propagator G and the total particle number N. The quantity N is the expectation value of the total number operator $2\sum_k c_k^\dagger c_k$(factor of 2 for spin) in the interacting ground state:

$$N = \left\langle \Psi_0 \left| 2\sum_k c_k^\dagger c_k \right| \Psi_0 \right\rangle = 2\sum_k \left\langle \Psi_0 \left| c_k^\dagger c_k \right| \Psi_0 \right\rangle \tag{9.32}$$

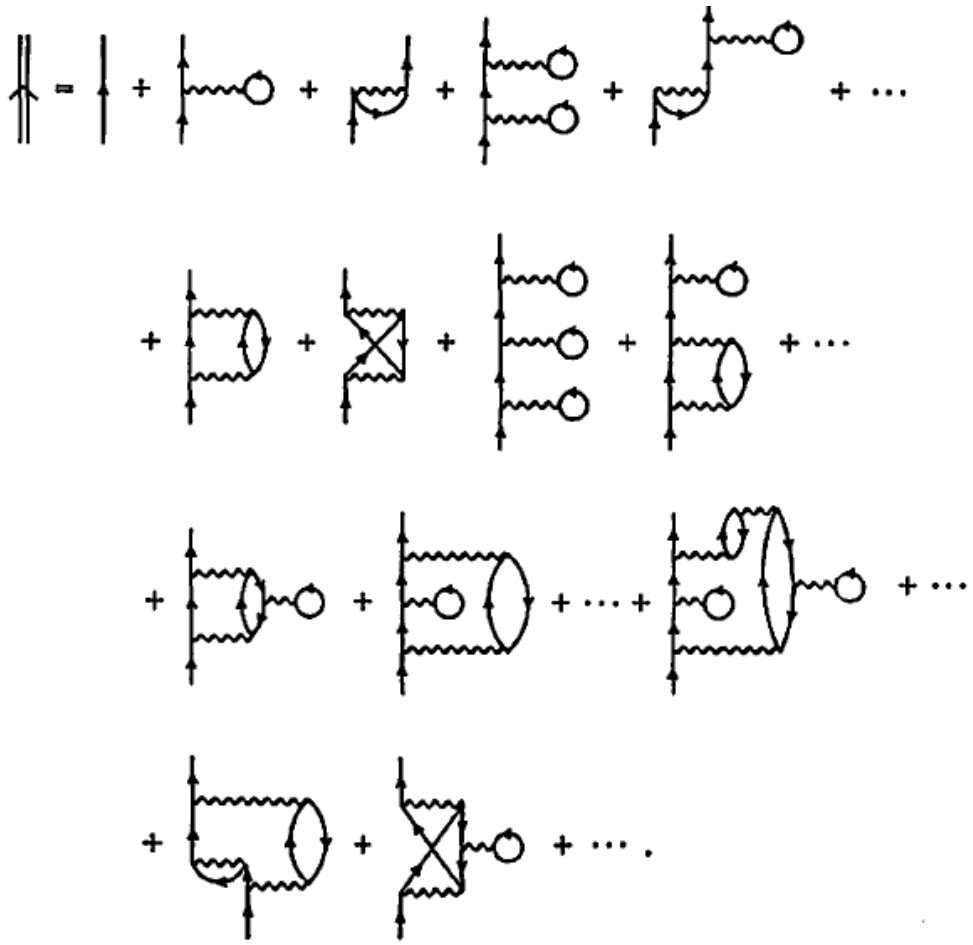
The summand is easily expressed in terms of $G(k_2, k_1, t_2 - t_1)$ by setting $t_2 = t, t_1 = 0, k_1 = k_2 = k$, then letting t approach zero from the left. This yields

$$N = 2\sum_k (-i) \times \lim_{t\to 0^-} G(k,t) = -2i \lim_{t\to 0^-} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \int \frac{d\omega}{2\pi} G(\mathbf{k},\omega) e^{-i\omega t} \tag{9.33}$$

which is the desired relation.

Imagine that we calculate an approximate G for the system by a partial summation over

some types of diagrams in



(9.34)

and then place this G in (9.33) to check and see if it yields $N = N_0$. Evidently, G will be a function of N_0, because each G_0 entering the calculation of G(approx.) depends on k_F, and k_F is related to N_0 by

$$N_0 = 2\sum_{k<k_P} 1 = \frac{2}{(2\pi)^3}\int_{k<k=} d^3\mathbf{k} = k_F^3/3\pi^2, \quad \text{or} \quad k_F = \left(3\pi^2 N_0\right)^{1/3} \tag{9.35}$$

Note that the Fermi energy is

$$c_F = k_F^2/2m = \frac{\left(3\pi^2 N_0\right)^{2/3}}{2m} \tag{9.36}$$

Hence N will be function of N_0. But, since G is only approximate, there is no guarantee that N will equal N_0.

It is simple to remove this difficulty by slightly modify the formalism. The method of doing this is to use the "grand canonical ensemble" at zero temperature. In this method we

no longer regard the system as isolated, with definite particle number N_0, but instead put it in contact with a particle reservior, so that it can gain or lose particles. Thus, particle number, N is variable throughout the calculation. The chemical potential of system, μ is fixed but unknown; its value is determined at the end of the calculation by setting the total particle number equal to N_0.

The modified Hamiltonian for this case is

$$H' = H - \mu N = H'_0 + H_1 \tag{9.37}$$

where

$$\begin{aligned} H'_0 &= \sum_k (\epsilon_k - \mu)\, c_k^\dagger c_k \\ H_1 &= \frac{1}{2} \sum_{klmn} V_{klmn} c_l^\dagger c_k^\dagger c_m c_n \end{aligned} \tag{9.38}$$

where N is the total particle number operator.

The ground state of the modified unperturbed Hamiltonian, H'_0, is obtained by selecting that number of particles, and that way of filling the energy levels which minimizes the energy. **It is easily seen that this means all levels filled up to $\epsilon_k = \mu$, i.e., up to $k_F^\mu = \sqrt{(2m\mu)}$** The corresponding particle number is $N = (3\pi^2)^{-1} \times (2m\mu)^{3/2}$. The free propagator for H'_0 is

$$G_0^\mu(\mathbf{k}, \omega) = \frac{1}{\omega - (\epsilon_k - \mu) + i\delta_k^\mu}, \quad \delta_k^\mu = \begin{cases} +\delta & \text{for } \epsilon_k > \mu \\ -\delta & \text{for } \epsilon_k < \mu \end{cases} \tag{9.39}$$

It will be convenient to define a new ω such that $\omega_{\text{new}} \equiv \omega + \mu$. In addition, in order to get the correct result when we do self-consistent Hartrec-Fock, it is necessary to re-write the infinitesimal in the form $i\,\text{sign}(\omega - \mu)\delta$ or $i(\omega - \mu)\delta$ for short, where $\omega \equiv \omega_{\text{new}}$. These two changes yield ($\omega \equiv \omega_{\text{new}}$)

$$G_0^\mu(\mathbf{k}, \omega) = \frac{1}{\omega - \epsilon_k + i(\omega - \mu)\delta} \tag{9.40}$$

Now N becomes a function of μ. If μ is now determined by setting

$$N(\mu) = N_0 \tag{9.41}$$

we guarantee that G(approx.) yields the correct number of particles. Using (9.33), (9.40),

and (9.41), and ignoring interactions we have:

$$N(\mu) = \frac{(k_P^\mu)^3}{(3\pi)^2} = \frac{(2m\mu)^{3/2}}{3\pi^2} = N_0 \tag{9.42}$$

so that $\mu = \epsilon_F$.

10 Dyson's Equation, Renormalization, RPA and Ladder Approximations

10.1 General types of partial sums

General type of diagrams summed over	Result
(1) All diagrams containing repeated proper (or 'irreducible') self-energy parts. (Summation is complete)	Dyson's equation
(2) All diagrams with "polarization parts" inserted in interaction lines	"dressed", "effective" or "renormalized" interactions
(3) All diagrams with self-energy parts' inserted in r ree particle and bole lines	"dressed" or "renormalized" particle and bole lines (self-consistent renormalization)
(4) All diagrams with 'irreducible vertex parts' inserted in place of a vertex	dressed vertices

10.2 Dyson's Equation

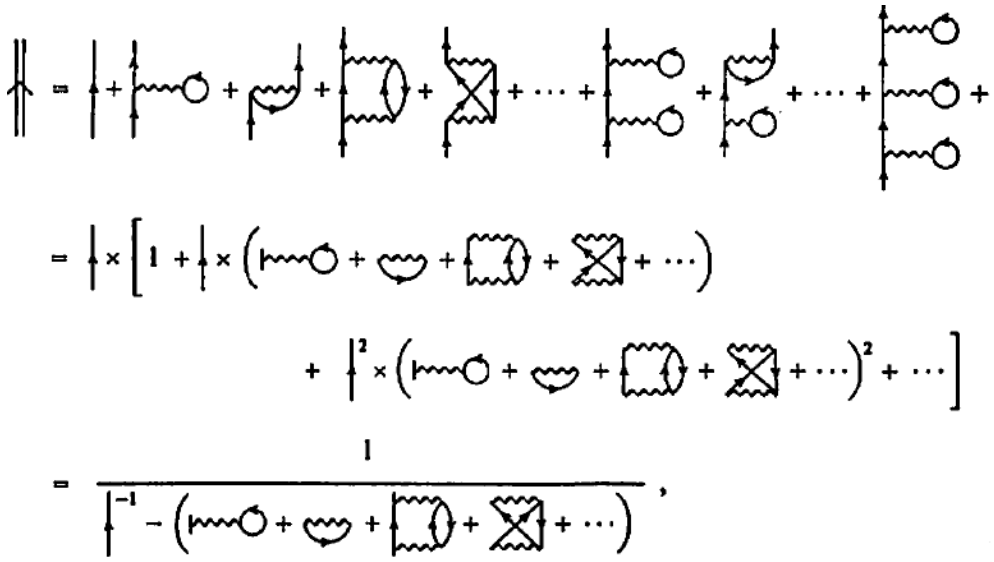
Let us first define "proper self-energy part" or "irreducible self-energy part". First we define:

Self-energy part: Any diagram without incoming and outgoing lines, which can be inserted into a particle or hole line.

Proper or irreducible self-energy part: A self-energy part which cannot be broken into two unconnected self-energy parts by removing one particle or hole line. Parts which can be

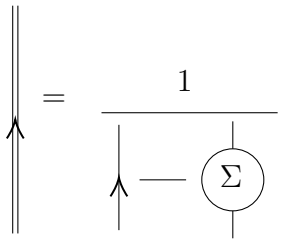
so broken are called 'improper' or 'reducible'.

In general it is possible to sum over all repetitions of all irreducible self-energy parts in a diagram expansion:



(10.1)

or



(10.2)

Translated into functions this becomes:

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_k - \Sigma(\mathbf{k},\omega) + i\delta_k} \tag{10.3}$$

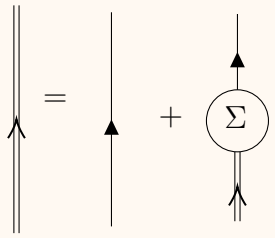
where

$$-i\Sigma(\mathbf{k},\omega) \equiv \tag{10.4}$$

It was necessary to restrict the sum to just repeated proper parts. If we had summed over repeated improper parts as well, diagrams would have been counted twice.

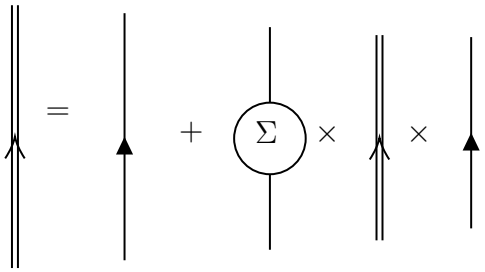
Equation (10.1) or (10.2) is called Dyson's equation and is the basic equation from which most propagator calculations start. $\Sigma(\mathbf{k},\omega)$ is a **generalized "effective field" or "effective potential" which the particle in state k sees because of its interaction with all the other particles of the system.** This field is $\omega-$dependent, which describes the motion of the quasi-particle cloud in $(\mathbf{k},t)$-space.

The form of (10.2) is only valid in the special cases of a system **with no external potential and with diagrams calculated in $(\mathbf{k},\omega)$-space.** A more general form of the Dyson equation which holds whenever the single-particle propagator expansion holds:



(10.5)

Equation (10.5) boils down to (10.2) for a system without external potential because the value of each diagram is the product of the values of its parts:



(10.6)

or

$$G(\mathbf{k},\omega) = G_0(\mathbf{k},\omega) + G(\mathbf{k},\omega)\Sigma(\mathbf{k},\omega)G_0(\mathbf{k},\omega) \tag{10.7}$$

Equation (10.5) is also valid when the diagrams do not factor. For example, in $(\mathbf{k},t)$-space we find

$$\begin{aligned} iG\left(\mathbf{k},t_2-t_1\right) &= iG_0\left(\mathbf{k},t_2-t_1\right) + \\ &+ \iint dt'dt'' iG_0\left(\mathbf{k},t_2-t''\right)(-i)\Sigma\left(\mathbf{k},t''-t'\right) iG\left(\mathbf{k},t'-t_1\right) \end{aligned} \tag{10.8}$$

Another example of (10.5) is the case of a system with an external potential. Then

$$iG\left(k_2,k_1;\omega\right)=iG_0\left(k_2,\omega\right)\delta_{k_2k_1}+ \\ +\sum_{k,k'}iG_0\left(k_2,\omega\right)\delta_{k_2k'}(-i)\Sigma\left(k',k;\omega\right)iG\left(k,k_1;\omega\right) \tag{10.9}$$

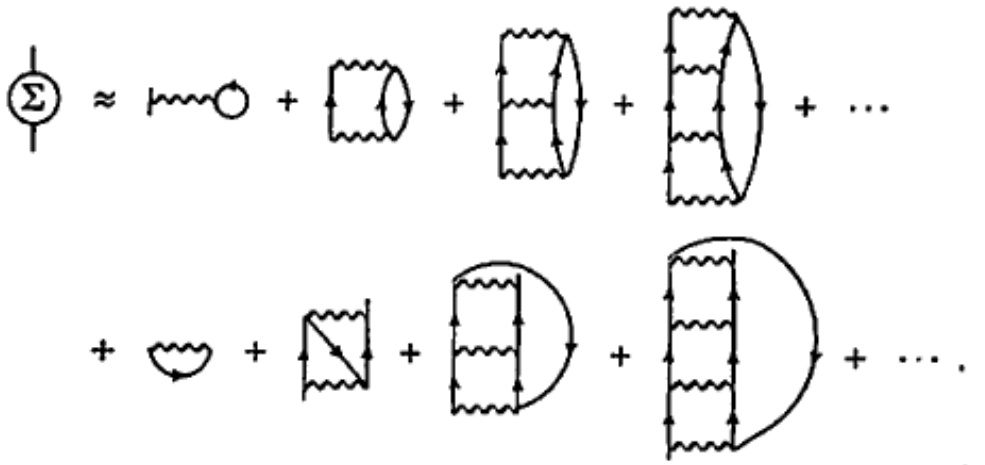
Note that now anomalous graphs must be included

10.3 Quasi particles in low-density Fermi system (ladder approximation)

We now describe the theory of Galitski for a system of particles interacting by means of short-range repulsive forces having range a, and with average distance between particles r_0. By 'low density' is meant that $a/r_0 \ll 1$. This can also be stated in terms of k_F since n, the number of particles/cm ^{3} is equal to $\frac{1}{3}\pi^{-2}k_F^3(9.42)$ and $n = 1/r_0^3$ so $1/r_0 \sim k_F$. Hence the low-density criterion is that $k_F a \ll 1$. Such a theory can be applied in a qualitative way to the case of nuclear matter, where $a/r_0 \sim \frac{1}{3}$, provided we neglect the attractive part of the nuclear potential.

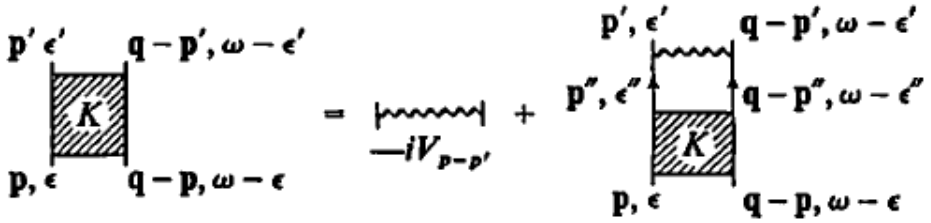
Let us first analyse which self-energy diagrams are the most important ones. We first notice that whenever there is a hole line, labelled by $\mathbf{p}$, there is an associated $\int d^3\mathbf{p}$ over $|\mathbf{p}| < k_F$. Particle lines have $\int d^3\mathbf{p}$ over $|\mathbf{p}| > k_F$. As mentioned before, $n \approx k_F^3$, so low density corresponds to low k_F. In low-density case, the contribution from the hole line integrals is negligible compared to those from particle line integral. Therefore, the dominant diagrams will be those with the least number of hole lines. We find for the sum of graphs

containing just one hole line the following:



(10.10)

These are called "ladder graphs". The sum of ladder graphs may be carried out with the aid of "K"-matrix. This is defined by:



(10.11)

which gives

$$K\left(\mathbf{p}'\boldsymbol{\epsilon}', \mathbf{p}, \epsilon; \mathbf{q}, \omega\right) = V_{p-p'} + i \int \frac{d^3\mathbf{p}'' d\epsilon''}{(2\pi)^4} V_{p''-p'} G_0^+\left(\mathbf{p}'', \epsilon''\right) G_0^+\left(\mathbf{q} - \mathbf{p}'', \omega - \epsilon''\right) \times K(\mathbf{p}'', \epsilon'', \mathbf{p}, \epsilon; \mathbf{q}, \omega) \tag{10.12}$$

10.4 Quasi particles In high-density electron gas (random phase approximation)

The electron gas was introduced as a theoretical metal consisting of N electrons moving against a smeared-out positive charge background. At zero temperature, the gas is characterized by a single parameter, **the average distance between electrons,** r_s. More precisely, r_s is given by

$$\frac{1}{n}\left(\frac{\mathrm{cm}^3}{\text{electron}}\right) = \frac{4}{3}\pi\left(r_s a_0\right)^3 \tag{10.13}$$

where n = electron density, and a_0 = Bohr radius = $\hbar^2/me^2$.

It is important to observe that the low density system with long-range interaction, like the electron gas, is physically different from the low-density system with short-range interaction, like nuclear matter. Hence ladder approximation is not applicable here.

The Hamiltonian for the electron gas in the smeared out positive background is given by

$$\begin{aligned} H = \sum_k \epsilon_k c_k^\dagger c_k + \frac{1}{2}\sum_{klmn} V_{klmn} c_l^\dagger c_k c_m c_n \\ H_{\substack{positive \\ background}} + H_{\substack{electron-positive \\ background}} \end{aligned} \tag{10.14}$$

This equation may be simplified since the V_0 part of the second sum can be used to cancel the last two terms as follows: The V_0 may be evaluated as (dropping spin factors for simplicity):

$$V_0 = V_{klkl} = \frac{1}{\Omega^2}\int d^3\mathbf{r} d^3\mathbf{r}' \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \tag{10.15}$$

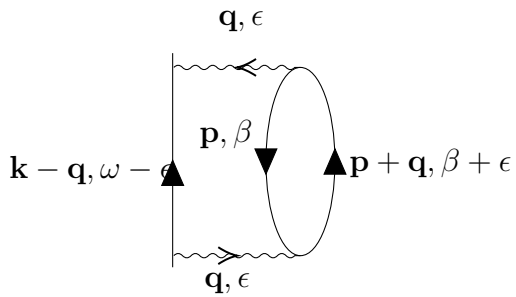
According to the commutation rule of $[c_l^\dagger, c_k]_+ = \delta_{lk}$, we have V_0 as:

$$\begin{aligned} \frac{V_0}{2}\sum_{kl} c_l^\dagger c_k^\dagger c_k c_l &= \frac{V_0}{2}\sum_{k=1}^{+} c_l^\dagger c_l c_k^\dagger c_k - \frac{V_0}{2}\sum_k c_k^\dagger c_k \\ &= \frac{V_0}{2}\left(N^2 - N\right) = \frac{1}{2}\frac{N^2 e^2}{\Omega^2}\int \frac{d^3 r d^3\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|} \end{aligned} \tag{10.16}$$

where we used the fact of $N^2 \gg N$.(10.16) is just the self-energy of a static uniform negative charge distribution. The static positive background is exactly equal to (10.16) while the electron-background term gives a contribution which is twice (10.16) and of opposite sign.(i.e., $V_{electron-positive} = \frac{N^2 eZ}{\Omega^2}\int \frac{d^3\mathbf{r} d^3\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}$. We don't have 1/2 here because electrons and are distinguiable from positive background). That is,

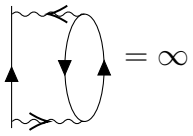
$$H = \sum_k \epsilon_k c_k^\dagger c_k + \frac{1}{2}\sum_{\substack{g,m,n \\ (q\neq 0)}} V_q c_{n-q}^\dagger c_{m+q}^\dagger c_m c_n \tag{10.17}$$

We can now find quasi particles in the electron gas, using (10.2) and (7.38). A typical irreducible self-energy part is:



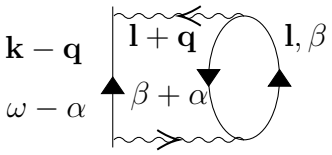
$$= (-1) \sum_{\mathbf{q},\mathbf{p}} \int \frac{d\epsilon d\beta}{(2\pi)^2} iG_0(k-q, \omega-\epsilon) \times iG_0(q+p, \beta+\epsilon) \times iG_0(\mathbf{p}, \beta) \times \frac{(4\pi e^2)^2}{\Omega^2 q^4} \tag{10.18}$$

Changing from a sum over q to an integral reveals that the above expression diverges at $\mathbf{q} = 0$ because of the q^4 in the denominator so that



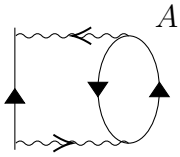
$$= \infty \tag{10.19}$$

However, the situation is saved by the partial summation method as follows: First we observe that each term in the self-energy is proportional to some power of r_s. To see this, we reproduce the integral for a 2-nd order self-energy part as:



$$= \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\alpha}{2\pi} (-iV_q)^2 \frac{i}{\omega - \alpha - \epsilon_{k-q} + i\delta_{k-q}} \times \times \left[-i\pi_0^A(\mathbf{q}, \alpha) + i\pi_0^B(\mathbf{q}, \alpha)\right] \tag{10.20}$$

Let us first examine the π_0^A-term:

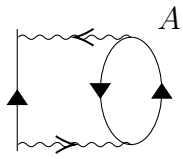


$$= (-2) \int \frac{d^3q}{(2\pi)^3} V_{q^2} \int_{\substack{l<k_F \\ |l+q|>k_F}} \frac{d^3\mathbf{l}}{(2\pi)^3} \int \frac{d\alpha}{2\pi} \times \frac{1}{\omega - \alpha - \epsilon_{k-q} + i\delta_{k-q}} \times \frac{1}{\epsilon_t - \epsilon_{l+q} + \alpha + i\delta} \tag{10.21}$$

The poles here, in the $\alpha-$integration are at

$$\alpha = -\epsilon_l + \epsilon_{l+q} - i\delta$$
$$\alpha = \omega - \epsilon_{k-q} + i\delta_{k-q}$$

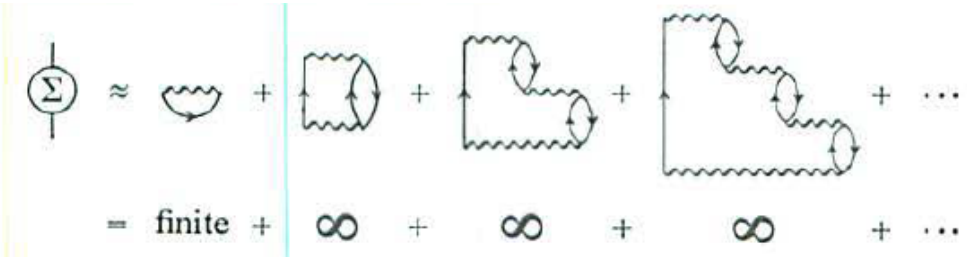
The integration is done by contours just as before. We see that $|\mathbf{k}-\mathbf{q}|$ must be $> k_F$, otherwise both poles are in the lower half-plane and we get zero.(remember the contour integration is always finished in a **counter-clockwise** fashion) The result is



$$= -i\Sigma^A(\mathrm{k},\omega) = (-2i) \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d^3\mathbf{l}}{(2\pi)^3} |V_q|^2 \frac{1}{\omega + \epsilon_l - \epsilon_{l+c} - \epsilon_{k-q} + i\delta}$$
$$l < k_F$$
$$|l+q| > k_r$$
$$|k-q| > k_F \tag{10.22}$$

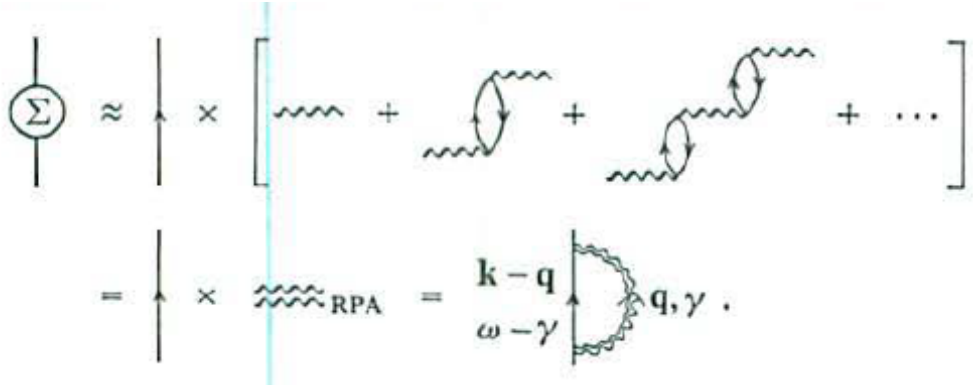
To make (10.22) dimensionless, express quantities in units of k_F (i.e.,set $q = q'k_F, \epsilon_1 = \epsilon_1' k_F^2$, etc.). Then we find that (10.22)$\sim k_F^3 \times k_F^3 \times k_F^{-4} \times k_F^{-2} = 1$ so that (10.22) has no explicit dependence on k_F. **In general, any nth-order term** $\sim r_s^{n-2}$.

Next, we arrange the diagrams according to degree of divergence (= number of factors q^2 in the denominator of the integrand) and dependence on r_s. Thus, for small r_s, i.e., high-density limit, **the dominant infinite terms are just those of lowest order in** r_{x}. **Hence in the high density limit**, the self-energy series is just the sum



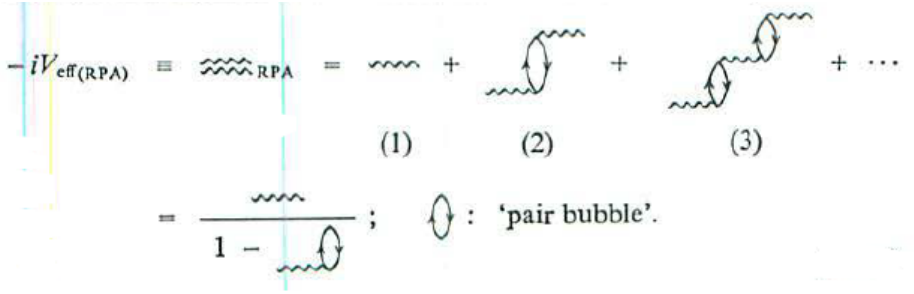
(10.23)

The sum over rings is easy. Factoring out a free propagator from each diagram in (10.23):



(10.24)

T he double wiggle is the "**effective interaction**" in RPA



(10.25)

Diagrams of form (1), (2), (3), ... , having one interaction line entering and one leaving are called 'polarization diagrams'. The reason for this is that they show how the interaction causes the medium to become 'virtually polarized' in all possible ways.

Equation (10.25) may be written in functional form as

$$V_{\text{eff(RPA)}}(\mathrm{q},\omega) = \frac{V_q}{1 + V_q \pi_0(\mathrm{q},\omega)} = \frac{V_q}{\epsilon_{\text{RPA}}(\mathrm{q},\omega)} \tag{10.26}$$

where

$$-i\pi_0(\mathbf{q},\omega) \equiv \overset{\mathbf{k}+\mathbf{q}}{\underset{\epsilon+\omega}{\text{◯}}}\ \mathbf{k},\epsilon \tag{10.27}$$

This has the form of an interaction taking place between two charges in a dielectric, with

$$\epsilon_{\text{RPA}}(q,\omega) = 1 + V_q \pi_0(\mathrm{q},\omega) \tag{10.28}$$

being the frequency-dependent or so-called 'generalized' dielectric constant

Box

The dielectric properties of a medium arise just because of the polarization of the medium by a field, and (10.25) is just the sum of diagrams representing the polarization of the electron gas by the field of one of the electrons in the gas itself. **If V_{eff} is Fourier transformed to (q,t) -space, it will thus be a time-dependent interaction; this is due to the inertia of the polarization charge.**

We may evaluate $\pi_0(\mathbf{q},\omega)$ by

$$-i\pi_0(\mathbf{q},\omega) = 2\times(-1)\int \frac{d^3\mathbf{k}d\epsilon}{(2\pi)^4}\frac{i}{\omega+\epsilon-c_{k+q}+i\delta_{k+q}}\times\frac{i}{\epsilon-\epsilon_k+i\delta_k} \tag{10.29}$$

where the factor of 2 comes from the sum over spins and the (-1) from the fermion loop. In the limit when ω=O and $\mathbf{q}$ is small, it is found that

$$\pi_0\left(q\ll k_F,\omega=0\right)=\frac{\lambda^2}{4\pi e^2},\quad \lambda^2=\frac{6\pi ne^2}{\epsilon_F}=\frac{4me^2k_F}{\pi}=\left(\frac{2}{\pi}\right)\left(\frac{4}{9\pi}\right)^{1/3}r_sk_F^2 \tag{10.30}$$

where n = electron density $=\frac{1}{3}\pi^{-2}k_F^3, \epsilon_F = k_F^2/2m$. Setting $\Omega=1$ and omitting spins for simplicity, we have

$$V_q=\frac{4\pi e^2}{q^2} \tag{10.31}$$

Substituting π_0 and V_q into (10.26) yields

$$V_{\text{eff(RPA)}}(\text{small q},0)=\frac{4\pi e^2}{q^2+\lambda^2} \tag{10.32}$$

We can now go on to the evaluation of $\Sigma_{RPA}(\mathbf{k},\omega)$ as:

$$\begin{aligned}-i\sum_{\text{RPA}}(\mathbf{k},\omega) &= \sum_{\mathbf{q}}\int\frac{d\gamma}{2\pi}\left[(-i)V_{\text{eff(RPA)}}(\mathbf{q},\omega)\right]\left[iG_0(\mathbf{k}-\mathbf{q},\omega-\gamma)\right]\\ &= \int\frac{d^3\mathbf{q}}{(2\pi)^3}\int\frac{d\gamma}{2\pi}\frac{4\pi e^2}{q^2\epsilon_{\text{RPA}}(\mathbf{q},\gamma)}\times\frac{1}{\omega-\gamma-\epsilon_{k-q}+i\delta_{k-q}}\end{aligned} \tag{10.33}$$

A Mismatch in subscript sequence

In chapter 7 we have shown that the "two-body" interaction in occupation number formalism is:

$$\mathcal{O}^{\text{occ}} = \frac{1}{2}\sum_{klmn} \mathcal{O}_{klmn} c_l^\dagger c_k^\dagger c_m c_n \tag{A.1}$$

where

$$\mathcal{O}_{klmn} = \int d^3\mathbf{r} \int d^3\mathbf{r}' \phi_k^*(\mathbf{r}) \phi_l^*(\mathbf{r}') \mathcal{O}(\mathbf{r}, \mathbf{r}'; \mathbf{p}, \mathbf{p}') \phi_m(\mathbf{r}) \phi_n(\mathbf{r}') \tag{A.2}$$

This appendix is dedicated to deal with the mismatch between the subscript of O_{klmn} and that of $c_l^\dagger c_k^\dagger c_m c_n$.

Using the Dirac notation, we have, for a state in the occupation number formalism:

$$\left\langle n_1, n_2, \ldots, n_i \ldots \right| = \overline{|n_1, n_2, \ldots, n_i\rangle} \tag{A.3}$$

where the overline means the Hermitian adjoint. However, for a product of operators we have

$$\left(\hat{\phi}_k \hat{\phi}_l\right)^\dagger = \hat{\phi}_l^\dagger \hat{\phi}_k^\dagger \tag{A.4}$$

Thus, for a two-body interaction $\hat{V}$ we have:

$$\begin{aligned} \hat{V} &= \frac{1}{2}\sum_{klmn} \langle k, l|V|m, n\rangle = \frac{1}{2}\sum_{klmn} \iint d\mathbf{r} d\mathbf{r}' \left(\hat{\phi}_k \hat{\phi}_l\right)^\dagger V(\mathbf{r} - \mathbf{r}') \hat{\phi}_m \hat{\phi}_n \\ &= \frac{1}{2}\sum_{klmn} \iint d\mathbf{r} d\mathbf{r}' \hat{\phi}_l^\dagger \hat{\phi}_k^\dagger V(\mathbf{r} - \mathbf{r}') \hat{\phi}_m \hat{\phi}_n = \frac{1}{2}\sum_{klmn} V_{klmn} c_l^\dagger c_k^\dagger c_m c_n \end{aligned} \tag{A.5}$$

where

$$V_{klmn} = \iint d\mathbf{r} d\mathbf{r}' \phi_k^\dagger \phi_l^\dagger V(\mathbf{r} - \mathbf{r}') \phi_m \phi_n \tag{A.6}$$

Thus we **don't have mismatches in Dirac notation to keep things intuitive, but we do need to take care of the effects of " † " when we translate the notation into integrals.**

B Spectral Density Function

B.1 Single-particle propagator

We shall derive only the expression for $A^+(\mathbf{k},\omega)$ in 9.19. Call Ψ_n^N, E_n^N the exact eigenstates and energies of the Hamiltonian H of the interacting N-particle system. The $G^+(\mathbf{k},t)$ may be expressed as a sum over these exact states by inserting the unit operator:

$$\sum_{n,N} \left|\Psi_n^{N'}\right\rangle \left\langle\Psi_n^{N'}\right|$$

into (9.6), letting $t_1 = 0, t_2 = t$, and noting that in the sum over N', all terms are zero except those for which $N' = N+1$:

$$\begin{aligned} G^+(\mathbf{k},t) &= -i\theta_t \sum_n \left\langle \Psi_0^N \left| e^{iHt} c_k \right| \Psi_n^{N+1} \right\rangle \left\langle \Psi_n^{N+1} \left| e^{-iHt} c_k^\dagger \right| \Psi_0^N \right\rangle \\ &= -i\theta_t \sum_n \left| \left\langle \Psi_n^{N+1} \left| c_k^\dagger \right| \Psi_0^N \right\rangle \right|^2 e^{-i\left(E_n^{N+1} - E_0^N\right)t} \\ &= -i\theta_t \sum_n \left| \left(c_k^\dagger\right)_{n0} \right|^2 e^{-i\left(E_n^{N+1} - E_0^N\right)t} \end{aligned} \tag{B.1}$$

Taking the Fourier transform of the above yields

$$G^+(\mathbf{k},\omega) = \sum_n \left| \left(c_k^\dagger\right)_{n0} \right|^2 \frac{1}{\omega - \left(E_n^{N+1} - E_0^N\right) + i\delta} \tag{B.2}$$

This shows that the poles of G^+ occur at the energies of the interacting $N+1$ particle system minus the ground state energy of the interacting N -particle system. The exponentials in the above may be expressed in terms of the chemical potential, thus:

$$E_n^{N+1} - E_0^N = \underbrace{E_n^{N+1} - E_0^{N+1}}_{w_{n0}^{N+1}} + \underbrace{E_0^{N+1} - E_0^N}_{\mu^{N+1}} \tag{B.3}$$

For large N we have

$$\begin{aligned} \mu^{N+1} &\approx \mu^N \equiv \mu \\ \omega_{n0}^{N+1} &\approx \omega_{n0}^N \equiv \omega_{n0} \end{aligned} \tag{B.4}$$

Giving

$$G^+(\mathbf{k},t) = -i\theta_t \sum_n \left| \left(c_k^\dagger\right)_{n_0} \right|^2 e^{-i(\omega_{n0}+\mu)t} \tag{B.5}$$

$$G^+(\mathbf{k},\omega) = \sum_n \left|\left(c_k^\dagger\right)_{n0}\right|^2 \frac{1}{\omega - (\omega_{n0}+\mu) + i\delta} \tag{B.6}$$

In a system with large volume, the energy levels are so closely spaced that we can go from a sum to an integral by introducing the spectral density function:

$$A^+(\mathbf{k},\omega)d\omega = \sum_{\omega<\omega_{n0}<\omega+d\omega} \left|\left(c_k^\dagger\right)_{n0}\right|^2 \tag{B.7}$$

or

$$A^+(\mathbf{k},\omega) = \sum_n \left|\left(c_k^\dagger\right)_{n0}\right|^2 \delta\left(\omega - \omega_{n0}\right) \tag{B.8}$$

This function is defined only for $\omega \geq 0$ because $\omega_{n0} \geq 0$. It gives **the probability that the state $|\Psi_0^N\rangle$ with an added particle in state k is an exact eigenstate of the $N+1$-particle system with energy between ω and $\omega + d\omega$**. Thus

$$G^+(\mathbf{k},t) = -i\theta_t \int_0^\infty A^+(\mathbf{k},\omega) e^{-i(\omega+\mu)t} d\omega \tag{B.9}$$

$$G^+(\mathbf{k},\omega) = \int_0^\infty d\omega' \frac{A^+(\mathbf{k},\omega')}{\omega - \omega' - \mu + i\delta} \tag{B.10}$$

A profound change takes place when we go from the sum (B.6) to the integral (B.10). The sum (B.6) has an infinite number of **real poles**, whereas the integral (B.10) has a small number of **complex poles**.

The physical meaning of the appearance of complex poles when we go from a sum to an integral may be seen by looking at the corresponding expressions for G in the time domain,i.e.,(B.5) and (B.9). Consider the sum(B.5) first. To analyse its behaviour, we note that there are two characteristic energies involved: First, it there is no interaction, then $(c_k^\dagger)_{n0} = \delta_{kn}$. But with interaction, in typical cases $(c_k^\dagger)_{n0}$ is spread out over a hand of energy levels from say n' to n'', having width $\Delta E = \omega_{n'',0} - \omega_{n',0}$. Secondly, there is the characteristic spacing between adjacent energy levels, $\Delta\epsilon \sim \omega_{n+1,0} - \omega_{n,0}$.

Now, at $t = 0$, all the terms in (B.5) are in phase and $G^+(t)$ is maximum. As t increases, the terms in (B.5) start to get out of phase with each other, and $G^+(t)$ decays in a characteristic time given by $\tau \sim \hbar/\Delta E$. However, if we wait a length of time $T \sim \hbar/\Delta\epsilon$, then the exponentials will start to get in phase with each other again, and $G^+(t)$ builds up

again to its value at $t = 0$. (This is just the 'beat' phenomenon observed when we add two signals $\cos(2\pi\nu_1 t)$ and $\cos(2\pi\nu_2 t)$: the beat frequency is $\nu_2 - \nu_1$ and the corresponding period for build-up of the beat is $T = 1/(\nu_2 - \nu_1)$.) Thus, the Green's function shows periodic behaviour.

The above holds for a finite system, with corresponding finite distance between energy levels. But if we go to the infinite volume limit, then $(\omega_{n+1,0} - \omega_{n,0}) \to 0$, and the build-up time $T \to \infty$. That is, $G^+(t)$ becomes aperiodic, decaying to zero in a time of order τ, and never building up again. This is just the quasi particle behaviour. Thus the discontinuous change from real poles to complex poles in the infinite volume limit, is associated with the discontinuous change of the propagator from a periodic to an aperiodic function.

In practice, it is not necessary to have volume$\to \infty$ since for a typical large system, we find that T is so large compared with the times invo lved in the experiment that build-up will not be observed. However, **in small systems, like atoms and light nuclei, The above considerations a re not valid: the energy levels are widely spaced, the propagator poles are real, and the quasi particle picture does not hold.**