Quantum Field Theory II
An introduction to Feynman diagrams

A course for MPAGS

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Preface

This course follows on from Quantum Field Theory I, and will introduce more advanced techniques such as Green's functions, and Feynman diagrams. It will begin with outlining the formalism required for such an approach, and follow on by applying the formalism to many examples within condensed matter physics, such as Fermi-liquid theory, disordered systems, and phonon interactions.

Prerequisites:

- A familiarity with basic complex analysis - such as the residue theorem, and evaluation of integrals by completing the contour in the upper or lower half planes.
- A familiarity with Fourier analysis - both Fourier series and Fourier transforms.
- The basics of second quantization, as taught last term in the Quantum Field Theory I module.

The course will also suppose some knowledge of condensed matter physics, at an undergraduate level (e.g. that given in either Kittel or Ashcroft and Mermin). While not strictly speaking necessary to follow the course, the entire content will be somewhat obscured if the reader has never met condensed matter physics before.

Suggested further reading

- Mattuck: A guide to Feynman diagrams in the many body problem - a very pedagogical introduction to the concepts behind diagrams. However, sometimes overly wordy when it comes to learning to actually calculate things.
- Mahan: Many Particle systems - contains basically everything in the subject area. Very terse to read, and too big to learn directly from, but as a reference book, is one of the best available.
- Abrikosov, Gorkov and Dzyaloshinskii (AGD): Methods of QFT in statistical physics - an excellent book, although the style takes some getting used to. A different emphasis from Mahan may make this book preferable to some people.
- Piers Coleman: (`http://www.physics.rutgers.edu/~coleman/mbody.html`) - an evolving monogram based on lectures given at Rutgers. Very comprehensive, including many more contemporary topics missing from the classic textbooks. An excellent compliment to these lecture notes.

The course will consist of ten official and two or three unofficial lectures of 2 hours each. Roughly speaking, each chapter of these notes should be one lecture, although the timing and division will not always work out as planned. Finally, I include two appendices with a brief review of complex integration and Fourier analysis as required by this course.

There are exercises scattered throughout the notes. As a good rule, it is worthwhile doing the exercises, as they are designed to demonstrate the concepts which the section describes. I believe that without attempting the exercises, the course (and the subject matter itself) will become increasingly difficult to follow.

The degree of difficulty of each exercise is labeled by a number of stars. One star (*) exercises should require relatively little calculation and should it should be possible to complete them in a relatively small amount of time. Two star (**) exercises will require a bit more time, and are often used to extend concepts. Three star (***) exercises will often require a deeper knowledge of the concepts involved, as well as an extended calculation. Completion of all of the three star exercises should indicate a reasonable proficiency in use of the technique of Feynman diagrams.

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Contents

1. Second quantization, elementary excitations and the free electron gas

In this section, we will review the important properties of second quantization, and try and understand the concept of an *elementary excitation.* As an example, we will begin our study of interacting electron systems by looking at some of the properties of a non-interacting degenerate Fermi gas.

1.1. Brief review of second quantization

Consider the time independent Schrodinger equation

$$-\frac{1}{2m}\nabla^2\Psi(\vec{r})+V(\vec{r})\Psi(\vec{r})=E\Psi(\vec{r}) \tag{1.1}$$

where to make everything finite, space will be confined to be within a box of volume V. The solutions of this equation are the eigenstates, $\phi_\lambda(\vec{r})$ which are labelled by a (discrete) parameter λ and have corresponding eigenvalues ϵ_λ. These states are

- Orthonormal: $\int d^3\vec{r}\phi^*_\lambda(\vec{r})\phi_\kappa(\vec{r})=\delta_{\lambda\kappa}$,
- Complete: $\sum_\lambda \phi^*_\lambda(\vec{r})\phi_\lambda(\vec{r}')=\delta(\vec{r}-\vec{r}')$.

The Hamiltonian can then be written in second-quantized form

$$\hat{H}=\sum_\lambda \epsilon_\lambda \hat{c}^\dagger_\lambda \hat{c}_\lambda \tag{1.2}$$

where $\hat{c}^\dagger_\lambda$ is the operator that creates a fermionic particle in state λ, satisfying the anticommutation relation $\{\hat{c}^\dagger_\lambda,\hat{c}_\kappa\}=\delta_{\lambda\kappa}$. The combination $\hat{c}^\dagger_\lambda\hat{c}_\lambda=\hat{n}_\lambda$ is the number operator.

We can then introduce the field operator $\hat{\Psi}^\dagger(\vec{r})$ defined by

$$\hat{c}^\dagger_\lambda=\int d^3\vec{r}\phi_\lambda(\vec{r})\hat{\Psi}^\dagger(\vec{r}). \tag{1.3}$$

From this expression, it is easy to see that the operator $\hat{\Psi}^\dagger(\vec{r})$ creates a particle at point $\vec{r}$. Taking the Hermitian conjugate gives the field annihilation operator

$$\hat{c}_\lambda=\int d^3\vec{r}\phi^*_\lambda(\vec{r})\hat{\Psi}(\vec{r}). \tag{1.4}$$

The orthonormality condition allows us to invert this relationship

$$\begin{aligned}\hat{\Psi}^\dagger(\vec{r}) &= \sum_\lambda \phi^*_\lambda(\vec{r})\hat{c}^\dagger_\lambda \\ \hat{\Psi}(\vec{r}) &= \sum_\lambda \phi_\lambda(\vec{r})\hat{c}_\lambda. \end{aligned} \tag{1.5}$$

From this, we can derive the anticommutation relation of the field operators:

$$\begin{aligned}\{\hat{\Psi}^\dagger(\vec{r}_1), \hat{\Psi}(\vec{r}_2)\} &= \sum_{\lambda\kappa} \phi^*_\lambda(\vec{r}_1)\phi_\kappa(\vec{r}_2)\underbrace{\{\hat{c}^\dagger_\lambda, \hat{c}_\kappa\}}_{=\delta_{\lambda\kappa}} \\ &= \sum_\lambda \phi^*_\lambda(\vec{r}_1)\phi_\lambda(\vec{r}_2) = \delta(\vec{r}_1 - \vec{r}_2). \end{aligned} \tag{1.6}$$

We also get the density operator

$$\hat{\rho}(\vec{r}) = \hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(\vec{r}) = \sum_{\lambda\kappa} \phi^*_\lambda(\vec{r})\phi_\kappa(\vec{r})\hat{c}^\dagger_\lambda\hat{c}_\kappa. \tag{1.7}$$

Example 1.1: Let $|0\rangle$ be the vacuum state, defined by

$$\hat{c}_\lambda|0\rangle = 0, \quad \forall\lambda. \tag{1.8}$$

Then a one-particle state is given by

$$|\mu\rangle = \hat{c}^\dagger_\mu|0\rangle. \tag{1.9}$$

It is then obvious that

$$\langle\mu|\hat{c}^\dagger_\lambda\hat{c}_\kappa|\mu\rangle = \begin{cases} 1 & \lambda = \kappa = \mu \\ 0 & \text{otherwise} \end{cases} \tag{1.10}$$

We therefore see that

$$\langle\mu|\hat{\rho}(\vec{r})|\mu\rangle = \phi^*_\mu(\vec{r})\phi_\mu(\vec{r}) = |\phi_\mu(\vec{r})|^2, \tag{1.11}$$

i.e. the probability of finding a particle in at position $\vec{r}$ in state μ is given by the modulus square of the wavefunction, exactly as we would expect.

1.2. Additive single body operators

An *additive single body operator* is an operator that may be written in the (first quantized) form

$$\hat{\mathcal{O}} = \sum_{n=1}^N \hat{o}_n \tag{1.12}$$

where $\hat{o}_n$ is an operator acting only on the n-th particle, in a state with N particles total. Examples of such operators are

- Kinetic energy: $\hat{T} = \sum_n \hat{p}_n^2/2m$,
- Particle density: $\hat{\rho}(\vec{r}) = \sum_n \delta(\vec{r} - \hat{\vec{r}}_n)$,
- Momentum (current) density: $\hat{\vec{j}}(\vec{r}) = \sum_n \hat{\vec{p}}_n \delta(\vec{r} - \hat{\vec{r}}_n)$,
- Angular momentum: $\hat{\vec{L}} = \sum_n \hat{\vec{p}}_n \times \hat{\vec{r}}_n$.

An example of an operator that cannot be written this way is an interaction term - this is more typically and *additive two body* operator.

In the second quantized form, it is easiest to write it in an orthonormal basis in which $\hat{o}$ is diagonal

$$\hat{\mathcal{O}} = \sum_{\lambda} \langle \lambda | \hat{o} | \lambda \rangle \hat{c}_{\lambda}^{\dagger} \hat{c}_{\lambda}. \tag{1.13}$$

However, this can then be rotated to any basis

$$\hat{\mathcal{O}} = \sum_{\mu\nu} \langle \mu | \hat{o} \nu \rangle \hat{c}_{\mu}^{\dagger} \hat{c}_{\nu}. \tag{1.14}$$

Example 1.2: Case of density operator. This is diagonal in position basis

$$\langle \vec{x} | \hat{\rho}(\vec{r}) | \vec{y} \rangle = \delta(\vec{x} - \vec{y}) \delta(\vec{r} - \vec{x}), \tag{1.15}$$

so in the eigenstate basis

$$\langle \mu | \hat{\rho}(\vec{r}) | \nu \rangle = \int d^3\vec{x} \int d^3\vec{y}\, \overbrace{\langle \mu | \vec{x} \rangle}^{=\phi_{\mu}^{*}(\vec{x})} \langle \vec{x} | \hat{\rho}(\vec{r}) | \vec{y} \rangle \overbrace{\langle \vec{y} | \nu \rangle}^{=\phi_{\nu}(\vec{y})} \tag{1.16}$$

giving us

$$\hat{\rho}(\vec{r}) = \sum_{\mu\nu} \phi_{\mu}^{*}(\vec{r}) \phi_{\nu}(\vec{r}) \hat{c}_{\mu}^{\dagger} \hat{c}_{\nu} \tag{1.17}$$

as we saw before in Eq. 1.7.

1.3. Free electron gas

We now specialize to a special case of Eq. 1.1 where $V(\vec{r}) = 0$, i.e. there is no external potential. This is known as the *free electron gas*. The eigenfunctions are then plane waves, labeled by their momentum $\vec{k}$:

$$\phi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}, \quad \epsilon_{\vec{k}} = \frac{k^2}{2m}, \tag{1.18}$$

where V is the volume of space. In all calculations, we keep V finite until the end, where we can safely take the limit $V \to \infty$. The relationship between the field operator $\hat{\Psi}^\dagger(\vec{r})$ and the eigenstate creation operator $\hat{c}^\dagger_{\vec{k}}$ is then just the Fourier series (which becomes the Fourier transform in the limit $\vec{V} \to \infty$):

$$\begin{aligned}\hat{\Psi}^\dagger_\sigma(\vec{r}) &= \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} \hat{c}^\dagger_{\vec{k}\sigma}, \\ \hat{c}^\dagger_{\vec{k}\sigma} &= \frac{1}{\sqrt{V}} \int d^3\vec{r} e^{i\vec{k}\cdot\vec{r}} \hat{\Psi}^\dagger_\sigma(\vec{r}), \end{aligned} \tag{1.19}$$

where $\sigma = \uparrow, \downarrow$ is the spin index. We then have the second quantized Hamiltonian and Number operator for the free electron gas

$$\begin{aligned}\hat{H} &= \sum_{\vec{k},\sigma} \epsilon_{\vec{k}} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma}, \quad \epsilon_{\vec{k}} = \frac{k^2}{2m} \\ \hat{N} &= \sum_{\vec{k},\sigma} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma}. \end{aligned} \tag{1.20}$$

1.3.1. Ground State and Kinetic Energy

We want to work with a system which has N particles in the volume V, i.e. a particle density of N/V. As these particles are Fermions, they can't all be in the same state - so to make the lowest energy state, put two particles (one spin up, one spin down) in the lowest energy state, then put the next two in the next lowest state, and so on until all N particles are there. This is the many-body Ground State $|GS\rangle$, and is mathematically defined from the vacuum as

$$|GS\rangle = \prod_{|\vec{k}|<k_F} \hat{c}^\dagger_{\vec{k},\uparrow} \hat{c}^\dagger_{\vec{k},\downarrow} |0\rangle. \tag{1.21}$$

It is easy to check that this state has the property that

$$\langle GS| \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}'\sigma'} |GS\rangle = \overbrace{\langle \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}'\sigma'} \rangle}^{\text{simplified notation}} = \begin{cases} \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'} & |\vec{k}| < k_F \\ 0 & \text{otherwise} \end{cases} \tag{1.22}$$

The parameter k_F, known as the *Fermi momentum* or *Fermi wavevector* is chosen so that the state has the correct number of particles

$$\langle \hat{N} \rangle = \overbrace{2}^{\text{spin}} \sum_{|\vec{k}|<k_F} 1 = N. \tag{1.23}$$

To do this sum, we now take the limit $V \to \infty$, where the sum becomes an integral

$$\frac{1}{V} \sum_{\vec{k}} \to \int \frac{d^3\vec{k}}{(2\pi)^3}, \tag{1.24}$$

i.e.

$$\frac{N}{V} = 2\int_{|\vec{k}|<k_F} \frac{d^3\vec{k}}{(2\pi)^3} = 2 \times \frac{4\pi}{(2\pi)^3} \int_0^{k_F} k^2 dk = \frac{k_F^3}{3\pi^2} \tag{1.25}$$

which gives

$$k_F = (3\pi^2 N/V)^{1/3}. \tag{1.26}$$

One can also estimate the total kinetic energy

$$T = \langle \hat{T} \rangle = 2 \sum_{|\vec{k}|<k_F} \frac{k^2}{2m} = 2\frac{V}{2\pi^2}\frac{1}{2m}\int_0^{k_F} k^4 dk = \frac{V}{2\pi^2 m}\frac{k_F^5}{5} \propto V\left(\frac{N}{V}\right)^{5/3}. \tag{1.27}$$

Hence the kinetic energy per particle can be related to the density by

$$\frac{\langle \hat{T} \rangle}{N} \propto \left(\frac{N}{V}\right)^{2/3}. \tag{1.28}$$

1.3.2. Single particle correlation function

We define the single particle correlation function as

$$G_{\sigma\sigma'}(\vec{x},\vec{y}) = \langle \hat{\Psi}^\dagger_\sigma(\vec{x})\hat{\Psi}_{\sigma'}(\vec{y})\rangle. \tag{1.29}$$

This is also known as the equal time propagator, or equal time Green function - we will discuss the meaning of this much more in the next chapter.

We now calculate $G_{\sigma\sigma'}(\vec{x},\vec{y})$ for the ground state $|GS\rangle$ of the free electron gas, as defined above.

$$\begin{aligned}
G_{\sigma\sigma'}(\vec{x},\vec{y}) &= \langle GS|\hat{\Psi}^{\dagger}_{\sigma}(\vec{x})\hat{\Psi}_{\sigma'}(\vec{y})|GS\rangle \\
&= \frac{1}{V}\sum_{\vec{k}_1,\vec{k}_2} e^{-i\vec{k}_1\cdot\vec{x}}e^{i\vec{k}_2\cdot\vec{y}} \qquad \underbrace{\langle \hat{c}^{\dagger}_{\vec{k}_1\sigma}\hat{c}_{\vec{k}_2\sigma'}\rangle}_{=\begin{cases}\delta_{\vec{k}_1\vec{k}_2}\delta_{\sigma\sigma'} & |\vec{k}|<k_F \\ 0 & \text{otherwise}\end{cases}} \\
&= \delta_{\sigma\sigma'}\frac{1}{V}\sum_{|\vec{k}|<k_F} e^{i\vec{k}\cdot(\vec{y}-\vec{x})} \\
&= \delta_{\sigma\sigma'}\int_{|\vec{k}|<k_F}\frac{d^3\vec{k}}{(2\pi)^3}e^{i\vec{k}\cdot(\vec{y}-\vec{x})} \\
&= \delta_{\sigma\sigma'}\frac{1}{(2\pi)^2}\int_0^{k_F} k^2 \int_{-1}^{1} d(\cos\theta)e^{ikr\cos\theta}, \qquad r=|\vec{x}-\vec{y}| \\
&= \delta_{\sigma\sigma'}\frac{1}{2\pi^2}\frac{1}{r}\int_0^{k_F} k\sin(kr)dk \\
&= \frac{\delta_{\sigma\sigma'}}{2\pi^2}\frac{\sin(k_F r)-k_F r\cos(k_F r)}{r^3} \\
&= \frac{\delta_{\sigma\sigma'}}{2\pi^2}\underbrace{k_F^3}_{=3\pi^2 N/V}\frac{j_1(k_F r)}{k_F r} \\
&= \delta_{\sigma\sigma'}\frac{3N}{2V}\frac{j_1(k_F r)}{k_F r}, \qquad (1.30)
\end{aligned}$$

where j_1 is the modified Bessel function

$$j_1(x) = \frac{\sin x - x\cos x}{x^2}. \qquad (1.31)$$

Example 1.3: We can obtain some more understanding of what this function $G(x-y)$ means by calculating it for a single particle state

$$|\lambda\rangle = \hat{c}^{\dagger}_{\lambda}|0\rangle. \qquad (1.32)$$

In this state,

$$\begin{aligned}
G(\vec{x},\vec{y}) &= \langle\lambda|\hat{\Psi}^{\dagger}(\vec{x})\hat{\Psi}(\vec{y})|\lambda\rangle \\
&= \sum_{\mu\nu}\phi^{*}_{\mu}(\vec{x})\phi_{\nu}(\vec{y}) \quad \underbrace{\langle\lambda|\hat{c}^{\dagger}_{\mu}\hat{c}_{\nu}|\lambda\rangle}_{=1 \text{ only if } \mu=\nu=\lambda} \\
&= \phi^{*}_{\lambda}(\vec{x})\phi_{\lambda}(\vec{y}), \qquad (1.33)
\end{aligned}$$

so we see that $G(\vec{x},\vec{y})$ is in some sense probing the wavefunction of the state.

Exercise 1.1: (*) We saw in the example that $G(\vec{x},\vec{y})$ is in some ways a probe of the wavefunction of the state. Now, the wavefunction of an N-particle state is a function of N coordinates, whereas $G(\vec{x},\vec{y})$ is a function of just two. To get some further insight into this, calculate $G(\vec{x},\vec{y})$ for a two particle state

$$|2\rangle = \hat{c}^{\dagger}_{\lambda_1}\hat{c}^{\dagger}_{\lambda_2}|0\rangle, \tag{1.34}$$

and for a three particle state

$$|3\rangle = \hat{c}^{\dagger}_{\lambda_1}\hat{c}^{\dagger}_{\lambda_2}\hat{c}^{\dagger}_{\lambda_3}|0\rangle. \tag{1.35}$$

Compare these with the actual (antisymmetrized) many body wavefunctions for these states.

1.3.3. Density-density correlation function

The (equal-time) density-density correlation function is defined as

$$D_{\sigma\sigma'}(\vec{x},\vec{y}) = \langle\hat{\rho}_\sigma(\vec{x})\hat{\rho}_{\sigma'}(\vec{y})\rangle. \tag{1.36}$$

Remembering that $\hat{\rho}_\sigma(\vec{x}) = \hat{\Psi}^{\dagger}_{\sigma}(\vec{x})\hat{\Psi}_\sigma(\vec{x})$, then evaluating this for the free electron gas gives

$$D_{\sigma\sigma'}(\vec{x},\vec{y}) = \frac{1}{V^2}\sum_{\vec{k}_1\vec{k}_2\vec{k}_3\vec{k}_4} e^{i(\vec{k}_2-\vec{k}_1)\cdot\vec{x}}e^{i(\vec{k}_4-\vec{k}_3)\cdot\vec{y}}\underbrace{\langle GS|\hat{c}^{\dagger}_{\vec{k}_1\sigma}\hat{c}_{\vec{k}_2\sigma}\hat{c}^{\dagger}_{\vec{k}_3\sigma'}\hat{c}_{\vec{k}_4\sigma'}|GS\rangle}. \tag{1.37}$$

To evaluate this, we need to learn how to take an expectation value of 4 operators. To read these expectation values, it is always easiest to start at the right hand side of the expression. In this case, we begin with the ground state. We then destroy the particle in state $\vec{k}_4\sigma'$, assuming there was a particle in this state to begin with. We then create one in state $\vec{k}_3\sigma'$, destroy one in $\vec{k}_2\sigma$ and create one in $\vec{k}_1\sigma$. We finally look at the overlap between this new state and the original ground state. Now, remembering that the Fock space we are using is orthonormal, this means to get a non-zero result, we must create particles in exactly the same states as we destroyed them. In other words, there are two chances for this expectation value to be non-zero:

- $\vec{k}_1 = \vec{k}_2$ and $\vec{k}_3 = \vec{k}_4$, with $|\vec{k}_1| < k_F$ and $|\vec{k}_3| < k_F$,
- $\vec{k}_1 = \vec{k}_4$, $\vec{k}_3 = \vec{k}_2$ and $\sigma = \sigma'$, with $|\vec{k}_4| < k_F$ and $|\vec{k}_3| > k_F$.

In both these cases, the expectation value is $\langle\ldots\rangle = 1$. In all other cases, it is zero.

This sum over all possible pairings is a specific example of something much more general known as Wick's theorem, which we will meet in full glory in later lectures.

Substituting these expectation values into Eq.1.37 gives

$$\begin{aligned} D_{\sigma\sigma'}(\vec{x},\vec{y}) &= \frac{1}{V^2}\sum_{|\vec{k}_1|<k_F}\sum_{|\vec{k}_3|<k_F} 1 \\ &+ \frac{\delta_{\sigma\sigma'}}{V^2}\sum_{|\vec{k}_1|<k_F}\sum_{|\vec{k}_2|>k_F} e^{i(\vec{k}_2-\vec{k}_1)\cdot(\vec{x}-\vec{y})}. \end{aligned} \tag{1.38}$$

Now, in the first term, we know from Eq. 1.23 that $\sum_{|\vec{k}_1|<k_F} 1 = N/2$, where the factor of $1/2$ comes from not summing over spin. Hence the first term is simply $N^2/4V^2$. In the second term, we rewrite the sum

$$\sum_{|\vec{k}_2|>k_F} = \sum_{\text{all } \vec{k}_2} - \sum_{|\vec{k}_2|<k_F}, \tag{1.39}$$

and we know (from Fourier series) that

$$\sum_{\text{all } \vec{k}_2} e^{i\vec{k}_2\dot{(}\vec{x}-\vec{y})} = V\delta(\vec{x}-\vec{y}) \tag{1.40}$$

is a delta function. Hence the second term in Eq. 1.38 becomes

$$\underbrace{\delta(\vec{x}-\vec{y})\left(\frac{1}{V}\sum_{|\vec{k}_1|<k_F}\overbrace{e^{-i\vec{k}_1\cdot(\vec{x}-\vec{y})}}^{=1}\right)}_{=N/2V} + \underbrace{\left(\frac{1}{V}\sum_{|\vec{k}_1|<k_F}e^{-i\vec{k}_1\cdot(\vec{x}-\vec{y})}\right)\left(\frac{1}{V}\sum_{|\vec{k}_2|<k_F}e^{i\vec{k}_2\cdot(\vec{x}-\vec{y})}\right)}_{\text{we did these sums in the previous section}}. \tag{1.41}$$

In the first term, the exponential is forced to be one, as the delta function forces $\vec{x}=\vec{y}$, so the sum becomes $N/2V$. In the second term, we are left with exactly the same sum we evaluated in Eq. 1.30 in the calculation of $G(\vec{x},\vec{y})$. Ultimately this gives us for the *normalized, connected* part of the pair correlation function

$$\begin{aligned} D^c_{\sigma\sigma'}(\vec{x},\vec{y}) &= \frac{\langle\hat{\rho}_\sigma(\vec{x})\hat{\rho}_{\sigma'}(\vec{y})\rangle - \langle\hat{\rho}_\sigma(\vec{x})\rangle^2}{\langle\hat{\rho}_\sigma(\vec{x})\rangle} \\ &= \delta_{\sigma\sigma'}\left[\delta(\vec{x}-\vec{y}) - \frac{N}{V}\left(\frac{3}{2}\frac{j_1(k_F|\vec{x}-\vec{y}|)}{k_F|\vec{x}-\vec{y}|}\right)^2\right]. \end{aligned} \tag{1.42}$$

Notice that although we are dealing with the non-interacting Fermi-gas, these expectation values and correlation functions still have a lot of structure. This is due to the presence of a length scale k_F^{-1} in the Fermi gas, even before interactions are added.

2. Introduction to Interactions

Although we have shown in the previous lecture that the non-interacting free-electron gas is not as simple as we might have thought, the real fun in many body physics comes when we add interactions, i.e. when the eigenstates of the Hamiltonian can no longer be written as slater determinants of single particle states. In this lecture, we introduce the concept of interactions within second quantization, attempt to calculate some properties within the perturbation theory we know from undergraduate courses, and see why a new framework is needed in order to make calculations of interacting many body systems tractable.

2.1. The Coulomb interaction in the free electron gas

Two-body interactions give an energy of the form

$$\int d^3\vec{x} \int d^3\vec{y} \;\; \rho(\vec{x}) U(\vec{x}-\vec{y}) \rho(\vec{y}). \tag{2.1}$$

For the Coulomb interaction, which will be what we are most interested in during this course, the interaction $U(\vec{r})$ is given by

$$U(\vec{r}) = \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\vec{r}|}. \tag{2.2}$$

We will use units in which $4\pi\epsilon_0 = 1$, so this simply becomes

$$U(\vec{r}) = \frac{e^2}{|\vec{r}|}. \tag{2.3}$$

Within second quantization, we simply replace the density $\rho(\vec{x})$ by the density operator $\hat{\rho}(\vec{x})$

$$\hat{H}_{\text{int}} = \int d^3\vec{x} \int d^3\vec{y} \;\; \hat{\rho}(\vec{x}) U(\vec{x}-\vec{y}) \hat{\rho}(\vec{y}). \tag{2.4}$$

If we immediately specialize to the free electron gas, then from the transformation 1.19, we obtain

$$\hat{H}_{\text{int}} = \frac{1}{V^2} \sum_{\vec{k}_1 \vec{k}_2 \vec{k}_3 \vec{k}_4} \hat{c}^\dagger_{\vec{k}_1} \hat{c}_{\vec{k}_2} \hat{c}^\dagger_{\vec{k}_3} \hat{c}_{\vec{k}_4} \underbrace{\int d^3\vec{x} \int d^3\vec{y} \, e^{i(\vec{k}_2-\vec{k}_1)\cdot\vec{x}} e^{i(\vec{k}_4-\vec{k}_5)\cdot\vec{y}} U(\vec{x}-\vec{y})}. \tag{2.5}$$

In the part which is underbraced, change variables to $\vec{r} = \vec{x} - \vec{y}$, so $\vec{x} = \vec{y} + \vec{r}$, which gives

$$\underbrace{\int d^3\vec{y} \, e^{i(\vec{k}_4-\vec{k}_3+\vec{k}_2-\vec{k}_1)\cdot\vec{y}}}_{=V\delta_{\vec{k}_4-\vec{k}_3+\vec{k}_2-\vec{k}_1}} \int d^3\vec{r} \, e^{i(\vec{k}_2-\vec{k}_1)\cdot\vec{r}} U(\vec{r}). \tag{2.6}$$

The delta function from the first integral is nothing but the law of conservation of momentum - the interaction $U(\vec{x}-\vec{y})$ depends only on the relative position of the two points, i.e. it respects the symmetry that space is homogeneous. This means that if two particles interact, the total momentum in the system can not be changed, which is how we interpret the delta function. We finally change variables again to $\vec{q}=\vec{k}_1-\vec{k}_2$ which leads to the final form of the interaction

$$\hat{H}_{\text{int}} = \frac{1}{V}\sum_{\vec{k}_1\vec{k}_2\vec{q}} \hat{c}^{\dagger}_{\vec{k}_1}\hat{c}_{\vec{k}_1-\vec{q}}\,U_{\vec{q}}\,\hat{c}^{\dagger}_{\vec{k}_2}\hat{c}_{\vec{k}_2+\vec{q}}, \tag{2.7}$$

where

$$U_{\vec{q}} = \int d^3\vec{r}\; e^{i\vec{q}\cdot\vec{r}}U(\vec{r}) \tag{2.8}$$

is the Fourier transform of the interaction potential. One can think of this as one particle with initial momentum $\vec{k}_1$ interacting with another particle with initial momentum $\vec{k}_2$ by exchanging a momentum $\vec{q}$. $U_{\vec{q}}$ is then the *matrix element* of such a process occuring - see the exercise. This view of the interaction will become much more clear when we start representing it as a Feynman diagram.

Exercise 2.1: (*) Suppose we are not dealing with a free electron gas, but the most general system with eigenstates $\phi_\lambda(\vec{x})$. What does the two body interaction look like (in terms of the $\hat{c}$ operators) in this general case?

Going back to the specific case of the Coulomb interaction in the free electron gas, let's evaluate the matrix element $U_{\vec{q}}$ (remembering that we will only be interested in this in the $V\to\infty$ limit):

$$\begin{aligned}
U_{\vec{q}} &= e^2\int d^3\vec{r}\,\frac{e^{i\vec{q}\cdot\vec{r}}}{|\vec{r}|} \\
&= 2\pi e^2\int_0^\infty dr\int_{-1}^{1} d(\cos\theta) r\, e^{irq\cos\theta} \qquad q=|\vec{q}| \\
&= \frac{4\pi e^2}{q}\int_0^\infty \sin(rq) \\
&= \frac{4\pi e^2}{q^2}\left[1-\cos(rq)|_{r\to\infty}\right].
\end{aligned} \tag{2.9}$$

The integral is badly defined, as the limit $r\to\infty$ doesn't really exist. However, if we just ignore this problem and assume $\cos(rq)$ goes away as $r\to 0$, we get the result

$$U_{\vec{q}} = \frac{4\pi e^2}{q^2}. \tag{2.10}$$

This is actually the correct answer, although the way we obtained it seems incredibly dodgy. The best way to see that the answer is correct is to take the inverse Fourier transform of $U_{\vec{q}}$ which turns out not to be ill defined and gives back our initial Coulomb potential. A couple of other ways of obtaining this result are as various limits, one by adding a small imaginary part to q in order to make the integral converge, the other as covered by the following exercise.

Exercise 2.2: (**) Consider the potential

$$U(\vec{r}) = \frac{e^2}{|\vec{r}|} e^{-\lambda|\vec{r}|}, \tag{2.11}$$

which is known in the high energy literature as the Yukawa potential. Show that

$$U_{\vec{q}} = \frac{4\pi e^2}{q^2 + \lambda^2}. \tag{2.12}$$

In the limit $\lambda \to 0$, the Yukawa potential becomes the plain Coulomb potential, and $U_{\vec{q}} \to 4\pi e^2/q^2$, as we would like.

To summarize so far, we have an interaction term corresponding to the Coulomb interaction between electrons in the free electron gas

$$\hat{H}_{\text{int}} = \frac{1}{V} \sum_{\vec{k}_1 \vec{k}_2 \vec{q}} \hat{c}^\dagger_{\vec{k}_1} \hat{c}_{\vec{k}_1 - \vec{q}} U_{\vec{q}} \hat{c}^\dagger_{\vec{k}_2} \hat{c}_{\vec{k}_2 + \vec{q}} \qquad U_{\vec{q}} = \frac{4\pi e^2}{q^2}. \tag{2.13}$$

There are two important comments to make about this

1. The matrix element $U_{\vec{q}}$ diverges as $q \to 0$. Now, zero momentum corresponds to something uniform in real space - in this case, the divergence comes from the fact that we have a uniform charge density over the whole of space, so we should have no surprise that energies will diverge. In fact, in a crystal, whereas the electrons alone do indeed have a uniform average charge density, this is cancelled out by the ions in the crystal lattice. Within the free electron gas picture, what we therefore want to do is add a uniform positive background charge density $-eN/V$ which cancels the average electronic charge to make space (i.e. our crystal) on average electrically neutral. The effect of this is to cancel the $\vec{q} = 0$ component of the interaction.

2. The Hamiltonian $\hat{H}_{\text{int}}$ as it stands has another problem: if it is applied to a one-particle state, it will give a non-zero answer. However, we know that electrons should not interact with themselves. The solution to this is something called *normal ordering*, where you place (by hand) all of the creation operators to the left of all of the annihilation operators. Let us demonstrate how this works by using the anticommutation relation

$$\{\hat{c}_{\vec{k}_1 - \vec{q}}, \hat{c}^\dagger_{\vec{k}_2}\} = \delta_{\vec{k}_1 - \vec{q}, \vec{k}_2} \tag{2.14}$$

to change the order of the operators in Eq. 2.13:

$$\begin{aligned}
&\frac{1}{V}\sum_{\vec{k}_1\vec{k}_2\vec{q}} \hat{c}^\dagger_{\vec{k}_1}\hat{c}_{\vec{k}_1-\vec{q}}U_{\vec{q}}\hat{c}^\dagger_{\vec{k}_2}\hat{c}_{\vec{k}_2+\vec{q}} \\
=\ &\frac{1}{V}\sum_{\vec{k}_1\vec{k}_2\vec{q}} \hat{c}^\dagger_{\vec{k}_1}\hat{c}^\dagger_{\vec{k}_2}U_{\vec{q}}\hat{c}_{\vec{k}_2+\vec{q}}\hat{c}_{\vec{k}_1-\vec{q}} + \frac{1}{V}\underbrace{\sum_{\vec{k}\vec{q}}\hat{c}^\dagger_{\vec{k}}\hat{c}_{\vec{k}}U_{\vec{q}}}_{\sum_{\vec{q}}U_{\vec{q}}=U(\vec{r}=0)}\ .
\end{aligned} \tag{2.15}$$

The last summation is the interaction potential at zero distance - i.e. is the self interaction of the electron and so should be ignored. The first term is the normal ordered form of the Hamiltonian.

2.2. THE Hamiltonian

We now come to what I will call “the Hamiltonian”, which corresponds to the electron gas interacting via the Coulomb interaction - which should describe many of the properties of electrons in a metal. We will spend the vast majority of this course analyzing the properties of this model, given by the Hamiltonian:

$$\begin{aligned}
\hat{H} &= \hat{H}_0 + \hat{H}_{\text{int}} \\
\hat{H}_0 &= \sum_{\vec{k}\sigma}\epsilon_0(\vec{k})\hat{c}^\dagger_{\vec{k}\sigma}\hat{c}_{\vec{k}\sigma} \\
\hat{H}_{\text{int}} &= \frac{1}{V}\sum_{\substack{\vec{k}_1\vec{k}_2\\ \vec{q}\neq 0\\ \sigma\sigma'}}\hat{c}^\dagger_{\vec{k}_1\sigma}\hat{c}^\dagger_{\vec{k}_2\sigma'}U_{\vec{q}}\hat{c}_{\vec{k}_2+\vec{q},\sigma'}\hat{c}_{\vec{k}_1-\vec{q},\sigma}
\end{aligned}$$

with

$$\epsilon_0(\vec{k}) = \frac{k^2}{2m}, \qquad U_{\vec{q}} = \frac{4\pi e^2}{q^2}. \tag{2.16}$$

To begin with, we will want to calculate the ground state of this model, or at least, correlation functions in the ground state.

2.3. First order perturbation theory - Hartree-Fock theory

Within first order perturbation theory in ordinary quantum mechanics, there is no change to the wavefunction, and the energy is calculated as the expectation value of the Hamiltonian in this state. In other words we will assume that $|GS\rangle$ is the non-interacting ground state, which we will denote henceforth by $|GS\rangle_0$ defined in the previous lecture by Eq. 1.21. Within solid state physics, this is known as the *Hartree-Fock* approximation.

The expectation value of $\langle \hat{H}_0 \rangle$ is then just the kinetic energy calculated in the previous lecture, so all that remains is to calculate the average *interaction energy*:

$$\begin{aligned} & {}_0\langle GS|\hat{H}_{\text{int}}|GS\rangle_0 \\ = \ & \frac{1}{V}\sum_{\substack{\vec{k}_1\vec{k}_2\\ \vec{q}\neq 0\\ \sigma\sigma'}} U_{\vec{q}} \quad {}_0\langle GS|\hat{c}^\dagger_{\vec{k}_1\sigma}\hat{c}^\dagger_{\vec{k}_2\sigma'}\hat{c}_{\vec{k}_2+\vec{q},\sigma'}\hat{c}_{\vec{k}_1-\vec{q},\sigma}|GS\rangle_0. \end{aligned} \tag{2.17}$$

As usual, we need to look at the possible pairings of the 4 operators within the expectation value

$$\langle \hat{c}^\dagger_{\vec{k}_1}\hat{c}^\dagger_{\vec{k}_2}\hat{c}_{\vec{k}_3}\hat{c}_{\vec{k}_4}\rangle, \qquad \langle \hat{c}^\dagger_{\vec{k}_1}\hat{c}^\dagger_{\vec{k}_2}\hat{c}_{\vec{k}_3}\hat{c}_{\vec{k}_4}\rangle. \tag{2.18}$$

In the first pairing, $\vec{k}_1 = \vec{k}_4$ and $\vec{k}_2 = \vec{k}_3$. Comparing this with the expression 2.17, we see that this corresponds to $\vec{q} = 0$. Now, the sum excludes the term $\vec{q} = 0$, so this pairing, known as the *Hartree* term, simply gives zero for this model.

The second pairing, known as the *Fock* term, by comparing again with Eq. 2.17 requires $\vec{k}_1 = \vec{k}_2 + \vec{q}$ and $\sigma = \sigma'$ to be non-zero. Furthermore, having made this pairing, one Fermionic swap is required to bring the order of the operators into the form of two number operators. Remembering that Fermionic operators anticommute, this swap gives us an extra minus sign, so the expectation value in the second pairing is $\langle \ldots \rangle = -1$, whenever the number operators give a non-zero result. Putting this together, Eq. 2.17 becomes:

$$\begin{aligned} \langle \hat{H}_{\text{int}} \rangle &= -\sum_{\vec{k},\sigma} \langle \hat{c}^\dagger_{\vec{k}\sigma}\hat{c}_{\vec{k}\sigma}\rangle \underbrace{\frac{1}{V}\sum_{\vec{q}\neq 0} U_{\vec{q}} \langle \hat{c}^\dagger_{\vec{k}+\vec{q},\sigma}\hat{c}_{\vec{k}+\vec{q},\sigma}\rangle}_{=-\epsilon_{\text{HF}}(\vec{k})} \\ &= \sum_{\vec{k},\sigma} \epsilon_{\text{HF}}(\vec{k})\langle \hat{c}^\dagger_{\vec{k}\sigma}\hat{c}_{\vec{k}\sigma}\rangle, \end{aligned} \tag{2.19}$$

where the underbraced section defines the function $\epsilon_{\text{HF}}(\vec{k})$. In principle, this function also depends on the spin orientation σ, however assuming no spontaneous symmetry breaking (i.e. Ferromagnetism - much more about this in later lectures), both spin directions are equivalent, so the function doesn't depend on spin.

We can now do something we aren't strictly allowed to do and remove the expectation values from the last expression, i.e. write an effective interaction Hamiltonian

$$\hat{H}^{\text{eff}}_{\text{int}} = \sum_{\vec{k},\sigma} \epsilon_{\text{HF}}(\vec{k})\hat{c}^\dagger_{\vec{k}\sigma}\hat{c}_{\vec{k}\sigma}, \tag{2.20}$$

where $\epsilon_{\text{HF}}(\vec{k})$ is still to be evaluated. This effective interaction Hamiltonian has the same expectation value (to first order in perturbation theory) as the original interaction Hamiltonian, but it has the property that it is now of the same form as the kinetic energy $\hat{H}_0$, i.e. the effective Hamiltonian is non-interacting. Hence the total Hamiltonian within this Hartree-Fock approximation is

$$\hat{H} = \sum_{\vec{k},\sigma} \epsilon(\vec{k}) \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma}, \tag{2.21}$$

which is a gas of non-interacting particles, but with a *renormalized* energy spectrum,

$$\epsilon(\vec{k}) = \epsilon_0(\vec{k}) + \epsilon_{\mathrm{HF}}(\vec{k}). \tag{2.22}$$

We can therefore interpret $\epsilon_{\mathrm{HF}}(\vec{k})$ as the average energy an electron with momentum $\vec{k}$ gains because of it's interactions with the other electrons in the system. Notice this is all on average though - within first order perturbation theory, correlations between the different particles are not taken into account.

Now that we understand the philosophy behind what we have done, we finally have to compute $\epsilon_{\mathrm{HF}}(\vec{k})$:

$$\begin{aligned} \epsilon_{\mathrm{HF}}(\vec{k}) &= -\frac{1}{V}\sum_{\vec{q}\neq 0} U_{\vec{q}} \langle \hat{c}^{\dagger}_{\vec{k}+\vec{q},\sigma} \hat{c}_{\vec{k}+\vec{q},\sigma} \rangle \\ &= -\frac{1}{V}\sum_{\vec{q}\neq 0} U_{\vec{q}-\vec{k}} \langle \hat{c}^{\dagger}_{\vec{q},\sigma} \hat{c}_{\vec{q},\sigma} \rangle \\ &= -\int_{|\vec{q}|<k_F} \frac{d^3\vec{q}}{(2\pi)^3} \frac{4\pi e^2}{|\vec{k}-\vec{q}|^2} \\ &= -\frac{e^2}{\pi}\int_0^{k_F} dq \int_{-1}^{1} d(\cos\theta) \frac{q^2}{q^2+k^2-2qk\cos\theta} \\ &= -\frac{e^2}{\pi k}\int_0^{k_F} dq\, q \ln\left|\frac{k+q}{k-q}\right| \\ &= -\frac{e^2 k_F}{\pi}\left(1+\frac{1-y^2}{2y}\ln\left|\frac{1+y}{1-y}\right|\right) \qquad y = k/k_F. \end{aligned} \tag{2.23}$$

It is convenient to write this as

$$\begin{aligned} \epsilon_{\mathrm{HF}}(\vec{k}) &= \frac{e^2 k_F}{\pi} S(|\vec{k}|/k_F), \\ S(y) &= -\left(1+\frac{1-y^2}{2y}\ln\left|\frac{1+y}{1-y}\right|\right). \end{aligned} \tag{2.24}$$

The function $S(y)$ is plotted in Fig. 2.1. A simple evaluation tells us that $S(0) = -2$ and $S(1) = -1$, however

$$\left.\frac{dS}{dy}\right|_{y=1} \to \infty, \tag{2.25}$$

i.e. the renormalized energy $\epsilon(\vec{k})$ has an infinite slope at $k = k_F$. Now, remembering that the Fermi-velocity is defined as $\frac{d\epsilon}{dk}$ at $k = k_F$, this means that within the Hartree-Fock approximation, there is an infinite Fermi velocity, and therefore the effective mass of the

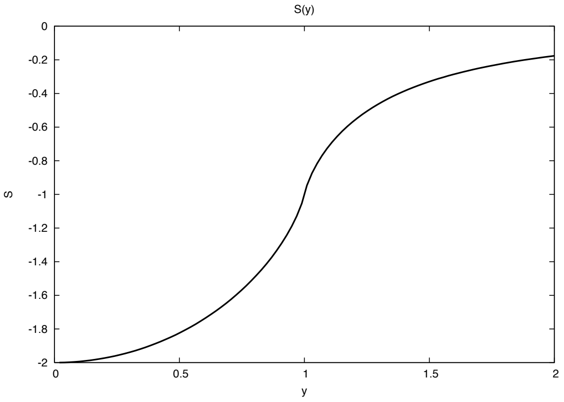


Figure 2.1.: A plot of the dimensionless renormalization of the energy, $S(y)$ from Eq. 2.24.

electron $m^* = 0$.[1] This would have observable consequences experimentally, for example a divergent specific heat capacity C_V which is not seen, so the first order perturbation theory is never going to be good enough.

Exercise 2.3: (**) Calculate $\langle \hat{H}_{\text{int}} \rangle$, i.e. finish the calculation started in this section by evaluating

$$\sum_{\vec{k}\sigma} \langle \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} \rangle \epsilon_{HF}(\vec{k}), \tag{2.28}$$

and show that

$$\frac{\langle \hat{H}_{\text{int}} \rangle}{N} \sim (N/V)^{1/3}. \tag{2.29}$$

This should be compared to the previously calculated average Kinetic energy Eq. 1.28, $\langle \hat{T} \rangle / N \sim (N/V)^{2/3}$. This means that for N/V large, i.e. a high density electron gas, it is actually the kinetic energy that is dominant (Fermi pressure), and the interactions are not terribly important. On the other hand, for a low density electron gas, it is the opposite limit and the interactions dominate the physics.

---

[1] The effective mass is defined by saying that near $k = k_F$, the renormalized energy spectrum behaves like the free one, but with an effective mass m^* instead of the real electron mass m:

$$\epsilon(k \approx k_F) \approx k^2/2m^*. \tag{2.26}$$

This allows us to define precisely what we mean by effective mass:

$$\frac{k_F}{m^*} = \left.\frac{d\epsilon}{dk}\right|_{k=k_F}. \tag{2.27}$$

This is the same definition of m^* as you may be familiar with from undergraduate work, the difference is that here it arises from interaction effects, whereas in undergraduate courses, it arose from band structure effects. Ultimately in a real material, both will play a role.

2.4. An attempt at second order perturbation theory

Having seen how spectacularly bad first order perturbation theory is at calculating anything, let us attempt second order pertrubation theory. If we look at for example Landau and Lifshitz, we find the result for second-order perturbation theory

$$E^{(2)} = \sum_j \frac{|V_{ij}|^2}{E_i^{(0)} - E_j^{(0)}}, \qquad \phi_i^{(1)} = \phi_i^{(0)} + \sum_j \frac{V_{ij}\phi_j}{E_i^{(0)} - E_j^{(0)}}, \tag{2.30}$$

where ϕ denotes the wavefunctions, E the energies, the sum is over all states and V_{ij} is the matrix element between state i and j through the perturbation. If we translate this into our usual second quantized form, it is easy to see that we get

$$|GS\rangle = |GS\rangle_0 + \sum_\phi \frac{{}_0\langle GS|\hat{H}_{\text{int}}|\phi\rangle}{E_i^{(0)} - E_\phi^{(0)}}|\phi\rangle, \tag{2.31}$$

where the sum is now over all many-body states, $|\phi\rangle$. We would then want to calculate a physically measurable quantity, for example the density-density correlation function

$$\langle GS|\hat{\rho}(\vec{x})\hat{\rho}(\vec{y})|GS\rangle = \ldots ??? \tag{2.32}$$

To evaluate this, we would need to form both $|GS\rangle$ and $\langle GS|$ from Eq. 2.31, and then we would have two sums over all states, and denominators involving the energies of them all. It doesn't look nice. Is there a better way to do this? In fact, is it even at all sensible to ask us to calculate the actual full state $|GS\rangle$, which is not a slater determinant, and is in principle a function of $3N$ variables?

The answer is of course, yes, there is a better way to proceed (I wouldn't have brought up the whole dreary subject otherwise!). What we want is to develop a perturbation theory that works directly with the correlation functions rather than the state itself. Before we can do this however, there is one ingredient missing: time. As we can see from the structure of the perturbation theory for states, Eq. 2.31, even if we try and work this directly with the static correlation functions we have so far dealt with rather than the states, we will still have those horrible energy denominators which will require energies of all many body states - something we want to avoid. The point is that the static correlation functions by themselves don't have quite enough information about the system to make a closed perturbation theory using them - we need to extend them to dynamical correlation functions. As an added bonus, in fact, most experiments probe dynamical correlation functions anyway - so this is something we would like to be able to calculate.

3. Time to add time: Schrödinger, Heisenberg, and the causal Green function

So far, all of the examples we have considered have been *static*, that is, there was no time dependence. In this lecture, we will look at how time dependence can be added into second quantization.

3.1. Schrödinger approach

In the Schrödinger approach, the time dependence is put into the wavefunction (i.e. the sates), which evolve via the Schrödinger equation

$$\hat{H}|\Psi(t)\rangle = i\frac{\partial}{\partial t}|\Psi(t)\rangle. \tag{3.1}$$

The operators themselves remain independent of time.

The formal operator solution of the Schrödinger equation is

$$|\Psi(t)\rangle = e^{-i\hat{H}t}|\Psi(0)\rangle, \tag{3.2}$$

where *by definition*, the exponential of an operator is defined by it's Taylor expansion:

$$e^{-i\hat{H}t} = 1 - i\hat{H}t + \frac{1}{2}\left(-i\hat{H}t\right)^2 + \ldots + \frac{1}{n!}\left(-i\hat{H}t\right)^n + \ldots \tag{3.3}$$

Note that if $|\Psi_E\rangle$ is an eigenstate of the Hamiltonian

$$\hat{H}|\Psi_E\rangle = E|\Psi_E\rangle, \tag{3.4}$$

then the operator solution simplifies

$$|\Psi_E(t)\rangle = e^{-iEt}|\Psi_E(0)\rangle. \tag{3.5}$$

The Schrödinger approach is nice and easy to understand, as it separates the operators, i.e. things you can do to the system from the state of the system, which is what evolves in time. However, it turns out to be calculationally inconvenient, as we have to deal directly with the complicated many body states. One can get around this by using another approach, as described in the following section.

3.2. Heisenberg approach

Now, the state itself is not a physical observable. For that, we need to calculate the expectation value of something, for example an operator $\hat{F}$. As the system evolves in time, the expectation value will change, i.e. it is time dependent:

$$\begin{aligned} F(t) &= \langle \Psi(t)|\hat{F}|\Psi(t)\rangle \\ &= \underbrace{\langle \Psi(0)|e^{i\hat{H}t}}\,\hat{F}\,\underbrace{e^{-i\hat{H}t}|\Psi(0)\rangle} \\ &= \langle \Psi(0)|\underbrace{e^{i\hat{H}t}\hat{F}e^{-i\hat{H}t}}_{=\hat{F}(t)}|\Psi(0)\rangle. \end{aligned} \tag{3.6}$$

We see that we can group the terms in two different ways - in the first, the states have the time dependence (which is the Schrödinger approach), in the second, the states remain time independent, at the expense of the operator acquiring time dependence

$$\hat{F}(t) = e^{i\hat{H}t}\hat{F}e^{-i\hat{H}t}. \tag{3.7}$$

This is the Heisenberg approach. If we differentiate this, we see that

$$\frac{\partial \hat{F}(t)}{\partial t} = i(\hat{H}\hat{F} - \hat{F}\hat{H}) = i\left[\hat{H}, \hat{F}\right]. \tag{3.8}$$

This is the Heisenberg form of the Schrödinger equation. There are three important points to note about this:

1. The time evolution of an operator $\hat{F}$ is given by it's *commutation* with the Hamiltonian $\hat{H}$. We haven't said anything about statistics here, so this is true for both Bosonic and Fermionic operators, i.e. for Fermions, although we are used to dealing with *anticommutation* relations, the time evolution is given by a *commutation.*

2. If the operator commutes with the Hamiltonian $[\hat{H}, \hat{F}] = 0$, then the expectation value of $\hat{F}$ does not change with time.

3. The commutation or anticommutation relations we know about operators for example $\left\{\hat{c}, \hat{c}^\dagger\right\} = 1$ are true only at *equal time*, so henceforth will be known as the equal time (anti-)commutation relations. Commutation or anticommutation relations between two operators at different times are not simple, and will involve the Hamiltonian. We won't say any more about this at present, as we will spend some time in later lectures studying this point.

3.3. Extended example: the double well potential

Let us consider a Hamiltonian with two states, specifically the well known double well potential shown in Fig. 3.1. The Hamiltoinan is

$$\hat{H} = -\omega \hat{c}_1^\dagger \hat{c}_2 - \omega \hat{c}_2^\dagger \hat{c}_1, \tag{3.9}$$

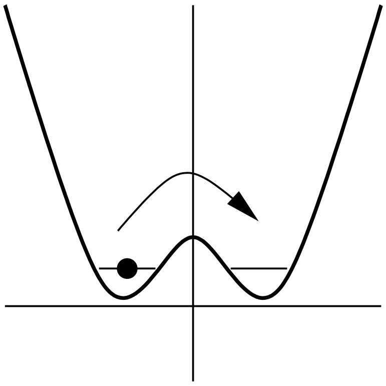


Figure 3.1.: A schematic of the double well potential - there are two states, one in the potential well on the left, and one in the potential well on the right. Furthermore, a particle has some probability ω of tunneling through the barrier in the middle between the two states. Another way of thinking of this is a tight binding model with only two lattice sites.

where $\hat{c}_1^\dagger$ creates a particle in the left well, $\hat{c}_2^\dagger$ creates a particle in the right well, and ω is the tunneling rate between these two states. We can then define two more operators corresponding to physical observables: the number operator $\hat{N}$ corresponding to the total number of particles in the system

$$\hat{N} = \hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2, \tag{3.10}$$

and the position operator $\hat{X}$ defined by

$$\hat{X} = \hat{c}_2^\dagger \hat{c}_2 - \hat{c}_1^\dagger \hat{c}_1, \tag{3.11}$$

where I have supposed that the right well is located at position $+1$ and the left well at position -1.

Let us prepare the system at time $t = 0$ in the state

$$|\Psi(t = 0)\rangle = \hat{c}_1^\dagger |0\rangle, \tag{3.12}$$

and we will ask what is the time evolution of this state, or more precisely, what is the time evolution of the expectation value of operators corresponding to a physical observable in this state?

We will answer the question in two ways, firstly using the Schrödinger representation, and secondly using the Heisenberg representation. However, there is something we must do first which is common to both methods, and this is to *diagonalize* the Hamiltonian.

To see why this is necessary, consider what we want to do: we want to evaluate

$$e^{i\hat{H}t}|\Psi\rangle, \tag{3.13}$$

and remembering that the exponential of an operator is defined via it's Taylor series, what we therefore need to calculate is $\hat{H}^n$ for arbitrary n. Now, raising a matrix (or operator - the two are basically equivalent) to an arbitrary power is easy if the matrix is diagonal - but it is not at all easy if the matrix is not diagonal. This is why we first diagonalize the operator.

The transformation we want in this case is to define two new variables via the linear transformation

$$\hat{d}_1^\dagger = \frac{1}{\sqrt{2}}\left(\hat{c}_1^\dagger + \hat{c}_2^\dagger\right), \qquad \hat{d}_2^\dagger = \frac{1}{\sqrt{2}}\left(\hat{c}_1^\dagger - \hat{c}_2^\dagger\right), \tag{3.14}$$

and their Hermitian conjugates.

Exercise 3.1: (*) Show that the new variables are indeed fermionic creation and annihilation operators, i.e. they satisfy the anticommutation relation $\left\{\hat{d}^\dagger_\alpha, \hat{d}_\beta\right\} = \delta_{\alpha\beta}$, and in terms of the new variables, the Hamiltonian becomes

$$\begin{aligned}\hat{H} &= \omega\left(\hat{d}^\dagger_2\hat{d}_2 - \hat{d}^\dagger_1\hat{d}_1\right) \\ &= \sum_{i=1}^{2}\epsilon_i\hat{d}^\dagger_i\hat{d}_i,\end{aligned} \tag{3.15}$$

where the two energy levels are $\epsilon_1 = -\omega$ and $\epsilon_2 = \omega$.

The inverse transformation is

$$\hat{c}^\dagger_1 = \frac{1}{\sqrt{2}}\left(\hat{d}^\dagger_1 + \hat{d}^\dagger_2\right), \qquad \hat{c}^\dagger_2 = \frac{1}{\sqrt{2}}\left(\hat{d}^\dagger_1 - \hat{d}^\dagger_2\right), \tag{3.16}$$

so we can write our initial $t = 0$ state as

$$|\Psi(t=0)\rangle = \hat{c}^\dagger_1|0\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle \tag{3.17}$$

where I have defined the two states

$$|1\rangle = \hat{d}^\dagger_1|0\rangle, \qquad |2\rangle = \hat{d}^\dagger_2|0\rangle. \tag{3.18}$$

3.3.1. Schrödinger

Now, we can specialize to the Schrödinger representation, where it is now easy to see that

$$\begin{aligned}|\Psi(t)\rangle &= e^{-i\hat{H}t}|\Psi(t=0)\rangle \\ &= \frac{1}{\sqrt{2}}e^{-i\hat{H}t}|1\rangle + \frac{1}{\sqrt{2}}e^{-i\hat{H}t}|2\rangle \\ &= \frac{1}{\sqrt{2}}e^{i\omega t}|1\rangle + \frac{1}{\sqrt{2}}e^{-i\omega t}|2\rangle\end{aligned} \tag{3.19}$$

Now, in our new diagonal representation, the operators we are interested in are

$$\begin{aligned}\hat{N} &= \hat{d}^\dagger_1\hat{d}_1 + \hat{d}^\dagger_2\hat{d}_2 \\ \hat{X} &= -\left(\hat{d}^\dagger_1\hat{d}_2 + \hat{d}^\dagger_2\hat{d}_1\right).\end{aligned} \tag{3.20}$$

It is then a trivial matter to work out the expectation values. First, the number operator

$$\langle\Psi(t)|\hat{N}|\Psi(t)\rangle = 1. \tag{3.21}$$

This is independent of time, which we could have predicted without calculation by noting that the Hamiltonian commutes with the number operator

$$\left[\hat{N}, \hat{H}\right] = 0. \tag{3.22}$$

Exercise 3.2: (*) Prove Eq. 3.22.

This commutation means that the Hamiltonian conserves the total number of particles. It can move a particle from the left well to the right well, or vice versa, but it can't create new particles, or annihilate existing ones. Outside the field of superconductivity, the vast majority of fermionic models we play with in condensed matter have this property - the number of electrons inside a piece of crystal is conserved. As we will see later though, phononic models in general don't have this property, phonons can be created ad destroyed dynamically.

Finally, we also evaluate the expectation value

$$\begin{aligned} \langle\Psi(t)|\hat{X}|\Psi(t)\rangle &= \frac{1}{2}e^{-2i\omega t}\langle 1|\hat{d}_1^\dagger\hat{d}_2|2\rangle - \frac{1}{2}e^{2i\omega t}\langle 2|\hat{d}_2^\dagger\hat{d}_1|1\rangle \\ &= -\cos(2\omega t). \end{aligned} \tag{3.23}$$

3.3.2. Heisenberg

We now repeat the same calculation in the Heisenberg representation. Now, that state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle \tag{3.24}$$

is independent of time, but the operators have a time dependence. The total number operator still commutes with the Hamiltonian so

$$\hat{N}(t) = \hat{d}_1^\dagger\hat{d}_1 + \hat{d}_2^\dagger\hat{d}_2 \tag{3.25}$$

independent of time. However, the position operator

$$\begin{aligned} \hat{X}(t) &= e^{i\hat{H}t}\hat{X}e^{-i\hat{H}t} \\ &= -e^{i\hat{H}t}\hat{d}_1^\dagger\hat{d}_2 e^{-i\hat{H}t} - e^{i\hat{H}t}\hat{d}_2^\dagger\hat{d}_1 e^{-i\hat{H}t} \\ &= -e^{-2i\omega t}\hat{d}_1^\dagger\hat{d}_2 - e^{2i\omega t}\hat{d}_2^\dagger\hat{d}_1. \end{aligned} \tag{3.26}$$

Finally, working out the expectation value gives

$$\langle\Psi|\hat{X}(t)|\Psi\rangle = -\cos(2\omega t), \tag{3.27}$$

as before.

In general, for calculations, we prefer the Heisenberg representation as it involves less dealing with states. It also means we can formally define an operator

$$\hat{\Psi}(\vec{x}, t), \tag{3.28}$$

i.e. the operator that creates a particle at point $\vec{x}$ and time t. The importance of this will become clear in the next section.

3.4. The casual Green function

The *causal* Green function, also known as the *Feynman propagator* is defined as

$$G_{\sigma\sigma'}(\vec{x}_1, t_1; \vec{x}_2, t_2) = -i\langle T\hat{\Psi}_\sigma(\vec{x}_1, t_1)\hat{\Psi}^\dagger_{\sigma'}(\vec{x}_2, t_2)\rangle, \tag{3.29}$$

where the expectation value $\langle \ldots \rangle$ is as usual a shortcut for $\langle GS| \ldots |GS\rangle$, i.e. it is the expectation value in the ground state of the system, and the symbol T stands for the time ordering operator

$$T\left(\hat{A}(t_1)\hat{B}(t_2)\right) = \begin{cases} \hat{A}(t_1)\hat{B}(t_2), & t_1 > t_2, \\ \pm\hat{B}(t_2)\hat{A}(t_1), & t_2 > t_1, \end{cases} \tag{3.30}$$

i.e. the operator places the operators from right to left in increasing order of time. This is the meaning of the word *causal.* When two operators are swapped by the time ordering operator, they gain an extra minus sign if they are fermionic operators.

When $t_1 > t_2$, the function $G_{\sigma\sigma'}(\vec{x}_1, t_1; \vec{x}_2, t_2)$ creates a particle at time t_1 and postition $\vec{x}_1$, then destroys it again at time t_2 and position $\vec{x}_2$, in other words, it measures the probability of a particle *propagating* from $(\vec{x}_1, t_1)$ to $(\vec{x}_2, t_2)$. We must remember though that we are in a system of many identical particles, so the particle removed may not be the same particle that was created (which is why even at equal times, G is non-zero, as we calculated in the first lecture.

We will now proceed to calculate $G_{\sigma\sigma'}(\vec{x}_1, t_1; \vec{x}_2, t_2)$ in the non-interacting Fermi gas. First, we see that in the absence of ferromagnetism (as is obviously absent in the non-interacting Fermi gas) that

$$G_{\sigma\sigma'}(\vec{x}_1, t_1; \vec{x}_2, t_2) = \delta_{\sigma\sigma'}G(\vec{x}_1, t_1; \vec{x}_2, t_2). \tag{3.31}$$

We shall therefore suppress the spin-indices throughout much of the calculation.

Let us expand the field operators Ψ in terms of the eigenstate creation and annihilation operators (Eq. 1.19). This gives us

$$G(\vec{x}_1, t_1; \vec{x}_2, t_2) = \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{x}_1 - \vec{x}_2)} G(\vec{k}, t_2 - t_1), \tag{3.32}$$

where

$$G(\vec{k}, t_2 - t_1) = -i\langle T\hat{c}_{\vec{k}}(t_1)\hat{c}^\dagger_{\vec{k}}(t_2)\rangle, \tag{3.33}$$

i.e. is the propagator of a particle of momentum $\vec{k}$ between times t_2 and t_1, or in other words, is the Fourier transform in space of the originally defined Green function. It's important to note that $G(\vec{x}_1, t_1; \vec{x}_2, t_2)$ in fact only depends on the difference $\vec{x}_1 - \vec{x}_2$. This is a consequence of the homogeneity of space, which the free electron model with zero external potential obviously satisfies. In fact, as already written in the equation, it will turn out also to be only a function of the time difference $t_2 - t_1$ and not the individual times separately. This is a consequence of homogeneity of time. We will discuss these concepts more in later lectures.

We now need to look at what the eigenstate creation $\hat{c}^\dagger_{\vec{k}}(t)$ and annihilation $\hat{c}_{\vec{k}}$ operators look like within the Heisenberg picture. We start with the creation operator

$$\hat{c}^\dagger_{\vec{k}}(t) = e^{i\hat{H}t}\hat{c}^\dagger_{\vec{k}\sigma}e^{-i\hat{H}t}. \tag{3.34}$$

Let's suppose this operator acts on an eigenstate $|\Psi_E\rangle$ of the system, with total energy E. Then

$$\hat{c}^\dagger_{\vec{k}}(t)|\Psi_E\rangle = e^{i\hat{H}t}\hat{c}^\dagger_{\vec{k}}\underbrace{e^{-i\hat{H}t}|\Psi_E\rangle}_{=e^{-iEt}|\Psi_E\rangle}. \tag{3.35}$$

When the operator $\hat{c}_{\vec{k}}$ acts on this state $|\Psi_E\rangle$, it either gives zero (if the single-particle state $\vec{k}$ is already occupied in the many body state $|\Psi_E\rangle$), or creates a state with energy $E + \epsilon_0(\vec{k})$. If the creation operator gives 0, we don't need to worry about the value of the other terms in the expression, as they will be multiplied by zero. Hence

$$e^{i\hat{H}t}\hat{c}^\dagger_{\vec{k}}|\Psi_E\rangle = e^{i(E+\epsilon_0(\vec{k})t}\hat{c}^\dagger_{\vec{k}}|\Psi_E\rangle. \tag{3.36}$$

Putting this together, we see that

$$\hat{c}^\dagger_{\vec{k}}(t)|\Psi_E\rangle = e^{i(E+\epsilon_0(\vec{k})t}\hat{c}^\dagger_{\vec{k}}e^{-iEt}|\Psi_E\rangle = e^{-i\epsilon_0(\vec{k})t}\hat{c}^\dagger_{\vec{k}}|\Psi_E(t)\rangle. \tag{3.37}$$

Notice that this final result is independent of the state $|\Psi_E(t)\rangle$, and as any arbitrary state can be written as a linear superposition of eigenstates, we can write this simply as an operator relation

$$\hat{c}^\dagger_{\vec{k}}(t) = e^{-i\epsilon_0(\vec{k})t}\hat{c}^\dagger_{\vec{k}}. \tag{3.38}$$

Doing an analogous calculation for the annihilation operator gives

$$\hat{c}_{\vec{k}}(t) = e^{i\epsilon_0(\vec{k})t}\hat{c}_{\vec{k}}. \tag{3.39}$$

We can now calculate

$$\langle T\hat{c}_{\vec{k}}(t_1)\hat{c}^\dagger_{\vec{k}}(t_2)\rangle = \begin{cases} e^{-i\epsilon_0(\vec{k})(t_2-t_1)}\left(1 - n_{\vec{k}}\right) & t_2 > t_1, \\ e^{-i\epsilon_0(\vec{k})(t_2-t_1)}n_{\vec{k}} & t_1 > t_2, \end{cases} \tag{3.40}$$

where

$$n_{\vec{k}} = \langle\hat{c}^\dagger_{\vec{k}}\hat{c}_{\vec{k}}\rangle = \begin{cases} 1 & |\vec{k}| < k_F, \\ 0 & \text{otherwise.} \end{cases} \tag{3.41}$$

Finally, let us calculate the Fourier transform of this in the time domain, which gives us the Green function in momentum-energy space:

$$\begin{aligned} G(\vec{k},\omega) &= -i\int_{-\infty}^{\infty} d(t_2-t_1)\; e^{i(t_2-t_1)\omega}\langle T\hat{c}_{\vec{k}}(t_1)\hat{c}^{\dagger}_{\vec{k}}(t_2)\rangle \\ &= \begin{cases} -i\int_{-\infty}^{0} dt\; e^{it(\omega-\epsilon_0(\vec{k}))} = i\int_0^{\infty} e^{-it(\omega-\epsilon_0(\vec{k}))} & |\vec{k}| > k_F, \\ -i\int_0^{\infty} dt\; e^{it(\omega-\epsilon_0(\vec{k}))} & |\vec{k}| > k_F. \end{cases} \end{aligned} \tag{3.42}$$

Example 3.1: Let us now take a brief interlude to look at integrals of the type

$$\int_0^{\infty} e^{ist} dt. \tag{3.43}$$

Technically, these integrals are badly defined as the integral doesn't converge as $t \to \infty$. To proceed, let us **define** such an integral as a limit:

$$\lim_{\delta\to 0^+}\int_0^{\infty} e^{ist-\delta t} dt = i\lim_{\delta\to 0^+}\frac{1}{s+i\delta}. \tag{3.44}$$

Very often, $\lim_{\delta\to 0^+}$ is not explicitly written, but is implied. Finally, we note that if we take the imaginary part of this

$$\Im\frac{1}{s+i\delta} = \lim_{\delta\to 0^+}\frac{-\delta}{s^2+\delta^2} = -\pi\delta(s). \tag{3.45}$$

We can now do the integrals, which gives us the Green function

$$G(\vec{k},\omega) = \begin{cases} \frac{1}{\omega-\epsilon_0(\vec{k})+i\delta} & |\vec{k}| > k_F, \\ \frac{1}{\omega-\epsilon_0(\vec{k})-i\delta} & |\vec{k}| < k_F. \end{cases} \tag{3.46}$$

The cases can be combined to give:

$$\boxed{G_0(\vec{k},\omega) = \frac{1}{\omega-\epsilon_0(\vec{k})+i\delta\,\mathrm{sign}(|\vec{k}|-k_F)} \qquad (3.47)}$$

We have put the subscript G_0 to indicate that this is the non-interacting Green function. This function is one of the most important components of the Feynman diagram expansion. We will spend the next few lectures deriving the diagrammatic perturbation expansion for G for an interacting system.

Just as a note, it will become convenient later on to measure all energies relative to the Fermi level, μ. If ω is measured relative to μ, then we can write

$$G_0(\vec{k},\omega) = \frac{1}{\omega-\xi_{\vec{k}}+i\delta\,\mathrm{sign}\,\xi_{\vec{k}}} \tag{3.48}$$

where

$$\xi_{\vec{k}} = \epsilon_0(\vec{k}) - \mu. \tag{3.49}$$

This will allow us to interpret positive energies as electron like excitations, and negative energies as hole like excitations.

4. Interaction representation and some theorems

To recap the previous lecture, we've seen that in the Schrödinger approach, the wavefunctions (states) have time dependence and operators are independent of time, whereas in the Heisenberg approach things are the other way around. We will now discuss one more approach which is a hybrid between these two methods, known as the *Interaction Representation.* This will turn out to be ideal for formulating perturbation theory. In this lecture we will develop all of the mathematical background necessary for deriving the Feynman rules.

4.1. Interaction Representation

Let us write a Hamiltonian rather generally as

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}. \tag{4.1}$$

In the example of the interacting electron gas, $\hat{H}_0$ is the kinetic energy part of the Hamiltonian and $\hat{H}_{\text{int}}$ is the Coulomb interaction, but in general the split is into a part we know how to solve,[1] $\hat{H}_0$ and a perturbation on this $\hat{H}_{\text{int}}$ which is usually an interaction term, but doesn't have to be. In general, we have that the two parts don't commute,

$$[\hat{H}_0, \hat{H}_{\text{int}}] \neq 0. \tag{4.2}$$

If the two parts did commute, then $\hat{H}_0$ and $\hat{H}_{\text{int}}$ could be diagonalized simultaneously, and the problem would be trivial.

Let us look at the expectation value of an operator $\hat{F}$ at time t:

$$\begin{aligned} & \langle\Psi|e^{i\hat{H}t}\hat{F}e^{-i\hat{H}t}|\Psi\rangle \\ = \; & \underbrace{\langle\Psi|e^{i\hat{H}t}e^{-i\hat{H}_0 t}}_{{}_I\langle\Psi(t)|}\underbrace{e^{i\hat{H}_0 t}\hat{F}e^{-i\hat{H}_0 t}}_{\hat{F}_I(t)}\underbrace{e^{i\hat{H}_0 t}e^{-i\hat{H}t}|\Psi\rangle}_{|\Psi(t)\rangle_I}. \end{aligned} \tag{4.3}$$

The division of the operators shown defines the interaction representation, where both operators and states gain time dependence.

---

[1] In fact, there is a further restriction that $\hat{H}_0$ must be *free*, i.e. be a quadratic Hamiltonian, in order for the techniques developed here, in particular Wick's theorem to hold. The subject of perturbation theory around solvable but non-free (e.g. integrable) starting points is facinating, but beyond the scope of these lectures.

In the interaction picture, operators are free:

$$\hat{F}_I(t) = e^{i\hat{H}_0 t}\hat{F}e^{-i\hat{H}_0 t}, \tag{4.4}$$

i.e. they evolve under time using only the non-interacting part of the Hamiltonian $\hat{H}_0$. It is easy to show that they satisfy a Schrödinger equation under $\hat{H}_0$:

$$\frac{\partial \hat{F}_I(t)}{\partial t} = i\left[\hat{H}_0, \hat{F}_I(t)\right]. \tag{4.5}$$

The states therefore evolve as

$$\begin{aligned} |\Psi(t)\rangle_I &= \hat{U}(t)|\Psi\rangle \\ \hat{U}(t) &= e^{i\hat{H}_0 t}e^{-i\hat{H}t}, \end{aligned} \tag{4.6}$$

where $\hat{U}(t)$ is known as the time evolution operator (in the interaction representation). It is important to note that

$$e^{i\hat{H}_0 t}e^{-i\hat{H}t} \neq e^{i\hat{H}_{\text{int}}t} \tag{4.7}$$

due to the non-commutation of $\hat{H}_0$ and $\hat{H}_{\text{int}}$. So how do the states evolve? If we take Eq. 4.6 and differentiate it, we get

$$\begin{aligned} \frac{\partial \hat{U}(t)}{\partial t} &= i\hat{H}_0 e^{i\hat{H}_0 t}e^{-i\hat{H}t} - ie^{i\hat{H}_0 t}\left(\hat{H}_0 + \hat{H}_{\text{int}}\right)e^{-i\hat{H}t} \\ &= i\hat{H}_0 \underbrace{e^{i\hat{H}_0 t}e^{-i\hat{H}t}}_{\hat{U}(t)} - i\underbrace{e^{i\hat{H}_0 t}\left(\hat{H}_0 + \hat{H}_{\text{int}}\right)e^{-i\hat{H}_0 t}}_{=\hat{H}_0 + \hat{H}_{\text{int}}(t)}\underbrace{e^{i\hat{H}_0 t}e^{-i\hat{H}t}}_{\hat{U}(t)} \\ &= -i\hat{H}_{int}(t)\hat{U}(t), \end{aligned} \tag{4.8}$$

where

$$\hat{H}_{int}(t) = e^{i\hat{H}_0 t}\hat{H}_{\text{int}}e^{-i\hat{H}_0 t}, \tag{4.9}$$

i.e. is an operator in the interaction representation.

Ultimately, this means that the states evolve under time only under the action of the perturbation

$$\frac{\partial|\Psi(t)\rangle_I}{\partial t} = -i\hat{H}_{\text{int}}(t)|\Psi(t)\rangle_I, \tag{4.10}$$

but with the caveat that $\hat{H}_{\text{int}}(t)$ now also evolves under time (under the action of $\hat{H}_0$). To summarize the interaction representation:

1. Operators are ‘free’.

2. States satisfy Schrödinger equation involving only the perturbation $\hat{H}_{\text{int}}$.

4.2. The U-matrix and the S-matrix

To proceed with calculations, we now need to solve the time evolution equation for the states, written in terms of the time evolution operator $\hat{U}(t)$ derived in Eq. 4.8:

$$\frac{\partial \hat{U}(t)}{\partial t} = -i\hat{H}_{int}(t)\hat{U}(t). \tag{4.11}$$

This is exactly like the regular Schrödinger equation, except that $\hat{H}_{int}$ is explicitly time dependent, which means the (classical) solution we would like to write $\hat{U}(t) = \exp\left[-i\int_0^t \hat{H}_{\rm int}(t')dt'\right]$ is incorrect, because in general $[\hat{H}_{\rm int}(t), \hat{H}_{\rm int}(t')] \neq 0$, i.e. $\hat{H}_{\rm int}$ doesn't commute with itself at different times.

4.2.1. Solution for $\hat{U}(t)$

Instead, let us solve Eq. 4.11 iteratively. We know the initial condition that $\hat{U}(0) = 1$, so let us take Eq. 4.11 and integrate it from 0 to t:

$$\begin{aligned} \hat{U}(t) - \underbrace{\hat{U}(0)}_{=1} &= -i\int_0^t \hat{H}_{\rm int}(t')\hat{U}(t')\,dt' \\ \Longrightarrow \hat{U}(t) &= 1 - i\int_0^t \hat{H}_{\rm int}(t')\underbrace{\hat{U}(t')}\,dt' \end{aligned} \tag{4.12}$$

Now take the $\hat{U}(t)$ on the right hand side of the equation, and substitute back in the same expression:

$$\begin{aligned} \hat{U}(t) &= 1 - i\int_0^t \hat{H}_{\rm int}(t')\left[1 - i\int_0^{t'} \hat{H}_{\rm int}(t'')\hat{U}(t'')\,dt''\right]dt' \\ &= 1 - i\int_0^t dt'\,\hat{H}_{\rm int}(t') + (-i)^2\int_0^t dt'\int_0^{t'} dt''\,\hat{H}_{\rm int}(t')\hat{H}_{\rm int}(t'')\underbrace{\hat{U}(t'')}. \end{aligned} \tag{4.13}$$

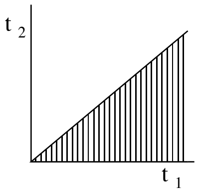
We can continue substituting in the expression for $\hat{U}(t'')$ on the right hand side, and eventually (after an infinite amount of time) we get the infinite sum

$$\hat{U}(t) = \sum_{n=0}^{\infty}(-i)^n\int_0^t dt_1\int_0^{t_1} dt_2\ldots\int_0^{t_{n-1}} dt_n\hat{H}_{\rm int}(t_1)\hat{H}_{\rm int}(t_2)\ldots\hat{H}_{\rm int}(t_n). \tag{4.14}$$

4.2.2. Symmetrized solution

While Eq. 4.14 is the correct solution for $\hat{U}(t)$, it is messy and asymmetric. The question is, can we write it in a more convenient and symmetric form? To do this, let us examine more carefully the case $n = 2$

$$\int_0^t dt_1 \int_0^{t_1} dt_2\, \hat{H}_{\text{int}}(t_1)\hat{H}_{\text{int}}(t_2), \qquad (4.15)$$



where the picture shows the integration region. Notice that $t_1 > t_2$ always, i.e. the operators in this expression are *time ordered*. We see therefore that

$$\begin{aligned}&\frac{1}{2!}\int_0^t dt_1 \int_0^t dt_2\, T\left[\hat{H}_{\text{int}}(t_1)\hat{H}_{\text{int}}(t_2)\right]\\ =\ &\frac{1}{2!}\int_0^t dt_1 \int_0^{t_1} dt_2\, \hat{H}_{\text{int}}(t_1)\hat{H}_{\text{int}}(t_2) + \frac{1}{2!}\int_0^t dt_2 \int_0^{t_2} dt_1\, \hat{H}_{\text{int}}(t_2)\hat{H}_{\text{int}}(t_1) \quad (4.16)\end{aligned}$$

which is identical to Eq. 4.15. It is not difficult to see the generalization of this to any term in the sum in Eq. 4.14 gives the final result

$$\boxed{\begin{aligned}\hat{U}(t) &= 1+\sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\int_0^t dt_1 \int_0^t dt_2 \ldots \int_0^t dt_n\, T\left[\hat{H}_{\text{int}}(t_1)\hat{H}_{\text{int}}(t_2)\ldots\hat{H}_{\text{int}}(t_n)\right]\\ &= T\exp\left\{-i\int_0^t dt'\,\hat{H}_{\text{int}}(t')\right\}. \qquad (4.17)\end{aligned}}$$

Note that the exponential form is just a short-hand way of writing the series.

4.2.3. The S-matrix (operator)

We now come to one of the most important constructions in diagrammatic perturbation theory, which is known as the S-matrix, although in our context it is more convenient to think of it as an operator than a matrix.[2]

We have discussed at length the time evolution operator $\hat{U}(t)$ which evolves the wavefunction in the interaction representation

$$|\Psi(t)\rangle_I = \hat{U}(t)|\Psi(0)\rangle_I. \qquad (4.18)$$

Now we would like to define a similar, but slightly more general object $\hat{S}(t,t')$, which evolves the system from time t' to time t:

$$|\Psi(t)\rangle_I = S(t,t')|\Psi(t')\rangle_I. \qquad (4.19)$$

Now, $|\Psi(t)\rangle_I = \hat{U}(t)|\Psi(0)\rangle$ and $|\Psi(t')\rangle_I = \hat{U}(t')|\Psi(0)\rangle$, so

$$\hat{U}(t)|\Psi(0)\rangle = \hat{S}(t,t')\hat{U}(t')|\Psi(0)\rangle, \qquad (4.20)$$

---

[2] Although one must remember that operators and matrices are basically the same things, and who cares about the name anyway?

or in other words

$$\hat{U}(t) = \hat{S}(t,t')\hat{U}(t') \implies \hat{S}(t,t') = \hat{U}(t)\hat{U}^{-1}(t'), \tag{4.21}$$

where $\hat{U}^{-1}(t')$ is the inverse operator to $\hat{U}(t)$, defined as

$$|\Psi(0)\rangle = \hat{U}^{-1}(t')|\Psi(t')\rangle_I, \tag{4.22}$$

i.e. $\hat{U}^{-1}(t')\hat{U}(t') = 1$. Following similar arguments as before, one sees that

$$\hat{U}^{-1}(t) = T\exp\left\{+i\int_0^t dt'\,\hat{H}_{\text{int}}(t')\right\} = \hat{U}^\dagger(t), \tag{4.23}$$

i.e. $\hat{U}(t)$ is a unitary operator. This gives us the important equation

$$\hat{S}(t,t') = \hat{U}(t)\hat{U}^\dagger(t'). \tag{4.24}$$

The S-matrix has a number of properties, all of which can be verified trivially:

1. $\hat{S}(t,t) = 1$,
2. $\hat{S}(t',t) = \hat{S}^\dagger(t,t')$,
3. $\hat{S}(t,t')\hat{S}(t',t'') = \hat{S}(t,t'')$, i.e. one can evolve from t to t'' by first evolving from t to t' and then from t' to t'', pretty much as we would expect.
4. Finally,
$$\frac{\partial}{\partial t}\hat{S}(t,t') = \frac{\partial}{\partial t}\hat{U}(t)\hat{U}^\dagger(t') = -i\hat{H}_{\text{int}}(t)\hat{S}(t,t'), \tag{4.25}$$
which can be solved as we did for $\hat{U}(t)$ to give us

$$\boxed{\hat{S}(t,t') = T\exp\left\{-i\int_{t'}^t dt_1\,\hat{H}_{\text{int}}(t_1)\right\}.} \tag{4.26}$$

4.2.4. Application to the Green function

We can now return to the Green function defined last lecture

$$G(\vec{x}_1,t_1;\vec{x}_2,t_2) = -i\langle T\hat{\Psi}_H(\vec{x}_1,t_1)\hat{\Psi}_H^\dagger(\vec{x}_2,t_2)\rangle, \tag{4.27}$$

It is important to note that in this definition, $\hat{\Psi}$ and $\hat{\Psi}^\dagger$ are in the Heisenberg representation. Now,

$$\begin{aligned}
\hat{\Psi}_H(t) &= e^{i\hat{H}t}\hat{\Psi}e^{-i\hat{H}t} \\
&= \underbrace{e^{i\hat{H}t}e^{-i\hat{H}_0t}}\,\underbrace{e^{i\hat{H}_0t}\hat{\Psi}e^{-i\hat{H}_0t}}\,\underbrace{e^{i\hat{H}_0t}e^{-i\hat{H}t}} \\
&= \hat{U}^\dagger(t)\hat{\Psi}_I(t)\hat{U}(t) \\
&= \hat{S}(0,t)\hat{\Psi}_I(t)\hat{S}(t,0).
\end{aligned} \tag{4.28}$$

We see that by using the S-matrix, we can transform operators in the Heisenberg representation to operators in the interaction representation. Hence the Green function can now be written

$$-i\langle GS|T[\hat{S}(0,t)\hat{\Psi}(\vec{x}_1,t_1)\underbrace{\hat{S}(t,0)\hat{S}(0,t')}_{=S(t,t')}\hat{\Psi}^\dagger(\vec{x}_2,t_2)\hat{S}(t',0)]|GS\rangle, \tag{4.29}$$

where all of the operators are now in the interaction representation, i.e. they evolve only under the action of $\hat{H}_0$, which we know how to solve. We also know what the S-matrix is in terms of a sum - so by calculating terms in this sum, we will have a perturbation theory for the Green function of the *interacting* system.

There is however one more important problem we must address before we can do this: and that is that $|GS\rangle$ must be the *interacting* ground state of the system, whereas so far we only know how to calculate expectation values in the non-interacting $|GS\rangle_0$. This will be addressed in the next section.

4.3. Gell-Mann and Low theorem

The Gell-Mann and Low theorem tells us that the interacting ground state of a system is related to the non-interacting ground state via the expression

$$\boxed{|GS\rangle = \hat{S}(0,-\infty)|GS\rangle_0. \qquad (4.30)}$$

We won't prove this theorem - for that we recommend reading the original paper [Phys. Rev. 84, 350 (1951)], particularly the appendix. We will however try to physically motivate this expression by using the *adiabatic* concept.

Consider a slight modification of our model

$$\hat{H} = \hat{H}_0 + e^{-\alpha|t|}\hat{H}_{\text{int}}, \tag{4.31}$$

which becomes our model in the limit $\alpha \to 0$. Consider first however α finite. Then in the distant (infinite) past, $t \to -\infty$, the system is non-interacting, so

$$|GS(t=-\infty)\rangle = |GS(t=-\infty)\rangle_0 = |GS\rangle_0 \tag{4.32}$$

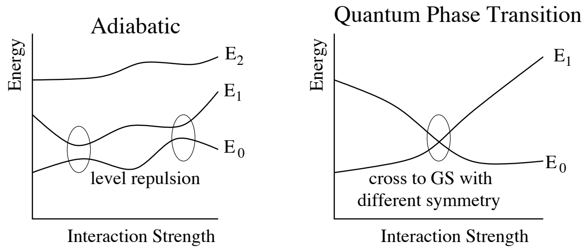
where the last equality follows because in the interaction representation, a non-interacting ground state does not evolve with time. Therefore

$$|GS(t=0\rangle = \hat{S}(0,-\infty)|GS(t=-\infty)\rangle = \hat{S}(0,-\infty)|GS\rangle_0, \tag{4.33}$$

where of course, now the S-matrix is that of the Hamiltonian 4.31, including α. What Gell-Mann and Low showed was that the limit $\alpha \to 0$ exists and gives the right answer, which gives us the Gell-Mann-Low theorem, Eq. 4.30.

We must be very careful however, that the adiabatic concept works only in the absence of any symmetry breaking quantum phase transitions - i.e. *if the interacting ground state*

Figure 4.1.: A schematic illustration of the difference between an adiabatic system and one with a quantum phase transition as the strength of the interaction is increased.



is not adiabatically connected to the non-interacting one, then the theorem is not true. This is illustrated schematically in Fig. 4.1.

One can also think of the limit $t \to +\infty$, where one must in the adiabatic case similarly return to the non-interacting ground state, but with a possible phase factor[3]

$$e^{iL} {}_0\langle GS|\hat{S}(\infty,0) = \langle GS|. \tag{4.34}$$

The phase factor e^{iL} is evaluated as $e^{iL} = {}_0\langle GS|\hat{S}(-\infty,\infty)|GS\rangle_0$.

If we now return to the Green function

$$G(\vec{x}_1,t_1;\vec{x}_2,t_2) = -i\frac{{}_0\langle GS|T\,\hat{S}(\infty,0)\hat{S}(0,t)\hat{\Psi}(\vec{x}_1,t_1)\hat{S}(t,t')\ \hat{\Psi}^\dagger(\vec{x}_2,t_2)\hat{S}(t',0)\hat{S}(0,-\infty)|GS\rangle_0}{{}_0\langle GS|\hat{S}(\infty,-\infty)|GS\rangle_0} \tag{4.35}$$

Finally, bearing in mind that the time ordering operator will place everything within the expectation value in order of increasing time anyway, it doesn't matter which order we write them, so we finally get a very compact expression for the Green function:

$$\boxed{\begin{aligned} G(\vec{x}_1,t_1;\vec{x}_2,t_2) &= -i\frac{\langle T\,\hat{\Psi}(\vec{x}_1,t_1)\hat{\Psi}^\dagger(\vec{x}_2,t_2)\hat{S}(\infty,-\infty)\rangle}{\langle\hat{S}(\infty,-\infty)\rangle}, \\ \hat{S}(\infty,-\infty) &= T\exp\left\{-i\int_{-\infty}^{\infty}\hat{H}_{\text{int}}(t')dt'\right\}. \qquad (4.36)\end{aligned}}$$

This is an expression for the *interacting* Green function, but

1. All expectation values are with respect to the non-interacting ground state $|GS\rangle_0$, and

2. All time dependence is in interaction representation, i.e. is only due to the non-interacting part, $\hat{H}_0$.

---

[3] Instead of continuing the evolution to $+\infty$, one could instead evolve back to $t = -\infty$, which is known as the Keldysh technique. This method is essential for systems out of equilibrium, where there is no reason to suppose the $t \to +\infty$ limit is the same as the $t \to -\infty$ limit. However, evolving forwards in time then backwards in time adds extra complications to the formalism and is technically more difficult so this technique is rarely used unless necessary.

Therefore, if we expand the S-matrix as a sum (which the exponential notation is shorthand for anyway), we get a perturbation expansion in the strength of the perturbation (interaction), where we calculate everything (expectation values and time evolution) with respect to the unperturbed system - i.e. we have achieved the goal we set in the second lecture. There is just one more thing to learn before this scheme becomes practical, and that is how to take (non-interacting) expectation values of large numbers of operators. This was something we hinted at in previous lectures, but now we see it in full detail.

4.4. Wick's theorem

We will demonstrate Wick's theorem via an example, to see how everything works, and from this, we will state the theorem in the general case. For a formal proof of the theorem, see the textbooks.

Suppose we want to calculate the expectation value

$$A(\vec{k}_1,\dots\vec{k}_6;t_1,\dots t_6) = \langle T\, \hat{c}^\dagger_{\vec{k}_1}(t_1)\hat{c}^\dagger_{\vec{k}_2}(t_2)\hat{c}^\dagger_{\vec{k}_3}(t_3)\hat{c}_{\vec{k}_4}(t_4)\hat{c}_{\vec{k}_5}(t_5)\hat{c}_{\vec{k}_6}(t_6)\rangle, \tag{4.37}$$

where everything is non-interacting. Now, aside from the time dependence, the time ordering, and the larger number of operators, this is very similar to what we achieved in the first lecture for Eq. 1.37.

We look at the time dependence first. In Lecture 3, (Eq. 3.38 and Eq. 3.39), we saw that if everything is non-interacting that the time dependent operators may simply be written

$$\hat{c}^\dagger_{\vec{k}}(t) = e^{-i\epsilon_0(\vec{k})t}\hat{c}^\dagger_{\vec{k}}, \qquad \hat{c}_{\vec{k}}(t) = e^{i\epsilon_0(\vec{k})t}\hat{c}_{\vec{k}}, \tag{4.38}$$

no matter which state they act on. Bearing this in mind, let us start as usual from the right:

- We start with $|GS\rangle_0$. This is an eigenstate of the non-interacting Hamiltonian.
- After the $\hat{c}_{\vec{k}_6}$ annihilation operator acts, we still have an eigenstate.
- Under time evolution, we gain a phase factor, but the state itself doesn't change.
- Therefore in order to have a non-zero overlap with ${}_0\langle GS|$, one of the operators $\hat{c}^\dagger_{\vec{k}_1}$, $\hat{c}^\dagger_{\vec{k}_2}$ or $\hat{c}^\dagger_{\vec{k}_3}$ must recreate this state again.
- Similarly for $\hat{c}_{\vec{k}_5}$ and $\hat{c}_{\vec{k}_4}$.

There are six possible pairings, which for convenience are shown explicitly in Figure 4.2. For each possible pairings, we can (by virtue of the anti-commutation relations) swap the operators so that the contracted ones are always together, and finally we insert $|GS\rangle_0\, {}_0\langle GS|$ between each pair of operators, which doesn't change anything, as we know after each pair we must get back to this state anyway. Put mathematically, we see that

$$\begin{aligned} & A(\vec{k}_1,\dots\vec{k}_6;t_1,\dots t_6) \\ = & \sum_{pairings} (-1)^P \langle T\hat{c}^\dagger_{\vec{k}_{p_1}}(t_{p_1})\hat{c}_{\vec{k}_{p_2}}(t_{p_2})\rangle\langle T\hat{c}^\dagger_{\vec{k}_{p_3}}(t_{p_3})\hat{c}_{\vec{k}_{p_4}}(t_{p_4})\rangle\langle T\hat{c}^\dagger_{\vec{k}_{p_5}}(t_{p_5})\hat{c}_{\vec{k}_{p_6}}(t_{p_6})\rangle, \end{aligned} \tag{4.39}$$

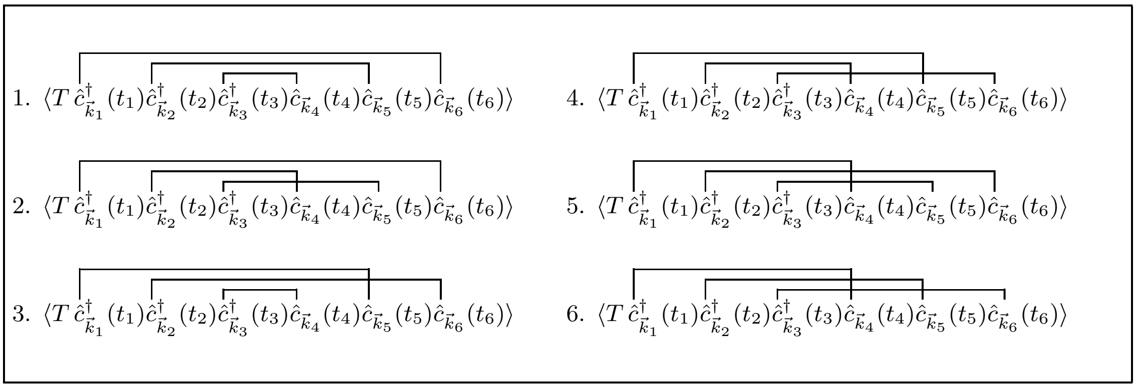


Figure 4.2.: The six different contractions of an expectation value with three creation and three annihilation operators.

where $\{p_1, \ldots, p_6\}$ is the permutation in question, and $(-1)^P$ is the parity of the permutation, i.e. it is ±1 depending on whether you had to swap an odd or even number of fermions to get to this state.

In writing Eq. 4.39, there is one more thing we should feel uneasy about - and that is the time ordering operator. In fact, there is nothing to worry about - the original time ordering operator puts the six original operators in some order, including a relevant minus sign depending on the number of fermionic swaps. From this moment onwards, the time may be taken out and expressed as the phase factors given by Eq. 4.38. The only thing we have to worry about is which creation operators are to the right or left of which annihilation operators. A little reflection will tell you that the time ordering operators in each individual expectation value in Eq. 4.39 will do the job correctly.

We therefore can finally write down:

Wick's theorem
Within a *non-interacting* system, the time ordered expectation value of a number of creation and annihilation operators may be written as the sum over all possible pairings of the product of the time ordered expectation value of each pair. Each term in the sum is weighted by the parity, which is plus or minus 1 depending on whether you have an odd or even no of Fermionic swaps to obtain the pairing.

It shouldn't have escaped your notice that each of the terms like $\langle T\hat{c}^\dagger_{\vec{k}_{p_1}}(t_{p_1})\hat{c}_{\vec{k}_{p_2}}(t_{p_2})\rangle = -\langle T\hat{c}_{\vec{k}_{p_2}}(t_{p_2})\hat{c}^\dagger_{\vec{k}_{p_1}}(t_{p_1})\rangle$ which appear on the R.H.S. of Eq. 4.39 are basically nothing but non-interacting Green functions, G_0, as we calculated in the second lecture (the reason the order we write the operators doesn't matter up to a minus sign is because the time-ordering operator will order them anyway). We finish this section with an example of Wick's theorem:

Example 4.1:

$$\begin{aligned}
&\langle T\,\hat{c}^{\dagger}_{\vec{k}_1}(t_1)\hat{c}^{\dagger}_{\vec{k}_2}(t_2)\hat{c}_{\vec{k}_3}(t_3)\hat{c}_{\vec{k}_4}(t_4)\rangle \\
=\;& -\langle T\,\hat{c}_{\vec{k}_3}(t_3)\hat{c}^{\dagger}_{\vec{k}_1}(t_1)\rangle\langle T\,\hat{c}_{\vec{k}_4}(t_4)\hat{c}^{\dagger}_{\vec{k}_2}(t_2)\rangle \\
& +\langle T\,\hat{c}_{\vec{k}_3}(t_3)\hat{c}^{\dagger}_{\vec{k}_2}(t_2)\rangle\langle T\,\hat{c}_{\vec{k}_4}(t_4)\hat{c}^{\dagger}_{\vec{k}_1}(t_1)\rangle \\
=\;& -\delta_{\vec{k}_3,\vec{k}_1}\delta_{\vec{k}_4,\vec{k}_2}\, iG_0(\vec{k}_3, t_3-t_1)\, iG_0(\vec{k}_4, t_4-t_2) \\
& +\delta_{\vec{k}_2,\vec{k}_3}\delta_{\vec{k}_4,\vec{k}_1}\, iG_0(\vec{k}_3, t_3-t_2)\, iG_0(\vec{k}_4, t_4-t_1).
\end{aligned} \tag{4.40}$$

We are now at a stage to put all of the bits and pieces we have learned in this lecture together and obtain the perturbation expansion for the zero-temperature Green function. This will be the topic of the next lecture.

5. Feynman Rules, Dyson series and self energy

In the last lecture, we paved the way to develop the diagrammatic expansion. In this lecture, we will put all of these concepts together to finally derive and develop the diagrammatic expansion. Now, it will turn out in condensed matter that very often, we need to go to infinite order in the perturbation theory to make any sense. To see how this works, we will look at the Dyson series, which leads us naturally to the important concept of self-energy.

5.1. Diagrams!

Let us go back to our equation for the interacting Green function Eq. 4.36, and expand out the exponential:

$$G(\vec{k},t-t') = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \ldots \int_{-\infty}^{\infty} dt_n \\ \times \frac{\langle T\, \hat{c}_{\vec{k}}(t) \hat{H}_{\text{int}}(t_1) \hat{H}_{\text{int}}(t_2) \ldots \hat{H}_{\text{int}}(t_n) \hat{c}^{\dagger}_{\vec{k}}(t') \rangle}{\langle S(\infty,-\infty) \rangle}. \tag{5.1}$$

Notice that we have also expressed the Green function in terms of the eigenstate creation and annihilation operators $\hat{c}^{\dagger}_{\vec{k}}$,$\hat{c}_{\vec{k}}$ rather than the field operators $\hat{\Psi}^{\dagger}(\vec{x})$,$\hat{\Psi}(\vec{x})$,[1] and we are continuing to ignore spin.

Let us for now ignore the denominator, which is just a number. Now, remembering that:

1. $\hat{H}_{\text{int}}$ itself is just a collection of creation and annihilation operators,
2. The expectation values are taken with respect to the non-interacting ground state, and
3. All operator are in the interaction representation, which is really just the Heisenberg representation for the non-interacting problem,

what we have done is write the interacting Green function as a sum of non-interacting expectation values. The n'th term in this series contains $\hat{H}_{\text{int}}$ precisely n times, so if the

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[1] the only difference this makes is simplicity - as we will see next lecture, we can carry out exactly the same procedure using the field operators instead of the eigenstate ones.

interaction has some parameter α governing it's strength, this is a perturbation theory in α.[2] Using Wick's theorem, we can write each term in this expansion in terms of non-interacting Green's functions. This is the general principle behind perturbation theory in quantum field theory. In fact, the rules for constructing the diagrams (which is what we are about to derive) depend on the exact form of $\hat{H}_{\text{int}}$, so we now will specialize to the case of two body interactions. If you are interested in a problem where $\hat{H}_{\text{int}}$ isn't of the form below, the Feynman diagram technique is still applicable, however you will need to come back to this step and derive the rules for your particular case. Some examples of this will be seen later in the course.

5.1.1. Two body interactions

Let us consider $\hat{H}_{\text{int}}$ to be a two body interaction which has the general form

$$\hat{H}_{\text{int}} = \frac{1}{V} \sum_{\vec{k}_1,\vec{k}_2,\vec{q}} \hat{c}^\dagger_{\vec{k}_1} \hat{c}^\dagger_{\vec{k}_2} \frac{U_{\vec{q}}}{2} \hat{c}_{\vec{k}_2+\vec{q}} \hat{c}_{\vec{k}_1-\vec{q}}. \tag{5.2}$$

Notice firstly the factor of 2 we have introduced, which at the moment is arbitrary but will turn out to be very convenient later on. Secondly, notice that we have an unrestricted sum over $\vec{q}$ - meaning that if we wish to use the Coulomb interaction

$$\frac{U_{\vec{q}}}{2} = 4\pi e^2/q^2 \qquad \Longrightarrow \qquad U_{\vec{q}} = 8\pi e^2/q^2, \tag{5.3}$$

we must also artificially set $U_{\vec{q}=0} = 0$ (c.f. discussion in Lecture 2). Finally note that the interaction $U_{\vec{q}}$ is independent of time.[3]

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[2] Note that while we say interaction, $\hat{H}_{\text{int}}$ could in principle be any perturbation to the Hamiltonian $\hat{H}_0$, in which case Eq. 5.1 gives a perturbation series in powers of the size of the perturbation. For concreteness, we will stick to the perturbation being an interaction for most of this course, although we will give a few different examples such as disorder or phonons near the end.

[3] While the static Coulomb interaction is generally enough for condensed matter physics, if one wants to study quantum electrodynamics (QED), one must (of course) put in the finite speed of light, which means that the interaction is no longer time independent. A time dependent interaction can be treated with Feynman diagrams (which were originally developed for QED) without problems, but the Feynman rules we derive are for the static case.

Example 5.1: A first order term

$$\begin{aligned}&\langle T\,\hat{c}_{\vec{k}}(t)\hat{H}_{\text{int}}(t_1)\hat{c}^{\dagger}_{\vec{k}}(t')\rangle\\ =\ & \frac{1}{V}\sum_{\vec{k}_1,\vec{k}_2,\vec{q}}\frac{U_{\vec{q}}}{2}\langle T\,\hat{c}_{\vec{k}}(t)\hat{c}^{\dagger}_{\vec{k}_1}(t_1)\hat{c}^{\dagger}_{\vec{k}_2}(t_1)\hat{c}_{\vec{k}_2+\vec{q}}(t_1)\hat{c}_{\vec{k}_1-\vec{q}}(t_1)\hat{c}^{\dagger}_{\vec{k}}(t')\rangle \qquad (5.4)\end{aligned}$$

contains 3 creation and 3 annihilation operators, therefore may be written in terms of sums of products of 3 Green functions.

A second order term,

$$\langle T\,\hat{c}_{\vec{k}}(t)\hat{H}_{\text{int}}(t_1)\hat{H}_{\text{int}}(t_2)\hat{c}^{\dagger}_{\vec{k}}(t')\rangle, \qquad (5.5)$$

will contain 5 creation and 5 annihilation operators, therefore may be written in terms of sums of products of 5 Green functions. And so on.

In fact, Eq. 5.4 in the example shows us one more thing that can happen which we must deal with before we write down the Feynman rules: very often, two operators will occur at the same time - in fact, in any term in the perturbation series the operators will come in sets of four with each of the four at identical times.

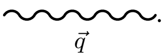
Now, we know back from Eq. 3.40 in Lecture 3 that the non-interacting Green function has a discontinuity at equal time $t - t' = 0$. In other words, at equal time, the time ordering operator doesn't know which way round to put the operators, and taking the limit from either side will yield different results. Realizing that that this ambiguity always comes from the operators in a single interaction term - which we know from Lecture 2 should be *normal ordered*, we make the final rule that:

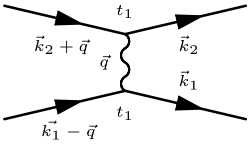
- If two operators occur at equal time, they should be normal ordered.

In practical terms, this means if we come across a Green function $G_0(\vec{k}, t = 0)$, this should be interpreted as $G_0(\vec{k}, t = 0^-)$, where 0^- means the limit as zero is approached from the negative side.

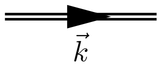
5.1.2. Representation as diagrams

We are finally ready to introduce what we have all been waiting for - Feynman diagrams. The diagrams are in fact nothing but a way of keeping track of the terms in the expansion Eq.5.1. The correspondence is given by:

- For every $G_0(\vec{k}, t - t')$, we have a line (with an arrow) – $t' \xrightarrow[\vec{k}]{\qquad} t$.
- For every $U_{\vec{q}}/2$ there is a wiggly line (which doesn't require an arrow) – .

- At the vertex, there is momentum conservation –  . The interaction links two points at equal time.

Now with this diagrammatic representation, let us look in more detail at the perturbation expansion for the interacting Green function (which we represent diagrammatically by a double line with an arrow):

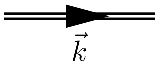
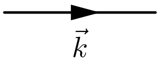
$G(\vec{k},t-t') =$ t'  t $= G^{(0)} + G^{(1)} + G^{(2)} + \dots,$ (5.6)

where we must remember that we are still ignoring the factor $\langle S(\infty,-\infty)\rangle$ in the denominator.

5.1.3. Zeroth order

To zeroth order, the S matrix is just one $S^{(0)} = 1$. This means that

$$G^{(0)}(\vec{k},t-t') = G_0(\vec{k},t-t') \tag{5.7}$$

t'  t $=$ t'  t $+\dots$

The interpretation of this is that the particle with momentum $\vec{k}$ introduced at time t' travels directly and gets to time t without interacting with (scattering off) any other particles. The first order terms will then be when it scatters once, second order when it scatters twice, and so on. According to quantum mechanics, we sum up the appropriate weight of all of these methods of getting from time t' to time t, to give us the total probability amplitude, G.

5.1.4. First order

The first order correction to the S matrix

$$S^{(1)} = -i\int_{-\infty}^{\infty} \hat{H}_{\text{int}}(t_1)dt_1. \tag{5.8}$$

This gives

$$G^{(1)} = (-i)^2\int_{-\infty}^{\infty} dt_1 \frac{1}{V}\sum_{\vec{k}_1,\vec{k}_2,\vec{q}} \frac{U_{\vec{q}}}{2} \underbrace{\langle T\, \hat{c}_{\vec{k}}(t)\hat{c}^\dagger_{\vec{k}_1}(t_1)\hat{c}^\dagger_{\vec{k}_2}(t_1)\hat{c}_{\vec{k}_2+\vec{q}}(t_1)\hat{c}_{\vec{k}_1-\vec{q}}(t_1)\hat{c}^\dagger_{\vec{k}}(t')\rangle} \tag{5.9}$$

One factor of $(-i)$ is from the expansion of S, the other is from the definition of G.

Now, we know from Fig. 4.2 that there are six possible pairings of this expectation value - hence there are six first order terms contributing to $G^{(1)}$, or as we say six *diagrams.* Let us consider the first pairing,

$$\langle T\, \overbrace{\hat{c}_{\vec{k}}(t)\hat{c}^\dagger_{\vec{k}_1}}(t_1)\overbrace{\hat{c}^\dagger_{\vec{k}_2}(t_1)\hat{c}_{\vec{k}_2+\vec{q}}}(t_1)\overbrace{\hat{c}_{\vec{k}_1-\vec{q}}(t_1)\hat{c}^\dagger_{\vec{k}}}(t')\rangle. \tag{5.10}$$

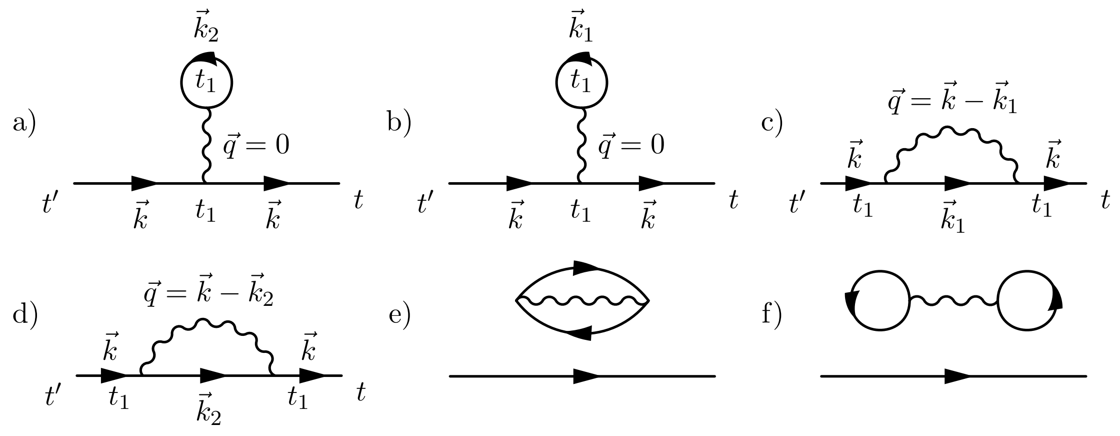


Figure 5.1.: The six first order diagrams, from the six Wick contractions.

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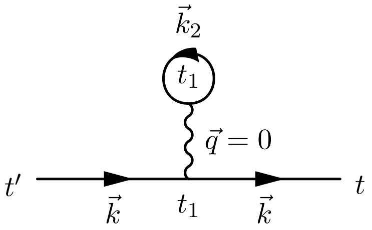
This gives

$$\begin{aligned} G^{(1a)} &= (-1)\int_{-\infty}^{\infty} dt_1 \frac{1}{V}\sum_{\vec{k}_1,\vec{k}_2,\vec{q}} \frac{U_{\vec{q}}}{2}\left\{-\underbrace{\langle T\,\hat{c}_{\vec{k}}(t)\hat{c}^{\dagger}_{\vec{k}_1}(t_1)\rangle}_{\vec{k}=\vec{k}_1}\underbrace{\langle T\,\hat{c}_{\vec{k}_2+\vec{q}}(t_1)\hat{c}^{\dagger}_{\vec{k}_2}(t_1)\rangle}_{\vec{q}=0}\underbrace{\langle T\,\hat{c}_{\vec{k}_1-\vec{q}}(t_1)\hat{c}^{\dagger}_{\vec{k}}(t')\rangle}_{\vec{k}=\vec{k}_1,\,\vec{q}=0}\right\} \\ &= i\int_{-\infty}^{\infty} dt_1 \frac{1}{V}\sum_{\vec{k}_2} \frac{U_{\vec{q}=0}}{2} G_0(\vec{k},t_1-t')G_0(\vec{k}_2,0^-)G_0(\vec{k},t-t_1). \end{aligned} \tag{5.11}$$

The corresponding diagram is:

$$G^{(1a)}(\vec{k},t-t') =$$



(5.12)

All six first order diagrams (including the one already studied) are shown in Figure 5.1. Notice that there are two pairs of diagrams, (a,b) and (c,d) which look identical to each other, and the last two, (e) and (f) are disconnected. We will come back to this in the next section.

Exercise 5.1: (**) Write down the remaining five Wick contractions of the first order expression. Which of your expressions corresponds to which diagram in Fig. 5.1? Put the momentum labels on diagrams (e) and (f).

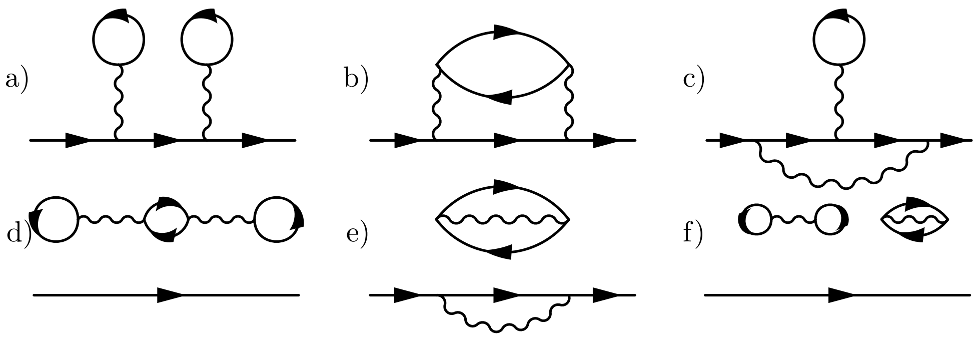


Figure 5.2.: A small selection of second order diagrams.

5.1.5. Second Order

The second order correction to the S matrix

$$S^{(2)} = \frac{(-i)^2}{2!} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \, \hat{H}_{\text{int}}(t_1) \hat{H}_{\text{int}}(t_2). \tag{5.13}$$

When this is substituted into the expression for G, we see that a second order diagram will consist of five fermionic lines and two interaction lines, and as there will be $5! = 120$ Wick contractions, there will in principle be 120 diagrams, although like the first order case, we may expect some of the diagrams to look identical to other ones.[4] A small selection of the second order diagrams are shown in Figure 5.2.

Exercise 5.2: (***) Draw all of the different second order diagrams. Unless I'm mistaken, I make 10 connected diagrams, and 11 disconnected ones.

We see that very quickly, the number of diagrams is becoming unmanageable. We are going to have to do some further work in reducing this if we are going to have a useful theory. This is exactly what we are going to do now.

5.2. Simplifications and cancellations in the diagrammatic expansion

While we now have the basics of what we are doing, there is still a bit of work to do. We still calculate first the perturbation expansion and Wick contractions, then draw diagrams to represent them. We would like to be able to do this the other way around - draw the diagrams, and then right the expression in the perturbation expansion for

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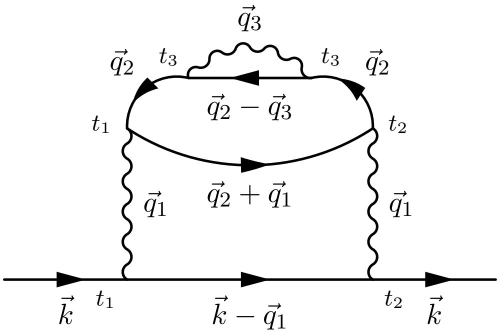
[4] As a brief glimpse ahead, once we have introduced symmetry factors, vacuum cancellations and Dyson series, these 120 diagrams will be reduced to 3 distinct, non-zero ones. Quite a saving! Read on.

which it corresponds, including factors of i, $1/n!$ and other things. We have also noticed that when we make all possible Wick contractions, some of the diagrams look identical to each other (and if you completed the exercise, you'll have seen that furthermore, the expressions are identical). We can ask ourselves if there is a way to consider the diagram only once, and be able to work out this *symmetry* factor. We also still have to work out what to do with the denominator. We will now look at a number of ways the number of diagrams may be reduced:

5.2.1. Multiple interaction symmetry factors

Let us, as usual, work by example. Consider a typical third order term:



- A third order term contains 3 interaction lines and 7 fermionic lines
- There are therefore $7! = 5040$ possible Wick contractions
- How can we tell how many will look the same?

This term arises from one particular contraction of

$$\langle T\, \hat{c}_{\vec{k}} \hat{H}_{\text{int}}(t_1) \hat{H}_{\text{int}}(t_2) \hat{H}_{\text{int}}(t_3) \hat{c}^\dagger_{\vec{k}} \rangle. \tag{5.14}$$

Now look carefully at the three interaction lines, which occur at t_1, t_2 and t_3, or as a label, I will say interaction lines $1, 2, 3$. Now imagine a different Wick contraction where instead of everything contracted with $\hat{H}_{\text{int}}(t_1)$, you contract it with $\hat{H}_{\text{int}}(t_2)$ and vice versa. This will create exactly the same diagram (i.e. exactly the same product of Green functions), except with the interaction lines in a different order, $2, 1, 3$. However, as we integrate over all t_1 and t_2 anyway, this change of label means nothing, so the contribution to $G^{(3)}$ from these two particular diagrams are identical. In fact, there are $3! = 6$ possible ways of labelling the three interaction lines: $(1, 2, 3), (1, 3, 2), (2, 1, 3), (2, 3, 1), (3, 1, 2), (3, 2, 1)$. We therefore only need to draw (and hence evaluate) the diagram once, then we multiply it by this factor $3!$, or in general $n!$ where n is the number of interaction lines, on in the words, the order of the perturbation expansion.

However, in the expansion of the S matrix, there is already a $1/n!$ term:

$$S(\infty, -\infty) = 1 - iT \int_{-\infty}^{\infty} dt_1\, \hat{H}_{\text{int}}(t_1) + \frac{(-i)^2}{2!} T \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2\, \hat{H}_{\text{int}}(t_1) \hat{H}_{\text{int}}(t_2) + \ldots \tag{5.15}$$

The $n!$ symmetry factor for each diagram exactly cancels the $1/n!$ in the expansion.

5.2.2. Single interaction symmetry factors

Now we look in detail at each individual interaction line. Each interaction line has two ends, so there are two possible ways of orienting it:

$$\text{(a)}\ \dots \hat{c}^\dagger_{\vec{k}_1}\, \hat{c}^\dagger_{\vec{k}_2}\, U_{\vec{q}}\, \hat{c}_{\vec{k}_2+\vec{q}}\, \hat{c}_{\vec{k}_1-\vec{q}} \dots \qquad \text{(b)}\ \dots \hat{c}^\dagger_{\vec{k}_1}\, \hat{c}^\dagger_{\vec{k}_2}\, U_{\vec{q}}\, \hat{c}_{\vec{k}_2+\vec{q}}\, \hat{c}_{\vec{k}_1-\vec{q}} \dots \tag{5.16}$$

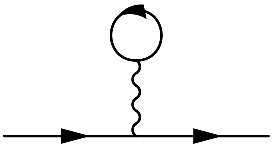
For every option (a) of contracting this particular interaction with whatever else, option (b) will give an identical result (when summed over all internal momenta). Summing over these two interaction line orientations is equivalent to making sure you draw only *topologically distinct* diagrams, and for each interaction line, you get a factor $U_{\vec{q}}$, instead of the $U_{\vec{q}}/2$ written in the Hamiltonian (this is where the factor of 2 comes in useful!).

5.2.3. Multiplicitive prefactors

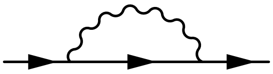
A typical term at order n has n interaction lines, and $2n+1$ Green functions. This means that if we draw an n'th order diagram, there must be a factor

$$\underbrace{(i)^{2n+1)}}_{\text{each } \langle \hat{c}_{\vec{k}} \hat{c}^\dagger_{\vec{k}} \rangle \text{ is } iG(\vec{k})} \times \underbrace{(-i)^n}_{\text{factor in } S\text{-matrix expansion}} \times \underbrace{(-i)}_{G=-i\langle \dots \rangle} = i^n. \tag{5.17}$$

What about the factors of ±1 from the number of fermionic swaps? Let us look at two first order diagrams:

1. 

$$\sim \langle T\, \hat{c}_{\vec{k}} \hat{c}^\dagger_{\vec{k}_1}\, \hat{c}^\dagger_{\vec{k}_2}\, U_{\vec{q}}\, \hat{c}_{\vec{k}_2+\vec{q}} \hat{c}_{\vec{k}_1-\vec{q}} \hat{c}^\dagger_{\vec{k}} \rangle \qquad \dots \text{factor } (-1)$$

2. 

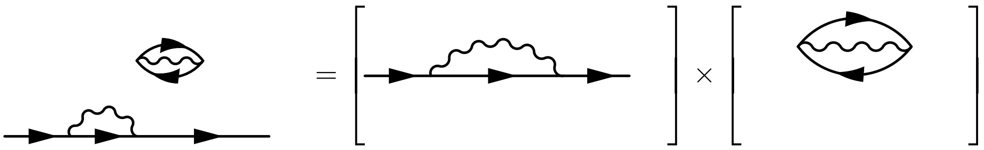
$$\sim \langle T\, \hat{c}_{\vec{k}} \hat{c}^\dagger_{\vec{k}_1}\, \hat{c}^\dagger_{\vec{k}_2}\, U_{\vec{q}}\, \hat{c}_{\vec{k}_2+\vec{q}} \hat{c}_{\vec{k}_1-\vec{q}} \hat{c}^\dagger_{\vec{k}} \rangle \qquad \dots \text{factor } (+1)$$

In the first case, the factor of (-1) arises because the middle contraction is in the wrong order to be a Green function, so there is one swap. In the second case, one swap is made to untangle the contractions, then a second one to get the middle contraction into the form of a Green function again, giving an overall factor of $(+1)$.

Is there any way to see from the pictures whether the factor will be ±1? The answer is yes, although I won't prove it. It turns out that with a bit of fiddling and doing a few examples that the correct factor is $(-1)^F$ where F is the number of closed fermionic loops - in the first diagram above, $F = 1$, in the second, $F = 0$. For a proof of this, it's best to play around a little yourself to see it is true, but failing that, any of the major textbooks will give a proof.

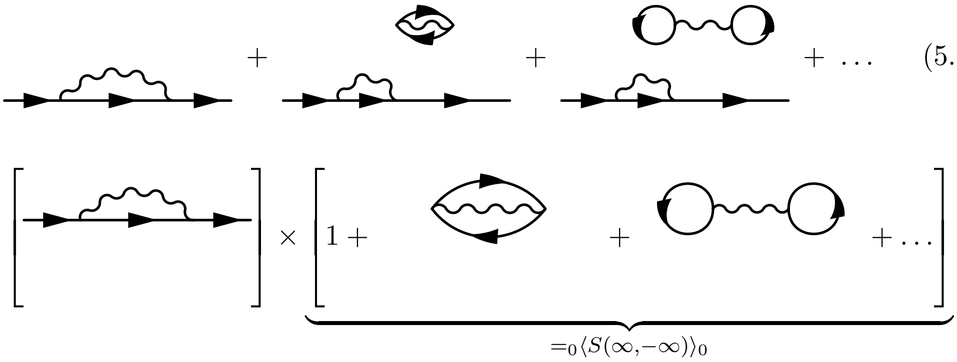
5.2.4. Vacuum graph cancellation

Notice something else interesting: at each order in perturbation theory, all of the prefactors are multiplicitive: the numerical prefactor $1/n!$ has cancelled, and all we are left with is factors of i or -1 which multiply together a certain number of times - meaning that *diagrams factorize*:[5]



(5.18)

In particular, we can see that



(5.19)

Graphs with no lines coming in or going out are exactly graphs that occur in the diagrammatic expansion of $_0\langle S(\infty,-\infty)\rangle_0$, i.e. the denominator in the expansion Eq. 5.1 which we have been so far ignoring. From the above factorization however, we see that by considering *only connected diagrams*, we cancel the denominator.

5.2.5. The Feynman Rules

We are now in a position to write down the Feynman rules for calculating $G(\vec{k}, t-t')$ to n^{th} order in perturbation theory:

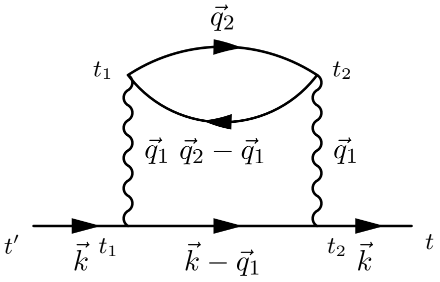
1. From all connected, topologically non-equivalent diagrams with $2n$ vertices, n wiggly lines and $2n+1$ directed solid lines (vertex=meeting of two solid and one wiggly line).
2. For each wiggly line, associate a time t_i, $i = 1 \ldots n$ and write down all momenta, such that momentum is conserved at each vertex.
3. For each solid line, associate a factor $G_0(\vec{k}_i, t_i - t_j)$.

---

[5] This is actually a special case of something called the linked cluster theorem. The factorization of diagrams is true for the expansion for the Green's function, but it is not true for some other perturbation expansions, for example that of the thermodynamic potential.

4. For each wiggly line, associate a factor $U_{\vec q}$.
5. Integrate over all intermediate times and sum over all intermediate momenta (and spins, if necessary).
6. Multiply by a factor $i^n(-1)^F$ where F is the number of closed fermionic loops.
7. If two ends of Green function are at equal times, interpret as $\lim_{t\to 0^-} G_0(\vec k, t)$.

Example 5.2: The following is an $n = 2$ diagram, and the corresponding expression it contributes to G:



$$\begin{aligned}&i^2(-1)^1\int dt_1\int dt_2\,\frac{1}{V}\sum_{\vec q_1}\frac{1}{V}\sum_{\vec q_2}\\ &\times G_0(\vec k, t_1-t')G_0(\vec k-\vec q_1, t_2-t_1)G_0(\vec k, t-t_2)\\ &\times (U_{\vec q_1})^2 G_0(\vec q_2, t_2-t_1)G_0(\vec q_2-\vec q_1, t_1-t_2).\end{aligned} \tag{5.20}$$

We will study all of the $n = 1$ diagrams much more carefully shortly. So for now:

Exercise 5.3: (**) In a previous exercise, you drew all 21 second order diagrams, of which only 10 were connected. Of these connected ones, in fact only 4 are non-zero (the important point being that the Coulomb interaction excludes the $\vec q = 0$ interaction lines). One of the non-zero diagrams is drawn above. Identify the other 3, and write the expression they correspond to.

5.3. The diagrammatic expansion in different representations

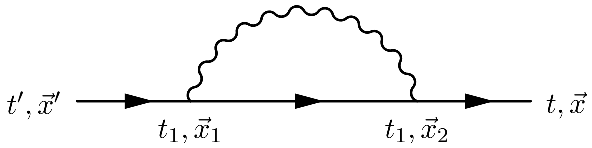
We have been working with the Green function in the momentum and time representation. We will now have a brief look at diagrams in the position-time representation (where we can get a very nice and easy physical interpretation), and a longer look at diagrams in the momentum-energy representation which will be by far the easiest to make calculations.

5.3.1. Real space

One can equally well write the interaction using real space

$$\hat H_{\text{int}} = \frac{1}{2}\int d^3\vec x_1\int d^3\vec x_2\,\hat\Psi(\vec x_1)\hat\Psi(\vec x_2)U(\vec x_1-\vec x_2)\hat\Psi(\vec x_2)\hat\Psi(\vec x_1). \tag{5.21}$$

The interaction, instead of carrying momentum $\vec{q}$ now links two positions $\vec{x}_1$ and $\vec{x}_2$, which are integrated over. A typical diagram for $G(\vec{x}-\vec{x}', t-t')$ therefore looks like



One can make the symmetry between space and time even more apparent by writing the interaction in the form

$$V(\vec{x}_1-\vec{x}_2, t_1-t_2) = V(\vec{x}_1-\vec{x}_2)\delta(t_1-t_2), \tag{5.22}$$

i.e. making it even more transparent that we are dealing with the instantaneous (static) Coulomb force.

We see that the only difference between momentum space and real space is that we integrate over intermediate positions, rather than intermediate momenta. In this representation however, the diagrams have a very nice physical interpretation: the Green function $G(\vec{x}-\vec{x}', t-t')$ is the probability amplitude for a particle to get from point $\vec{x}'$ at time t' to point $\vec{x}$ at time t.[6] The Feynman expansion then basically is saying that the electron can get between these two points in all possible ways (weighted by the appropriate amplitude). The zeroth order Feynman graph is then the direct path, the one drawn above can be interpreted as at first travels to point $\vec{x}_1, t_1$ where it interacts with another electron at point $\vec{x}_2$. This electron at $\vec{x}_2$ then travels to the finish point where it is taken out, with another electron at $\vec{x}_1$ traveling to $\vec{x}_2$ in order to leave the system in the same state it started in.

While this representation is nice for interpretation, unfortunately $G_0(\vec{x}-\vec{x}', t-t')$ in this representation is a horrible looking function, which we don't really want to be multiplying together and integrating. On the other hand, this representation will prove useful later on when we add disorder - i.e. when the system no longer has translational invariance, and therefore conservation of momentum will not apply. We postpone a discussion of such things until Lecture 9 however, and for now, return to our study of the Coulomb interacting electron gas.

5.3.2. Momentum/Frequency space

We must remember that the nicest expression we have for the non-interacting Green function is in momentum and frequency space, Eq. 3.47:

$$G_0(\vec{k}, \omega) = \frac{1}{\omega - \epsilon_0(\vec{k}) + i\delta\,\mathrm{sign}(|\vec{k}| - k_F)}. \tag{5.23}$$

---

[6] although we must remember that this is in a sea of identical electrons, so the electron that comes out isn't necessarily the same electron that went in - in fact, within the theory of identical particles this is not even a sensible question to be asking.

We can see that it will therefore be much easier to actually evaluate some of these integrals if we can make the diagrammatic expansion in this representation.

Now, when we went from real space to momentum space, what this came down to was a Fourier transform between $\vec{x}$ and $\vec{k}$. Furthermore, as a result of translational invariance, the interaction turned out to conserve momentum at every vertex.

Completely analogously, when we go from time to frequency space, we make a Fourier transform for t to ω, and as a consequence of temporal invariance, the interaction will conserve energy (frequency) at every vertex.[7]

Therefore, we will make our diagrammatic expansion analogously, except instead of associating a time to each vertex, we will associate an energy with each line (both fermionic and interaction), making sure that energy is conserved at each vertex.

By doing this, we see that interaction lines now carry an energy as well as a momentum. So what is $U(\vec{q},\omega)$?

$$\begin{aligned} U(\vec{q},\omega) &= \int d(t_2-t_1)\, e^{i\omega(t_2-t_1)} U(\vec{q},t_2-t_1) \\ &= \int d(t_2-t_1)\, e^{i\omega(t_2-t_1)} U(\vec{q})\delta(t_2-t_1) = U(\vec{q}) \end{aligned} \tag{5.24}$$

i.e. the static Coulomb interaction is independent of energy. We still need to write down the energy carried by the interaction lines on the diagrams, in order to conserve energy at each vertex, but the amplitude of the diagram is *independent* of these interaction energies.[8]

For the sake of completeness, let us now write down explicitly the Feynman rules for constructing $G(\vec{k},\omega)$ to n^{th} order in perturbation theory:

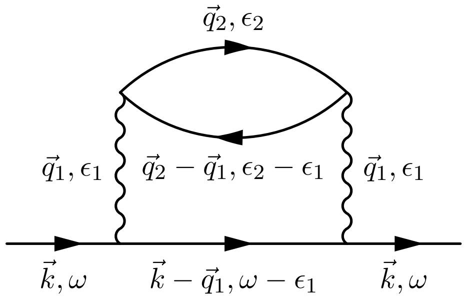
1. From all connected, topologically non-equivalent diagrams with $2n$ vertices, n wiggly lines and $2n+1$ directed solid lines (vertex=meeting of two solid and one wiggly line).
2. For each line (solid and wiggly), write down the momentum and energy, such that both are conserved at each vertex.
3. For each solid line, associate a factor $G_0(\vec{k}_i,\omega_i)$.
4. For each wiggly line, associate a factor $U_{\vec{q}}$.
5. Integrate over all intermediate energies and sum over all intermediate momenta (and spins, if necessary).
6. Multiply by a factor $i^n(-1)^F$ where F is the number of closed fermionic loops.

---

[7] This conservation of energy/momentum is technically due to a property of convolution in the theory of Fourier transforms. For a more formal derivation of the diagrammatic expansion in momentum/energy space, see any of the textbooks.

[8] Again, remember that this is for the special case of the static Coulomb interaction. We will see examples in later chapters where this is not true.

Example 5.3: Let us see how this all works by looking at the same example as before:



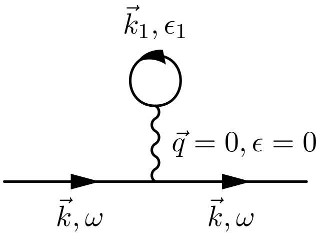
$$i^2(-1) \int \frac{d\epsilon_1}{(2\pi)^3} \int \frac{d\epsilon_2}{(2\pi)^3} \frac{1}{V} \sum_{\vec{q}_1} \frac{1}{V} \sum_{\vec{q}_2} \times G_0^2(\vec{k}, \omega) G_0(\vec{k} - \vec{q}_1, \omega - \epsilon_1) \times (U_{\vec{q}_1})^2 G_0(\vec{q}_2, \epsilon_2) G_0(\vec{q}_2 - \vec{q}_1, \epsilon_2 - \epsilon_1). \tag{5.25}$$

5.4. Infinite sums: Dyson series, and self energy

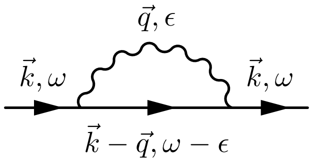
Whereas perturbation theory is fine in some cases, it turns out that in many cases one needs to sum over whole classes of diagrams to get a reasonable answer. For example, we will see in the next lecture that the spectrum of the interacting model is given by the poles of the Green function, which is something we wouldn't expect to be able to change at any finite order in perturbation theory. Fortunately, there is a way to sum up infinite classes of diagrams, as we will now see.

There are two first order diagrams, having discounted duplicates and disconnected diagrams:

a)



b)

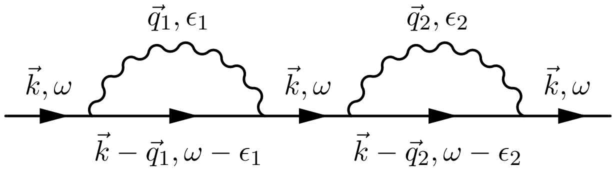


(a) is known as the Hartree term, (b) is the Fock term. In fact, as we already saw back in Lecture 2, the Hartree term gives zero for the case of the Coulomb interaction. This is also clear from the diagram: to conserve momentum, the interaction line must have $\vec{q} = 0$.

Let us therefore look more closely at the Fock term (b), which gives a contribution

$$\underbrace{i \int \frac{d\epsilon}{2\pi} \frac{1}{V} \sum_{\vec{q}} U_{\vec{q}} G_0(\vec{k} - \vec{q}, \omega - \epsilon)}_{\text{call this } \Sigma(\vec{k},\omega)} \, G_0^2(\vec{k}, \omega). \tag{5.26}$$

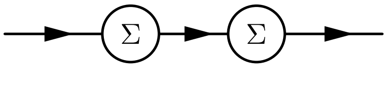
Now consider one of the $n = 2$ diagrams:



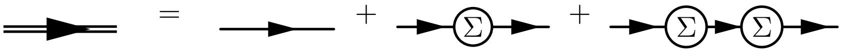
which it is not difficult to see has a contribution

$$G_0(\vec{k},\omega)\Sigma(\vec{k},\omega)G_0(\vec{k},\omega)\Sigma(\vec{k},\omega)G_0(\vec{k},\omega) \tag{5.27}$$

where $\Sigma(\vec{k},\omega)$ is defined as before. One might therefore represent this diagrammatically as



In fact, we could have a whole series of these, known as a Dyson series:



$$\begin{aligned} G(\vec{k},\omega) &= G_0(\vec{k},\omega) + G_0\Sigma G_0 + G_0\Sigma G_0\Sigma G_0 + \dots \qquad (5.28) \\ &= G_0(\vec{k},\omega)\sum_{n=0}^{\infty}\Big[G_0(\vec{k},\omega)\Sigma(\vec{k},\omega)\Big]^n \\ &= \frac{G_0(\vec{k},\omega)}{1 - G_0(\vec{k},\omega)\Sigma(\vec{k},\omega)} = \frac{1}{G_0^{-1}(\vec{k},\omega) - \Sigma(\vec{k},\omega)} \end{aligned}$$

Finally, remembering the form of G_0, we get

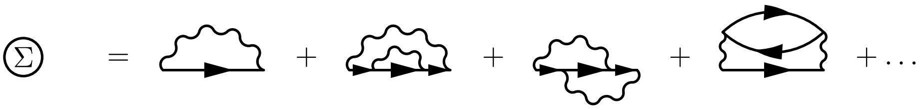
$$G(\vec{k},\omega) = \frac{1}{\omega - \xi_{\vec{k}} - \Sigma(\vec{k},\omega) + i\,\mathrm{sign}\,\xi_{\vec{k}}}. \tag{5.29}$$

The function $\Sigma(\vec{k},\omega)$ is known as the self-energy, for reasons that will become apparent as we start to calculate things.

In fact, Eq. 5.29 is completely general, so long as we define the self-energy in a general way:

Self Energy: The self-energy $\Sigma(\vec{k},\omega)$ is defined as the sum of all diagrams that *cannot be split into two by breaking a single fermion line.* Note that there must be an momentum $\vec{k}$ and energy ω coming in from the left and going out to the right of the self energy diagrams, although the Green function lines which carry this energy and momentum to the first vertex and away from the last vertex are not included.

In diagrammatic terms,



(5.30)

There are a few important consequences of the Dyson series:

- Less independent diagrams to calculate
- The interacting G now looks like the Green function of non-interacting fermions, but with a renormalized energy spectrum:

$$\xi_{\vec{k}} \to \xi_{\vec{k}} - \Sigma(\vec{k}\underbrace{,\ \ \omega)} \tag{5.31}$$

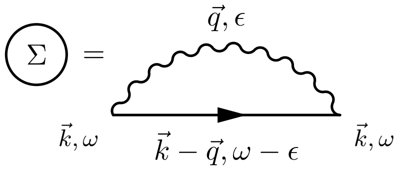
- Hence the name self energy.

If Σ depended only on $\vec{k}$, this really would be nothing but a renormalized energy spectrum. We will come back to the consequences of Σ also being a function of energy later.

5.5. Hartree-Fock theory revisited

To finish this lecture, lets actually calculate the self-energy to lowest order (where there is now only one diagram left). As this will be our first solid calculation using the diagrammatic technique, we will go through it in some detail.

The diagram in question is:



$$\Sigma(\vec{k}, \omega) = i \int \frac{d^3\vec{q}}{(2\pi)^3} U_{\vec{q}} \underbrace{\int \frac{d\epsilon}{2\pi} G_0(\vec{k} - \vec{q}, \omega - \epsilon)}\,. \tag{5.32}$$

Notice that we have already written the sum over $\vec{q}$ as an integral. Let's look at the energy integral - change variables $\epsilon \longrightarrow \omega - \epsilon$, and write $\vec{p} = \vec{k} - \vec{q}$. We are then left to calculate

$$\int \frac{d\epsilon}{2\pi} G_0(\vec{p}, \epsilon). \tag{5.33}$$

It is important to realize that this came about from the Fourier transform of an equal time Green function (in fact, any integral which appears in the diagrammatic expansion which can be reduced by a change of variables to the form above will come from an equal time Green function). We know the prescription for equal time is to allow time to approach zero from below, so this integral actually means

$$\lim_{t \to 0^-} \int \frac{d\epsilon}{2\pi}\, e^{-i\epsilon t} G_0(\vec{p}, \epsilon) = \lim_{t \to 0^-} \int \frac{d\epsilon}{2\pi}\, \frac{e^{-i\epsilon t}}{\epsilon - \xi_{\vec{k}} + i \operatorname{sign} \xi_{\vec{k}}}. \tag{5.34}$$

Now, the factor of $e^{i\epsilon 0^+}$ means that we can evaluate this integral as a contour integral, so long as we complete the contour in the upper 1/2 plane.

Now, there is a pole at $\epsilon = \xi_{\vec{k}} - i\,\mathrm{sign}\,\xi_{\vec{k}}$. Therefore, if $\xi_{\vec{k}} > 0$, there are no poles in the upper half plane, and the integral is zero. On the other hand, if $\xi_{\vec{k}} < 0$, there is one pole in the upper half plane, with a residue of $1/2\pi$, so the integral is i. In other words

$$i \int \frac{d\epsilon}{2\pi} G_0(\vec{k}-\vec{q}, \omega - \epsilon) = -n(\vec{k}-\vec{q}), \tag{5.35}$$

where

$$n(\vec{k}-\vec{q}) = \theta(-\xi_{\vec{k}-\vec{q}}) \text{ is the Fermi function.} \tag{5.36}$$

Therefore, to first order in the diagrammatic expansion,

$$\begin{aligned} \Sigma(\vec{k},\omega) &= -\int \frac{d^3\vec{q}}{(2\pi)^3}\, U_{\vec{q}} n_{\vec{k}-\vec{q}} \;=\; -\int \frac{d^3\vec{q}}{(2\pi)^3}\, U_{\vec{k}-\vec{q}} n_{\vec{q}} \\ &= -\int_{|\vec{q}|<k_F} \frac{d^3\vec{q}}{(2\pi)^3}\, \frac{4\pi e^2}{|\vec{k}-\vec{q}|^2} \\ &= -\frac{e^2 k_F}{\pi}\left(1 + \frac{1-\left(\frac{k}{k_F}\right)^2}{2\left(\frac{k}{k_F}\right)} \ln\left|\frac{k_F+k}{k_F-k}\right|\right), \end{aligned} \tag{5.37}$$

where you should recognize this integral from Lecture 2.

Notice that at this level in perturbation theory, $\Sigma(\vec{k},\omega)$ is indeed independent of ω, so the Green function does indeed look identical to the non-interacting one, with

$$\xi_{\vec{k}} \to \xi_{\vec{k}} + \Sigma(\vec{k}). \tag{5.38}$$

This is of course identical to the Hartree-Fock result we calculated in Lecture 2. However, now we understand much better the concept of renormalized spectrum, and furthermore, we are now within a framework where we can go beyond this result when we want to.

Exercise 5.4: (***) For the model of the free Fermi gas interacting via the Coulomb interaction, we have seen that the only non-zero first order diagram for the self energy is the Fock diagram. For this model, draw all of the (non-zero) 2nd and 3rd order diagrams for the self energy $\Sigma(\vec{k},\omega)$. For the 2nd order diagrams, give the expressions the diagrams correspond to (but without doing the integrals).

Unless I am mistaken, I believe there are three 2nd order diagrams and twenty 3rd order diagrams.

6. All about Green functions

In the previous lecture, we learn how to calculate the Green function for an interacting system, at least perturbatively. In this lecture, we will learn what we can do with the Green function once we have it. We will look at general properties of the Green function (now, no longer restricted to the non-interacting case), in order to understand what the Green function will tell us about the system in question.

6.1. Spectral (Lehmann) representation

Let us consider the (in general interacting) Green function for $t > t'$

$$\begin{aligned} G(\vec{k}, t-t') &= -i\langle GS\hat{c}_{\vec{k}}(t)\hat{c}^{\dagger}_{\vec{k}}(t')|GS\rangle, && t > t' \\ &= -i\sum_{\phi_n}\langle GS|\hat{c}_{\vec{k}}(t)|\phi_n\rangle\langle\phi_n|\hat{c}^{\dagger}_{\vec{k}}(t')|GS\rangle, \end{aligned} \tag{6.1}$$

where in the second line, we have inserted a resolution of the identity

$$1 = \sum_{\phi_n}|\phi_n\rangle\langle\phi_n| \tag{6.2}$$

where the sum is over all possible many body states $|\phi_n\rangle$, which have energy E_n. Note that in general, we do not necessarily know what these states or energies are, but we do know they exist.

The Green function is written in terms of Heisenberg operators, let us go over to Schrödinger operators:

$$\begin{aligned} \hat{c}_{\vec{k}}(t) &= e^{i\hat{H}t}\hat{c}_{\vec{k}}e^{-i\hat{H}t} \\ e^{-i\hat{H}t}|GS\rangle &= e^{-iE_0t}|GS\rangle \\ e^{-i\hat{H}t'}|\phi_n\rangle &= e^{-iE_nt'}|GS\rangle. \end{aligned} \tag{6.3}$$

We can therefore write our Green function 6.1 as

$$\begin{aligned} G(\vec{k}, t-t') &= -i\sum_n c_{0n}(\vec{k})c^{\dagger}_{n0}(\vec{k})e^{i(E_n-E_0)(t-t')}, && c_{0n}(\vec{k}) = \langle GS|\hat{c}_{\vec{k}}|\phi_n\rangle \\ &= -i\sum_n |c_{0n}(\vec{k})|^2 e^{i(E_n-E_0)(t-t')}, && t > t'. \end{aligned} \tag{6.4}$$

Making an analogous calculation for $t < t'$ gives the answer

$$G(\vec{k}, t-t') = \begin{cases} -i\sum_n |c_{0n}(\vec{k})|^2 e^{i(E_n-E_0)(t-t')}, & t > t' \\ i\sum_{n'} |c_{n'0}(\vec{k})|^2 e^{i(E_{n'}-E_0)(t-t')}, & t < t'. \end{cases} \tag{6.5}$$

where $c_{0n}(\vec{k}) = \langle GS|\hat{c}_{\vec{k}}|\phi_n\rangle$ and $c_{n'0}(\vec{k}) = \langle \phi_{n'}|\hat{c}_{\vec{k}}|GS\rangle$ are matrix elements.

Now, suppose the $|GS\rangle$ has N particles in it. Then c_{0n} is only non-zero when $|\phi_n\rangle$ is a state with $N+1$ particles in it, and $c_{n'0}$ is only non-zero when $|\phi_{n'}\rangle$ is a state with $N-1$ particles. In other words

$$\begin{cases} \text{for } t > t', & \sum_n \text{ is over states with } N+1 \text{ particles,} \\ \text{for } t < t', & \sum_{n'} \text{ is over states with } N-1 \text{ particles.} \end{cases} \tag{6.6}$$

Now, let us *define*

$$\begin{aligned} \epsilon_n &= E_n - E_0(N+1), \\ \mu &= E_0(N+1) - E_0(N). \end{aligned} \tag{6.7}$$

Here, $E_0(N)$ is the ground state energy for the system with N particles[1], E_n is the energy of state $|\phi_n\rangle$ which is an $N+1$ particle state. One can understand μ as being the energy required to add one more particle to the system - which is a generalized definition of the chemical potential, beyond our earlier non-interacting definition. Also notice that by definition of ground state, $\epsilon_n > 0$.

Now,

$$E_n - E_0(N) = E_n - E_0(N+1) + (E_0(N+1) - E_0(N)) = \epsilon_n + \mu. \tag{6.8}$$

Similarly, define:

$$\begin{aligned} \epsilon'_n &= E_{n'} - E_0(N-1), \\ \mu' &= E_0(N-1) - E_0(N). \end{aligned}$$

Note that in the thermodynamic limit, $\epsilon_n = \epsilon'_n$ and $\mu = \mu'$ up to corrections of order $1/N$.

This time, $E_{n'}$ is the energy of an $N-1$ particle state. Hence as before

$$E_{n'} - E_0(N) = \epsilon'_n - \mu'. \tag{6.9}$$

Substituting these definitions into Eq. 6.5 gives us (in the thermodynamic limit)

$$G(\vec{k}, t-t') = \begin{cases} -i\sum_n |c_{0n}(\vec{k})|^2 e^{-i(\mu+\epsilon_n)(t-t')}, & t > t' \\ i\sum_n |c_{n0}(\vec{k})|^2 e^{-i(\mu-\epsilon_n)(t-t')}, & t < t'. \end{cases} \tag{6.10}$$

Now, let us take the Fourier transform, to express this in the momentum/energy representation:

$$G(\vec{k}, \omega) = \int d(t-t')\, e^{i\omega(t-t')} G(\vec{k}, t-t') \tag{6.11}$$

This integral must be split up into the two parts: $t > t'$ and $t < t'$. If we cast our minds back to Lecture 3 and Eq. 3.44, we will recall that

$$\int_0^\infty e^{i\alpha t} dt = \frac{i}{\alpha + i\delta}, \qquad \int_{-\infty}^0 e^{i\alpha t} dt = \frac{-i}{\alpha - i\delta}. \tag{6.12}$$

---

[1] Remember that this is the true ground state energy for the interacting system. Here, it may seem that I'm making things much more complicated than they have to be, but the point is to completely avoid any reference to single particle states, as we are in an interacting system.

With this knowledge, we can execute the integral in Eq. 6.11 to obtain

$$G(\vec{k},\omega) = \sum_n \frac{|c_{on}|^2}{\omega - \epsilon_n - \mu + i\delta} + \sum_{n'} \frac{|c_{n'0}|^2}{\omega - \epsilon_{n'} - \mu - i\delta}. \tag{6.13}$$

Exercise 6.1: (**) Show that if we substitute the matrix elements and energies of the non-interacting free Fermi gas into Eq. 6.13, we obtain our known expression, Eq. 3.47 for $G_0(\vec{k},\omega)$.

Now define:

$$\begin{aligned} A^+(\vec{k},E) &= \sum_n |c_{0n}(\vec{k})|^2 \delta(E-\epsilon_n), \\ A^-(\vec{k},E) &= \sum_{n'} |c_{n'}(\vec{k})|^2 \delta(E-\epsilon_{n'}). \end{aligned} \tag{6.14}$$

These functions, roughly known as spectral functions, are something like a partial density of states. Examining the expression for A^+, we see that the matrix elements

$$c_{0n}(\vec{k}) = \langle GS|\hat{c}_{\vec{k}}|\phi_n\rangle \tag{6.15}$$

are zero unless state n is carrying momentum $\vec{k}$, as we know that after removing a particle with momentum $\vec{k}$ we must obtain the ground state, which is carrying no overall momentum. We therefore very roughly are looking at how many states which have momentum $\vec{k}$ also have energy E. One can make a similar analysis to explain the physical significance of A^- - except using holes instead of electrons.

Remembering from the definition that ϵ_n are positive, one can easily see that $A^+(\vec{k},E)$ and $A^-(\vec{k},E)$ are only non-zero for $E > 0$. One can therefore put the two of them together to define *the spectral function*

$$\begin{aligned} A(\vec{k},\omega) &= \begin{cases} A^+(\vec{k},\omega), & \omega > 0, \\ A^-(\vec{k},-\omega), & \omega < 0, \end{cases} = A^+(\vec{k},\omega) + A^-(\vec{k},-\omega) \\ &= \sum_n |\langle\phi_n|c^\dagger_{\vec{k}}|\mathrm{GS}\rangle|^2 \delta(\omega-\epsilon_n) + \sum_n |\langle\phi_n|c_{\vec{k}}|\mathrm{GS}\rangle|^2 \delta(\omega+\epsilon_n), \end{aligned} \tag{6.16}$$

It is also important to note that the function A is very roughly what is measured in angle resolved photo-emmision spectroscopy (ARPES) measurements. For more information on this, however, I refer you to the MPGAS course on probes.

Mathematically, $A^+, A^- \geq 0$, i.e. these two functions are both non-negative definite (they are the sums of the modulus squared of something). Also, we can now write the Green function in it's final form

$$G(\vec{k},\omega) = \int_0^\infty \left[\frac{A^+(\vec{k},E)}{\omega - E - \mu + i\delta} + \frac{A^-(\vec{k},E)}{\omega + E - \mu - i\delta} \right] dE. \tag{6.17}$$

This is know as the *spectral representation*, or the *Lehmann representation*, after the guy who first studied such things.[2]

---

[2] In a joint paper between Dr. Spectral and Prof. Lehmann...

It is now easy to see that

$$\operatorname{Im} G(\vec{k},\omega) = \begin{cases} -\pi A^{+}(\vec{k},\omega-\mu) & \omega > \mu, \\ \pi A^{-}(\vec{k},\mu-\omega) & \omega < \mu. \end{cases} \tag{6.18}$$

This has two important consequences, both of which we will discuss further shortly:

- The imaginary part of the Green function changes sign at $\omega = \mu$. This means that the causal Green function has very strange analytic properties on the complex plane.
- The spectral functions (which we have seen have the meaning of partial densites of states) can be obtained from the imaginary part of the Green function. Hence, by calculating the Green function by means of the diagrammatic expansion we have been learning, one can actually obtain real experimental predictions for the system.

Exercise 6.2: (***) We have discussed the physical meaning of the spectral function $A(\vec{k},\omega)$ as defined by Eq. 6.16. By manipulating this expression (and performing the integrals), discuss the physical meaning of:

1. $$f(\vec{k}) = \int \frac{d\omega}{2\pi} A(\vec{k},\omega). \tag{6.19}$$

2. $$g(\omega) = \int \frac{d^3\vec{k}}{(2\pi)^3} A(\vec{k},\omega). \tag{6.20}$$

3. $$h(\vec{k}) = \int \frac{d\omega}{2\pi} n_F(\omega) A(\vec{k},\omega), \tag{6.21}$$

   where

   $$n_F(\omega) = \begin{cases} 1 & \omega < \mu \\ 0 & \omega > \mu \end{cases} \tag{6.22}$$

   is the Fermi function.

6.2. Beyond Casual: Advanced and Retarded

Let us consider a function, $G_R(\vec{k},\omega)$ defined in a very similar way to Eq. 6.17:

$$G_R(\vec{k},\omega) = \int_0^\infty \left[\frac{A^{+}(\vec{k},E)}{\omega - E - \mu + i\delta} + \frac{A^{-}(\vec{k},E)}{\omega + E - \mu + i\delta} \right] dE. \tag{6.23}$$

The only change between this and Eq. 6.17 is the change of sign of the $i\delta$ in the second term. However, this change of sign means that all of the poles of the function $G_R(\vec{k}, \omega$ are in the lower half plane (in ω - we always assume $\vec{k}$ remains fixed when we talk about the analytic properties of a Green function). This means that G_R is *analytic in the upper half plane*. Perhaps the most important property of G_R however, is it's relation to the physically important spectral function. Comparing Eq. 6.16 and Eq. 6.23, it is easy to see that

$$A(\vec{k}, \omega) = -\frac{1}{\pi} \mathrm{Im}\, G_R(\vec{k}, \omega - \mu), \tag{6.24}$$

or if we measure all energies relative to the Fermi energy as we so often do,

$$A(\vec{k}, \omega) = -\frac{1}{\pi} \mathrm{Im}\, G_R(\vec{k}, \omega). \tag{6.25}$$

G_R is know as the *retarded Green function.* While the retarded Green function is in a sense much nicer than the causal one, we cannot do perturbation theory directly with the retarded Green function: the time ordering operator in the expansion of the S-matrix means we require the causal Green function. The usual approach therefore is to calculate the causal Green function using a diagrammatic expansion, then from this try to evaluate the retarded Green function.[3] Again, comparing Eq. 6.17 with Eq. 6.23, we can see that

$$G_R(\vec{k}, \omega) = \begin{cases} G(\vec{k}, \omega) & \omega > \mu, \\ G^*(\vec{k}, \omega) & \omega < \mu. \end{cases} \tag{6.26}$$

A comparison of Eq. 6.17 with Eq. 6.23 will also give the relation

$$G_R(\vec{k}, \omega) = G(\vec{k}, \omega - i\delta), \tag{6.27}$$

which in many cases will be the most useful, although it is not always possible to make the appropriate analytic continuation.

Let us now consider now for a moment where the $-i\delta$ came from in Eq. 6.17. If we cast our minds back to Eq. 6.11, we can see that the $-i\delta$ arose from the Fourier transform of the causal Green function at $t < 0$. If we had $t > 0$ on this part, we would have got $+i\delta$, as we have in G_R. Hence,[4] we can see that we will obtain the expression Eq. 6.23 after Fourier transform if we take our original definition of the retarded Green function to be

$$G_R(x - x', t - t') = \begin{cases} -i\langle \hat{\Psi}(\vec{x}, t)\hat{\Psi}^\dagger(\vec{x}', t') + \hat{\Psi}^\dagger(\vec{x}', t') hat\Psi(\vec{x}, t)\rangle & t > t', \\ 0 & t < t'. \end{cases} \tag{6.28}$$

This is more conventionally written as a *different time anti-commutator*

$$G_R(x - x', t - t') = \begin{cases} -i\langle \Big\{ \hat{\Psi}(\vec{x}, t), \hat{\Psi}^\dagger(\vec{x}', t') \Big\}\rangle & t > t', \\ 0 & t < t'. \end{cases} \tag{6.29}$$

---

[3] In fact, it is possible to make a diagrammatic expansion using the retarded Green function within the Keldysh technique, but again this is at the cost of extra complexity arising from having two branches for time to sit on.

[4] As usual, see the standard textbooks for more formal derivations

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Exercise 6.3: (*) Starting from Eq. 6.29, express G_R using the spectral representation, and show you do indeed obtain Eq. 6.23.

For completeness, one can also define the *advanced Green function*:

$$G_A(x-x',t-t') = \begin{cases} 0 & t > t' \\ i\langle\Big\{\hat{\Psi}(\vec{x},t),\hat{\Psi}^\dagger(\vec{x}',t')\Big\}\rangle & t < t'. \end{cases} \tag{6.30}$$

It has the property that $G_A(\vec{k},\omega) = G_R^*(\vec{k},\omega)$, and is therefore analytic in the lower half plane. We will rarely however be using G_A within this lecture course.

6.3. The meaning of the poles

As we've seen with the free Green function, G_0, if we express it in momentum-energy representation:

$$G_0(\vec{k},\omega) = \frac{1}{\omega - \xi_{\vec{k}} + i\delta\,\mathrm{sign}\,\xi_{\vec{k}}}, \tag{6.31}$$

there are poles at the points

$$\omega = \xi_{\vec{k}}, \tag{6.32}$$

i.e. on the spectrum of single-particle excitations. Similarly, if we consider the Hartree-Fock Green function, there are poles on the spectrum of renormalized single particle excitations.

We may wonder whether this interpretation of the poles may be extended to the general interacting case. Consider taking $G_0(\vec{k},\omega)$ and Fourier transforming back to $(\vec{k},t)$ representation:

$$G(\vec{k},t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,e^{-i\omega t}G(\vec{k},\omega). \tag{6.33}$$

We would like to study this integral using the techniques of complex analysis. However, as we have seen above, $G(\vec{k},\omega)$ has somewhat dubious analytic properties. Let us therefore divide the integral into two parts (where we are using the notation that all energies are measured relative to the chemical potential, μ)

$$\begin{array}{lll} -\infty < \omega < 0 & \text{where} & G = G_A, \\ 0 < \infty < \infty & \text{where} & G = G_R. \end{array} \tag{6.34}$$

Now, G_A is analytic in the lower half plane, so we can deform the contour down, as shown in Fig. 6.1(a). We can deform it as low as we want, which will make $e^{-\omega t}$ as small as we want, so the only part of the first integral which remains is the vertical line

$$\int_{-i\infty}^{0}\frac{d\omega}{2\pi}\,e^{-i\omega t}G_A(\vec{k},\omega). \tag{6.35}$$

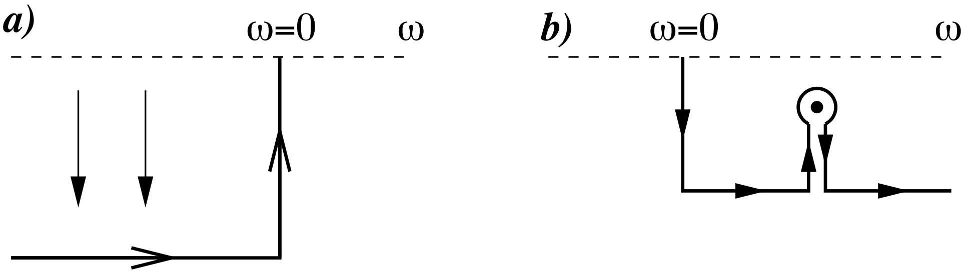


Figure 6.1.: The deformation of the contours for (a) $\omega < 0$ and (b) $\omega > 0$.

On the other hand, G_R does have poles in the lower half plane. Suppose there is a pole at the position $\omega = \epsilon(\vec{k} - i\gamma$. Then we may deform the contour down being careful to bypass the pole, as shown in Fig. 6.1(b). We can't however move the contour all the way down to $-i\infty$ as there may be more poles.

However, by choosing t *sufficiently* long (where exactly how long *sufficiently* means depends on the full structure of the poles), we can make the horizontal contribution to the integral as small as we want. One can also show (see textbooks for details) that if $t \gg \epsilon(\vec{k})^{-1}$, then the vertical contributions are small.

Therefore, in the long time limit, this leaves the only contribution to $G(\vec{k}, t)$ coming from around the pole, i.e.

$$G(\vec{k}, t) \sim a e^{-i\epsilon(\vec{k})t} e^{-\gamma t}, \tag{6.36}$$

where a is the residue at the pole. Now remembering that $G(\vec{k}, t)$ is a probability amplitude until time t of the propagation of a state with momentum $\vec{k}$ introduced at time 0. Therefore, this form of G looks exactly like a quasi-particle of energy $\epsilon(\vec{k})$, decaying with a lifetime $1/\gamma$.

So we see that the poles of the Green function (in $\vec{k}, \omega$ space) give the single-particle quasi-particle spectrum of the interacting model - with the real part being the energy of the quasi-particle excitation, and the imaginary part being it's inverse lifetime.

Exercise 6.4: (***) In general, the self energy will have both a real and an imaginary part:

$$\Sigma(\vec{k}, \omega - i\delta) = \Sigma'(\vec{k}, \omega) + i\Gamma(\vec{k}, \omega), \tag{6.37}$$

so the spectral function

$$A(\vec{k}, \omega) = -\frac{1}{\pi} \mathrm{Im}\, G(\vec{k}, \omega - i\delta) = \frac{\Gamma(\vec{k}, \omega)}{|\omega - \epsilon_{\vec{k}} - \Sigma'(\vec{k}, \omega)|^2 + \Gamma(\vec{k}, \omega)^2}. \tag{6.38}$$

If the self energy is small (how small?), this is a Lorenzian of width Γ, centered around a renormalized energy

$$\epsilon^*_{\vec{k}} = \epsilon(\vec{k}) + \Sigma'(\vec{k}, \epsilon^*_{\vec{k}}). \tag{6.39}$$

By expanding the Lorenzian about this point, show that near the renormalized energy, the Green function can be written

$$G(\vec{k}, \omega - i\delta) = \frac{Z_{\vec{k}}}{\omega - \epsilon^*_{\vec{k}} - i\Gamma^*_{\vec{k}}}, \tag{6.40}$$

where

$$Z^{-1}_{\vec{k}} = \left(1 - \frac{\partial}{\partial\omega}\Sigma'(\vec{k}, \omega)\Big|_{\omega=\epsilon^*_{\vec{k}}}\right) \tag{6.41}$$

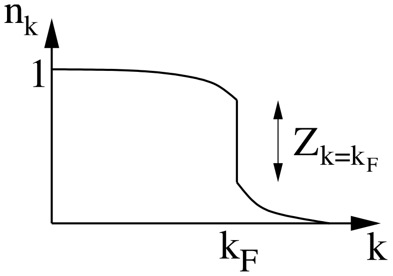
and

$$\Gamma_{\vec{k}} = Z_{\vec{k}}\Gamma(\vec{k}, \epsilon^*_{\vec{k}}). \tag{6.42}$$

$\Gamma^*_{\vec{k}}$ can be interpreted as the inverse lifetime of a particle of momentum $\vec{k}$. The meaning of $Z_{\vec{k}}$ becomes clear when we look at the momentum distribution

$$n_{\vec{k}} = \langle GS|\hat{c}^\dagger_{\vec{k}}\hat{c}_{\vec{k}}|GS\rangle. \tag{6.43}$$

Show that for the form of G given above in Eq. 6.40, the momentum distribution curve $n_{\vec{k}}$ looks like:



i.e. $n_{\vec{k}}$ is smoothed out by interactions, but there is still a sudden drop of magnitude $Z_{|\vec{k}|=k_F} < 1$ at the Fermi surface. In other words, the Fermi surface is still sharp. (Hint: can you relate $n_{\vec{k}}$ to the expression in Eq. 6.21 which you met in a previous exercise?)

What would $Z_{|\vec{k}|=k_F} = 0$ imply?

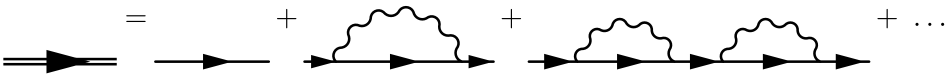
For the free electron gas, and the treatment of interactions within Hartree-Fock, the poles of the Green function are all on the real axis, hence the lifetime of all single particle excitations is infinite. Now we know (for example, from experiment) that this is not that case. In the next lecture, we will start looking at the diagrams which give processes to allow the quasi-particles to decay.

7. The Random Phase approximation: screened interactions and plasmons

Let us have a brief recap of where we have reached so far:

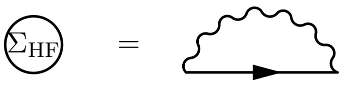
- We've seen how to look at time dependence within many-body physics (second quantization).
- We've studied the single particle Green function - and how to obtain physically observable properties of the system from it.
- We've looked at the perturbation expansion of the Green function via Wick's theorem, the Gell-mann-Low theorem, and Feynman diagrams.
- We've learned how to resum certain classes of these diagrams via Dyson series. In particular, we've looked at the self-energy, and calculated this to first order for the interacting electron gas (Hartree Fock).

The Hartree-Fock theory is given by the diagrams



(7.1)

In other words,

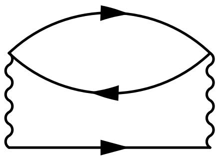


(7.2)

There is a problem though, as Hartree-Fock theory gives

- Zero effective mass, $m^* = 0$, and
- Infinite lifetime, $\tau \to 0$.

Neither of these are supported by experiment. Therefore, to make a more meaningful calculation, we must go beyond Hartree-Fock. In other words, we must start looking at second order diagrams for self-energy, for example



(7.3)

The new feature that this diagram contains is the fermionic *bubble*, also known as a polarization loop for reasons that will become apparent presently. In fact, it turns out that these bubbles are so important in quantum field theory (at least in the condensed matter variant thereof) that before we return to this diagram, we will spend some time examining just the bubble. We will spend some time examining where it comes from and it's significance before evaluating it for the Coulomb interacting free electron gas. We will then see how to make a Dyson series out of these bubbles, which is known as the Random Phase Approximation (RPA), and finally we will see how this leads to the concepts of screened interaction, and plasmon excitations.

7.1. The two particle Green function

We have so far only considered the single particle Green function $G(\vec{k},\omega)$. Let us now consider the (causal) density-density Green function, defined by

$$X(\vec{q},t) = i\langle GS|T\,\hat{\rho}_{\vec{q}}(t)\hat{\rho}^\dagger_{\vec{q}}(0)|GS\rangle, \tag{7.4}$$

where (as usual) the Fourier transform of the density operator is given by

$$\hat{\rho}_{\vec{q}}(t) = \sum_{\vec{k}\sigma} \hat{c}^\dagger_{\vec{k},\sigma}(t) c_{\vec{k}+\vec{q},\sigma}(t). \tag{7.5}$$

Notice that for a the single-particle Green function, you add an extra particle and let it propagate. Here, we make a density fluctuation, or in other words, a particle-hole pair, and let it propagate. So $X_0(\vec{q},t)$ will contain information about the actual excitation spectrum of our Fermi-gas which has a fixed number of particles. Substituting Eq. 7.5 into Eq. 7.4, we get

$$X(\vec{q},t) = i\sum_{\vec{k},\vec{k}'}\sum_{\sigma,\sigma'}\langle GS|T\,\hat{c}^\dagger_{\vec{k},\sigma}(t)\hat{c}_{\vec{k}+\vec{q},\sigma}(t)\hat{c}^\dagger_{\vec{k}'+\vec{q},\sigma'}\hat{c}_{\vec{k}',\sigma'}|GS\rangle. \tag{7.6}$$

Let us evaluate this for the non-interacting electron gas, to obtain the *bare bubble*, $X_0(\vec{q},t)$. We will do this (as always) using Wick's theorem. There are two possible contractions:

$$1.\ \wick{\c1{\hat{c}}^\dagger_{\vec{k},\sigma}(t)\c1{\hat{c}}_{\vec{k}+\vec{q},\sigma}(t)\c2{\hat{c}}^\dagger_{\vec{k}'+\vec{q},\sigma'}\c2{\hat{c}}_{\vec{k}',\sigma'}}, \qquad 2.\ \wick{\c1{\hat{c}}^\dagger_{\vec{k},\sigma}(t)\c2{\hat{c}}_{\vec{k}+\vec{q},\sigma}(t)\c2{\hat{c}}^\dagger_{\vec{k}'+\vec{q},\sigma'}\c1{\hat{c}}_{\vec{k}',\sigma'}} \tag{7.7}$$

For now, let us ignore the special case of $\vec{q} = 0$.

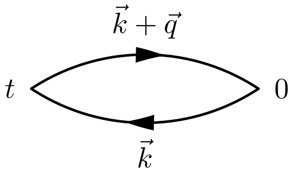
Exercise 7.1: (*) Why will we, in fact, never care about $X_0(\vec{q} = 0, \omega)$?

The first contraction requires $\vec{q} = 0$ in order to be non-zero, so given that we will not be worrying about this case, there is only one possible contraction, and we can write

$$X_0(\vec{q}, \omega) = 2i \sum_{\vec{k}} G_0(\vec{k} + \vec{q}, t) G_0(\vec{k}, -t), \tag{7.8}$$

where the factor of 2 comes from the sum over spin, and the definition $G_0 = -i \langle T \, \hat{c} \, \hat{c}^\dagger \rangle$ and three Fermionic swaps give the factor $+i$. In diagrammatic notation, we therefore see that

$-iX_0(\vec{q}, t) =$ (7.9)



Within the diagram, $\vec{q}$ is an external momentum, whereas the internal momentum $\vec{k}$ is summed over. Within this diagram, there is also an internal spin - which is also implicitly summed over.

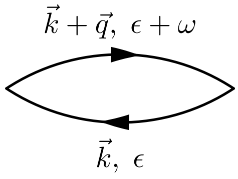
Now, one can think of a hole as an electron propagating backwards in time, which is why this is known as a particle-hole, or polarization loop.

It is now easy to take the Fourier transform of this to go into our favourite momentum-energy representation:

$$X_0(\vec{q}, \omega) = \int_{-\infty}^{\infty} dt \, e^{-i\omega t} X_0(\vec{q}, t) = 2i \sum_{\vec{k}} \int \frac{d\epsilon}{2\pi} G_0(\vec{k} + \vec{q}, \epsilon + \omega) G_0(\vec{k}, \epsilon), \tag{7.10}$$

or diagrammatically as

$-iX_0(\vec{q}, \omega) =$ (7.11)



Now, we recall that

$$G_0(\vec{k}, \epsilon) = \frac{1}{\epsilon - \xi_{\vec{k}} + i\delta \, \mathrm{sign} \, \xi_{\vec{k}}}, \tag{7.12}$$

so

$$\begin{aligned} X_0(\vec{q}, \omega) &= -2 \sum_{\vec{k}} \int \frac{d\epsilon}{2\pi i} \, G_0(\vec{k} + \vec{q}, \epsilon + \omega) G_0(\vec{k}, \epsilon) \\ &= -2 \sum_{\vec{k}} \int \frac{d\epsilon}{2\pi i} \, \frac{1}{\epsilon + \omega - \xi_{\vec{k}+\vec{q}} + i\delta \, \mathrm{sign} \, \xi_{\vec{k}+\vec{q}}} \, \frac{1}{\epsilon - \xi_{\vec{k}} + i\delta \, \mathrm{sign} \, \xi_{\vec{k}}} \end{aligned} \tag{7.13}$$

We are now left with the trifling matter of actually evaluating the integral. To do this, we will use the residue theorem, and employ a common trick in quantum field theory. Suppose $\xi_{\vec{k}+\vec{q}}$ and $\xi_{\vec{k}}$ are both > 0. Then in the complex ϵ plane, the only poles are in the lower half plane. In this case, complete the integral in the upper half plane[1], where there are no poles and the asymptotic value of the integral is of order $1/\epsilon^2$, so the answer is zero.

Similarly, if both $\xi_{\vec{k}+\vec{q}} > 0$ and $\xi_{\vec{k}} > 0$, then complete in the upper half plane, and get the same result.

The only way to get a non zero answer is if $\xi_{\vec{k}+\vec{q}}$ and $\xi_{\vec{k}}$ have opposite signs. In these case, we evaluate the residue, and obtain

$$X_0(\vec{q},\omega) = -2\sum_{\vec{k}}\left[\frac{\theta(\xi_{\vec{k}+\vec{q}})\theta(-\xi_{\vec{k}})}{\omega - \xi_{\vec{k}+\vec{q}} + \xi_{\vec{k}} + i\delta} - \frac{\theta(-\xi_{\vec{k}+\vec{q}})\theta(\xi_{\vec{k}})}{\omega - \xi_{\vec{k}+\vec{q}} + \xi_{\vec{k}} - i\delta}\right]. \tag{7.14}$$

Notice that the theta functions can be written in a more physically transparent way as the particle and hole distribution functions

$$n_{\text{part}} = n^0(\vec{k}) = \theta(-\xi_{\vec{k}}), \qquad n_{\text{hole}} = 1 - n^0(\vec{k}) = \theta(\xi_{\vec{k}}). \tag{7.15}$$

We see then that the first term in Eq. 7.14 looks like the propagator of a particle-hole pair, with $|\vec{k}+\vec{q}| > k_F$ and $|\vec{k}| < k_F$, which means that the excitation energy $\omega_{\vec{q}} = \xi_{\vec{k}+\vec{q}} - \xi_{\vec{k}}$ is positive. The second term has the momenta of the particle and hole reversed – it looks like the first term after a time reversal operation. In other words, we can see that a causal Green function (in this case, the two-particle causal Green function, but also the single particle Green function as discussed in Lecture 6) is a superposition of advanced and retarded Green functions.

7.2. The dynamical form factor

Let us consider the imaginary part of X_0, which is known as the dynamical form factor

$$S_0(\vec{q},\omega) = \frac{1}{\pi}\,\mathrm{Im}\,X_0(\vec{q},\omega). \tag{7.16}$$

Now, reminding ourselves that $\mathrm{Im}\left[\frac{1}{x-i\delta}\right] = \pi\delta(x)$, we see from Eq. 7.14 that for $\omega > 0$

$$S_0(\vec{q},\omega) = 2\int\frac{d^3\vec{k}}{(2\pi)^3}\,\underbrace{n^0(\vec{k})\left[1 - n^0(\vec{k}+\vec{q})\right]}_{\text{hole }\vec{k},\text{ particle }\vec{k}+\vec{q}}\,\underbrace{\delta(\omega - \xi_{\vec{k}+\vec{q}} + \xi_{\vec{k}})}_{\text{conservation of energy}} \tag{7.17}$$

where we have anticipated actually evaluating this so converted the sum into an integral. Notice that as with the spectral function, the delta function enforces conservation of energy - hence the dynamical form factor contains information about real processes.

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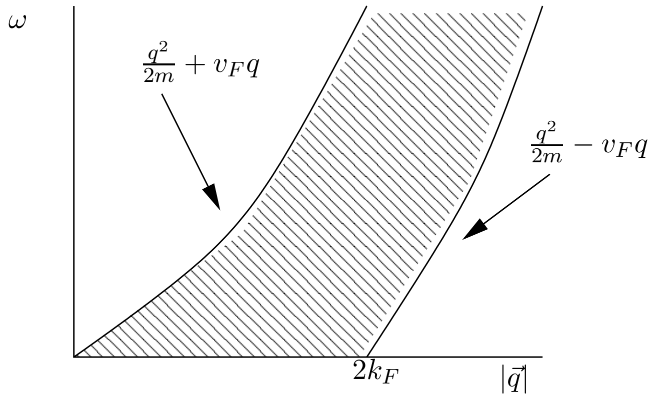
[1] Note that for this diagram, there is no issue of equal time Green functions - so there is no factor of $e^{i\epsilon 0-}$ forcing to complete in the upper half plane, as there was for the Fock diagram.

Exercise 7.2: (*) What is $S_0(\vec{q},\omega)$ for $\omega < 0$?

If we look at our expression for S_0, Eq. 7.17 more closely, we can interpret it physically. The first $n_0(\vec{k})$ ensures the state with momentum $\vec{k}$ is already occupied, i.e. an excitation with this momentum will be a hole. Similarly, the excitation with $\vec{k}+\vec{q}$ must be a particle. So we are forming all possible particle-hole pairs which carry momentum $\vec{q}$, and satisfy energy conservation. In other words, we are looking at the spectrum of the *real excitations of the Fermi gas* (i.e. a particle being promoted to a higher energy, which creates a particle-hole pair).

In fact, a spectral analysis similar to that carried out for G in Lecture 6 will show that, with the addition of matrix elements, the above analysis is completely generic, even for interacting systems.

Exercise 7.3: (***) By inserting the free gas spectrum $\xi_{\vec{k}} = k^2/2m - \mu$ into Eq. 7.17 and executing the integral, show that $S_0(\vec{q},\omega > 0)$ is only non zero in the region shown in the diagram:



and is given by

$$S_0(\vec{q},\omega>0) = \begin{cases} \frac{N_F}{2}\frac{\omega}{qv_F} & 0 \le \omega \le qv_F - \frac{q^2}{2m}, \\ \frac{N_F}{2}\frac{k_F}{2q}\left[1 - \frac{1}{qv_F}\left(\omega - \frac{q^2}{2m}\right)^2\right] & |qv_F - \frac{q^2}{2m}| \le \omega \le qv_F + \frac{q^2}{2m}, \\ 0 & \text{otherwise}, \end{cases} \tag{7.18}$$

where $q = |\vec{q}|$, $v_F = k_F/m$ is the Fermi velocity, and $N_F = mk_F/\pi^2$ is the density of states at the Fermi level.

Let us now ask ourselves the question: suppose we make a (particle-hole) excitation with momentum $\vec{q}$ in our non-interacting Fermi gas. What is the energy of this excitation?

Well, if we look at the diagram above, we see that in general, even having fixed $\vec{q}$, $S_0(\vec{q}, \omega)$ is still nonzero for a wide range of energies. In other words, our excitation could have a wide range of energies - it is known as an *incoherent* excitation. For the free Fermi gas in three dimensions, we can see from the above figure that all particle-hole excitations are incoherent. This should be strongly contrasted with the form of the spectral function for the free Fermi gas

$$A_0(\vec{q}, \omega) = \delta(\omega - \xi_{\vec{q}}), \tag{7.19}$$

which shows that single particle excitations are *coherent*.

Exercise 7.4: (***) So far, we have been discussing the three dimensional result. What is $S_0(\vec{q}, \omega)$ in one dimension? Explain the difference between the 3D and 1D results.[2]

7.3. The Lindhard function

Now, let us consider the real part of X_0, which is known as the *Lindhard formula*. By simply taking the real part of Eq. 7.14 and some elementary algebra, we see that

$$\mathrm{Re}\, X_0(\vec{q}, \omega) = 2 \int \frac{d^3\vec{k}}{(2\pi)^3} \frac{n^0(\vec{k}) - n^0(\vec{k} + \vec{q})}{\omega - \xi_{\vec{k}+\vec{q}} + \xi_{\vec{k}}}. \tag{7.20}$$

While the imaginary part, the dynamical form factor contains information about the real excitations of the system, the Lindhard function has also information about the probability (and phases) of all possible virtual processes. I'm not sure terribly much physical information can be extracted from the Lindhard function as compared to the dynamical form factor, however the Lindhard function is essential when we will go beyond the non-interacting system - as according to the principles of quantum mechanics, all possible paths must be added, not just the *on-shell* (i.e. energy conserving) ones.

---

[2] If you have answered this question correctly, you will see that in one dimension, there is a region for small $\vec{q}$ and small ω where the particle-hole excitations are *almost* coherent. It is this curious property of the one-dimensional Fermi gas that gives rise to techniques such as Bosonization which treat some forms of interaction exactly. Unfortunately however, this is way beyond the scope of this course.

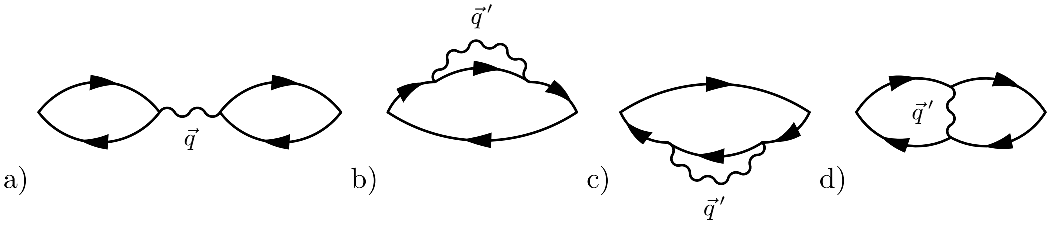


Figure 7.1.: The four first order diagrams for $X(\vec{k},\omega)$.

Exercise 7.5: (***) Evaluate the integral in Eq. 7.20 to show that

$$\mathrm{Re}\, X_0(\vec{q},\omega) = N_F F(\,|\vec{q}|/2k_F,\ \omega/4\epsilon_F) \tag{7.21}$$

where

$$\begin{aligned} F(\bar{q},\bar{\omega}) &= \frac{1}{8\bar{q}}\left\{\left[1-\left(\bar{q}+\frac{\bar{\omega}}{\bar{q}}\right)^2\right]\ln\left|\frac{\bar{q}+\bar{\omega}/\bar{q}+1}{\bar{q}+\bar{\omega}/\bar{q}-1}\right|\right. \\ &\quad \left.+\left[1-\left(\bar{q}-\frac{\bar{\omega}}{\bar{q}}\right)^2\right]\ln\left|\frac{\bar{q}-\bar{\omega}/\bar{q}+1}{\bar{q}-\bar{\omega}/\bar{q}-1}\right|\right\}+\frac{1}{2}, \end{aligned} \tag{7.22}$$

and N_F is the density of states as the Fermi energy ϵ_F, as before.

Notice that the expression obtained in the exercise has no poles in the complex plane, only branch cuts. This is another way of seeing that there is no coherent particle hole excitations in the three dimensional non-interacting free Fermi gas.

7.4. The Random Phase Approximation

Having spent some time considering the significance of $X(\vec{q},\omega)$ and calculating it for a non-interacting Fermi gas, we can now ask what about interactions? By the same arguments as in Lecture 5, we can see that

$$X(\vec{q},\omega) = i\frac{{}_0\langle GS|T\,\hat{\rho}_{\vec{q}}(t)\hat{\rho}^\dagger_{\vec{q}}(0)S(\infty,-\infty)|GS\rangle_0}{{}_0\langle GS|S(-\infty,\infty)|GS\rangle_0}, \tag{7.23}$$

with everything in the interaction representation, and all expectation values with respect to the non-interacting ground state. We can therefore use exactly the same diagrammatic rules we learnt to express any order in the perturbation expansion in terms of integrals of products of Green functions.

We have examined in great length X_0, the zeroth order approximation X. The first order terms for $X(\vec{q},\omega)$ are shown in Fig. 7.1. It might be tempting, given that we know

$$X_0(\vec{q},\omega) = -2\sum_{\vec{k}}\int\frac{d\epsilon}{2\pi i}\,G_0(\vec{k}+\vec{q},\epsilon+\omega)G_0(\vec{k},\epsilon), \tag{7.24}$$

to think that if we replace the G_0's with G's in this formula, we would obtain X. However, this is **not true**. Looking at Fig. 7.1, we see that diagrams (b) and (c) would indeed by reproduced by replacing G_0 with G, however diagrams (a) and (d)[3] would not.

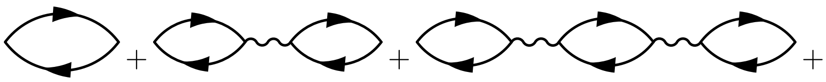
This shouldn't be surprising. The interacting many-body wavefunction which can not be written as a slater determinant is a function of a macroscopic number of variables. It would be inconceivable to be able to describe it fully by knowledge of the Green function.[4] In other words, even if we knew exactly what $G(\vec{k},\omega)$ is for an interacting system, this alone wouldn't enable us to be able to determine $X(\vec{q},\omega)$ exactly.

Now, let us go back to the diagrams in Figure 7.1, and let us suppose we are interested in long wavelength, low energy properties of the material (i.e. small $|\vec{q}|$ and ω). If we remember that the Coulomb interaction $U_{\vec{q}} \sim 1/q^2$, then we see that diagram (a), which involves an interaction line *at the external momentum*, $\vec{q}$, gives a much larger contribution that the other three diagrams in which the interaction line momentum, $\vec{q}'$ is integrated over.

In fact, we can make a Dyson series of such diagrams, which is known as the Random Phase Approximation (RPA):

$$X_{\mathrm{RPA}}(\vec{q},\omega) \tag{7.25}$$

=



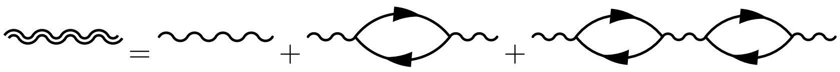
$+ \ldots$

$$\begin{aligned} &= X_0(\vec{q},\omega) + X_0(\vec{q},\omega)\left[-U_{\vec{q}}X_0(\vec{q},\omega)\right] + X_0(\vec{q},\omega)\left[-U_{\vec{q}}X_0(\vec{q},\omega)\right]^2 + \ldots \\ &= \frac{X_0(\vec{q},\omega)}{1+U_{\vec{q}}X_0(\vec{q},\omega)} \end{aligned}$$

We will come back to look at some of the physical consequences of this form of $X(\vec{q},\omega)$. We shall first have a short interlude to a closely related topic - that of screening.

7.5. Screened Interaction

Let us consider a different interpretation of the RPA sum of bubbles - as an effective interaction, which we will represent diagrammatically by a double wiggle line:



$+ \ldots \quad (7.26)$

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[3] These two diagrams roughly fall into a category known amongst those in the know as *vertex corrections.* At least, strictly speaking, (d) is a vertex correction, (a) is just plain old RPA - as we will see shortly.

[4] This is not completely true for a small class of models known as *integrable* - but I digress.

Physically, we could say that two particles could interact via the direct interaction, or the interaction from one particle induces a density fluctuation in the electron sea, which in turns interacts with the second particle, or they could interact via two intermediate density fluctuations, and so on.

Mathematically, we see that

$$\begin{aligned} U_{\mathrm{RPA}}(\vec{q},\omega) &= \overbrace{U_{\vec{q}}}^{\text{independent of }\omega} + U_{\vec{q}}\left[-X_0(\vec{q},\omega)U_{\vec{q}}\right] + U_{\vec{q}}\left[-X_0(\vec{q},\omega)U_{\vec{q}}\right]^2 + \dots \\ &= \frac{U_{\vec{q}}}{1+U_{\vec{q}}X_0(\vec{q},\omega)}. \end{aligned} \tag{7.27}$$

Notice that the effective interaction is now ω-dependent - which Fourier transformed back to time space means that it isn't instantaneous any more. Which is what we would expect - although the direct interaction is instantaneous, interacting via density fluctuations certainly isn't.

For simplicity, however, let us first consider static screening, i.e. we will look at the effective interaction in the limit $\omega = 0$. We have already evaluated $X_0(\vec{q},\omega)$ in general in the exercise - with the answer given by Eq. 7.21 and Eq. 7.18. From these general expressions or otherwise, we can therefore see that

$$X_0(\vec{q}\to 0, \omega = 0) = N_F \frac{mk_F}{\pi^2} = \frac{3}{2}\frac{n}{\epsilon_F}, \tag{7.28}$$

where $n = N/V$ is the average particle density, and notice that in this limit, the imaginary part is zero.

Exercise 7.6: (*) Derive Eq. 7.28.

From this, we see that

$$1 + U_{\vec{q}}X_0(\vec{q},\omega=0) = 1 + \frac{6\pi n e^2}{q^2\epsilon_F}, \tag{7.29}$$

so therefore

$$U_{\mathrm{RPA}}(\vec{q},\omega=0) = \frac{4\pi e^2}{q^2+\kappa^2} \tag{7.30}$$

where

$$\kappa = \frac{1}{\xi_{\mathrm{TF}}} = \left(\frac{6\pi n e^2}{\epsilon_F}\right)^{1/2} \tag{7.31}$$

is the inverse Thomas-Fermi screening length. Casting our memory back to Lecture 2, we see that this is the Yukawa potential, so corresponds to the *screened Coulomb interaction*

$$U(\vec{r}) = \frac{e^2}{|\vec{r}|}e^{-\kappa|\vec{r}|} = \frac{e^2}{|\vec{r}|}e^{-|\vec{r}|/\xi_{\mathrm{TF}}}. \tag{7.32}$$

In other words, in the presence of the polarizable medium (the electron sea), the long range Coulomb interaction actually becomes short range. This has a nice physical interpretation: suppose there is a point of higher than average density (i.e. negative charge). Then the electrons in the nearby vicinity will be repelled from this region, creating a region around this point of lower than average density, i.e. a screening region of positive charge. At a long distance, another electron sees not only the initial negative charge, but also the screening region around it, which almost cancel each other, hence making the Coulomb interaction effectively short ranged.

Exercise 7.7: (***) While we usually think of long-distance effects being equivalent to small-momentum effects, and therefore the expression in Eq. 7.32 which was derived in the $\vec{q} \to 0$ limit as being the correct long distance behaviour of the effective Coulomb interaction, there is in a fact a further twist in the tale.

Let us remain in the static limit, and look at the full function

$$X_0(q, \omega = 0), \qquad q = |\vec{q}|, \tag{7.33}$$

which can be read off from Eq. 7.21 (Notice from Eq. 7.18 that $\operatorname{Im} X_0(\vec{q}, \omega = 0) = 0$. Show that

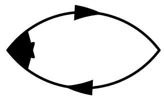
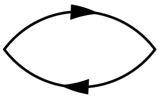
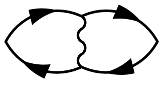
$$\frac{dX_0(q, \omega = 0)}{dq} \tag{7.34}$$

is singular at $q = 2k_F$. Explain the origin of this singularity (which is known in the literature as the *Kohn anomaly.* Show that it gives rise to an oscillating term in the RPA screened potential:

$$U_{\mathrm{RPA}}(\vec{r}) \propto \frac{\cos(2k_F|\vec{r}\,| + \varphi)}{|\vec{r}\,|^3}, \tag{7.35}$$

where φ is an unimportant phase. At long distances, this term term will be much more important than the exponential drop.

It's worth pointing out as an epilogue to this section, that analogous to the self energy, one can define the exact irreducible polarization bubble, $\Pi(\vec{q}, \omega)$ as the sum over all bubble diagrams which *cannot be cut into two by splitting a single interaction line*, i.e.

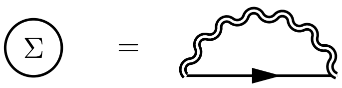
$\Pi(\vec{q}, \omega) =$  $=$  $+$  $+ \dots$ (7.36)

The RPA resummation then becomes exact (c.f. the generic expression for the Green function in terms of self energy):

$$= U_{\mathrm{exact}}(\vec{q}, \omega) = \frac{U_{\vec{q}}}{1 + U_{\vec{q}}\Pi(\vec{q}, \omega)}. \tag{7.37}$$

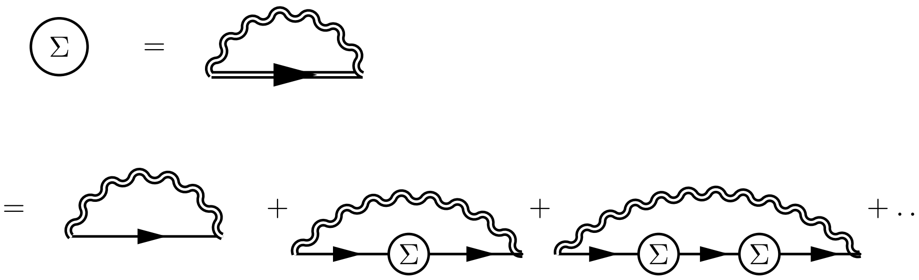
7.6. Beyond Hartree-Fock

Before we return to extract information from the bubble itself, let us have a brief look at how what we have learned so far in this lecture can help us calculate the self energy beyond the Hartree-Fock approximation. At an initial level, we could imagine that in the Fock diagram, we can replace the *bare interaction* by the *effective interaction* (which is often in the literature also called the *dressed interaction*):



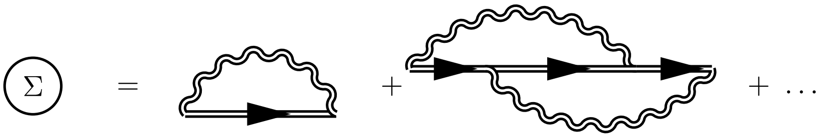
(7.38)

We could even replace the *bare Green function* line by the true Green function including self-energy corrections



(7.39)

which should of course be solved self-consistently.[5] Of course one can go even further:[6]



(7.40)

The art in condensed matter is to be able to associate physical processes to each diagram, and understand why you either need to include them, or they can be ignored (remembering that each diagram corresponds to an expression which, in order to understand anything, must be evaluated).

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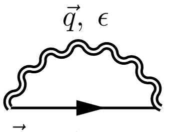
[5] A technique known unsurprisingly as self-consistent Hartree-Fock (SCHF).

[6] While the use of the "doubled" lines significantly reduces the number of diagrams, one must be very careful to make sure no diagram is double counted.

Exercise 7.8: (***) We recall that within the Hartree Fock approximation, we obtained the unphysical result of zero effective mass $m^* = 0$. The simplest way of going beyond Hartree-Fock will be the diagram in Eq. 7.38. In fact, even this diagram in general is unnecessarily difficult to calculate. Let us therefore replace it by something slightly simpler:

$$\Sigma(\vec{k},\omega) =$$



,

$$= U_{\mathrm{RPA}}(\vec{q},\omega) \qquad (7.41)$$

and approximating the RPA effective interaction by it's static small-$\vec{q}$ limit

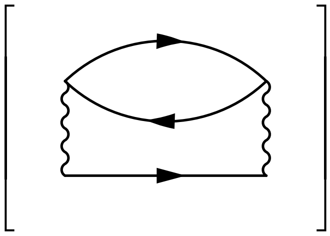
$$U_{\mathrm{RPA}}(\vec{q}) \approx \frac{4\pi e^2}{q^2+\kappa^2}. \qquad (7.42)$$

Within this approximation, calculate $\Sigma(\vec{k},\omega)$, and show that the effective mass m^* is now finite.

While in this exercise we see that going beyond Hartree-Fock gets rid of the unphysical $m^* = 0$ and gives a finite effective mass, we still find that the self energy is real, and therefore the quasi-particles still have an infinite lifetime. In fact, it turns out that it is the static interaction approximation that gives this result - but unfortunately calculating $\Sigma(\vec{k},\omega)$ using the full ω-dependence of U_{RPA} gives integrals of unfeasible difficulty. In the following exercise, we will calculate only the simplest diagram to give a finite lifetime.

Exercise 7.9: (***) Let us consider the simplest polarization correction to the self-energy, and for simplicity, let us calculate only the imaginary part of it:

$$\Gamma(\vec{k},\omega) = \mathrm{Im}$$



$$, \qquad (7.43)$$

where the notation is as in Eq. 6.37.

To evaluate this, first obtain the expression for this diagram (which in fact, you should have done in a previous exercise in Lecture 5). First, execute the two energy integrals by contour integration (in an analogous way to the evaluation of X_0), then take the imaginary part (analogous to the way we obtained S_0), which should give you a number of terms looking something like

$$-2\pi \int_{|\vec{q}_1|>k_F} \frac{d^3\vec{q}_1}{(2\pi)^3} \int_{|\vec{q}_2|<k_F,|\vec{k}+\vec{q}_1-\vec{q}_2|>k_F} \frac{d^3\vec{q}_2}{(2\pi)^3} |U_{\vec{q}_1-\vec{q}_2}|^2 \delta(\omega+\xi_{\vec{q}_2}-\xi_{\vec{q}_1}-\xi_{\vec{k}-\vec{q}_1+\vec{q}_2}). \qquad (7.44)$$

From evaluating these integrals, you can obtain the lifetime (as defined in Eq. 6.42) to be

$$\frac{1}{\tau_{\vec{k}}} = \Gamma(\vec{k}, \xi_{\vec{k}}) \propto \frac{(|\vec{k}\,| - k_F)^2}{2m}. \tag{7.45}$$

This demonstrates the Fermi-liquid principle.

7.7. Plasmons

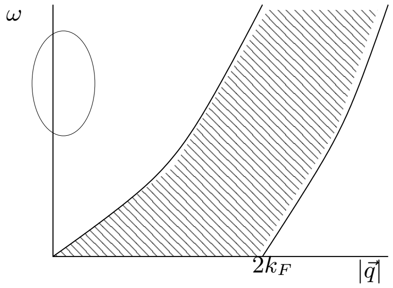
Let us now return to the polarization bubble:

$$X(\vec{q}, t) = i\langle GS|T\ \hat{\rho}_{\vec{q}}(t)\hat{\rho}^{\dagger}_{\vec{q}}|GS\rangle \tag{7.46}$$

which is given with the RPA as

$$X_{\mathrm{RPA}}(\vec{q}, \omega) = \frac{X_0(\vec{q}, \omega)}{1 + U_{\vec{q}} X_0(\vec{q}, \omega)}. \tag{7.47}$$

Now, recall that Im X_0 is only non-zero in the following region:



Let us now consider the circled bit on the diagram, i.e. large ω and small $\vec{q}$ (so Im $X_0 = 0$). Then X_0 is given by the Lindhard formula, Eq. 7.20

$$\mathrm{Re}\, X_0(\vec{q}, \omega) = 2\int \frac{d^3\vec{k}}{(2\pi)^3}\, \frac{n^0(\vec{k}+\vec{q}) - n^0(\vec{k})}{\omega - \xi_{\vec{k}+\vec{q}} + \xi_{\vec{k}}}. \tag{7.48}$$

Let us expand in small-$\vec{q}$:

$$n^0(\vec{k}+\vec{q}) - n^0(\vec{k}) \approx \vec{q}\cdot\frac{\partial n^0(\vec{k})}{\partial\vec{k}}. \tag{7.49}$$

Now,

$$n^0(\vec{k}) = \theta(\frac{k_F^2}{2m} - \frac{k^2}{2m}) \qquad \Longrightarrow \qquad \frac{\partial n^0(\vec{k})}{\partial \vec{k}} = \frac{-\vec{k}}{m}\delta(\xi_{\vec{k}}). \tag{7.50}$$

Similarly,

$$\xi_{\vec{k}+\vec{q}} - \xi_{\vec{k}} \approx \vec{q}\cdot\frac{\partial\xi_{\vec{k}}}{\partial\vec{k}} = \vec{q}\cdot\frac{\vec{k}}{m}. \tag{7.51}$$

Therefore, for small $|\vec{q}\,|$, we have

$$X_0 \approx 2\int \frac{d^3\vec{k}}{(2\pi)^3}\,\frac{-\vec{k}\cdot\vec{q}}{m\omega-\vec{k}\cdot\vec{q}}\,\delta(\xi_{\vec{k}}). \tag{7.52}$$

Now, not only is $|\vec{q}\,|$ small, but we want the limit where ω is large, so we can expand

$$\frac{1}{m\omega-\vec{k}\cdot\vec{q}} \approx \frac{1}{m\omega}\left[1+\frac{\vec{k}\cdot\vec{q}}{m\omega}+\dots\right]. \tag{7.53}$$

We can now evaluate the integral in polar coordinates, where $\vec{k}\cdot\vec{q} = |\vec{k}\,|\,|\vec{q}\,|\cos\theta = k_F|\vec{q}\,|\cos\theta$ as the delta-function forces $|\vec{k}\,| = k_F$, so (with the usual notation that $q = |\vec{q}\,|$

$$\begin{aligned} X_0 &\approx \frac{-4\pi}{(2\pi)^3}\int_{-1}^{1} d(\cos\theta)\,\frac{k_F q\cos\theta}{m\omega}\left[1+\frac{k_F q\cos\theta}{m\omega}+\dots\right] \qquad \underbrace{\times k_F^2\frac{m}{k_F}}_{\text{from the integral over }\delta(\xi_k)} \\ &= \frac{-4\pi}{(2\pi)^3}\,\frac{2}{3}\,\frac{k_F^2 q^2}{m^2\omega^2}mk_F = -\frac{1}{3\pi^2}\,\frac{k_F^3 q^2}{m\omega^2}+O(q^4). \end{aligned} \tag{7.54}$$

Hence the denominator of the RPA expression is

$$1+U_{\vec{q}}X_0(\vec{q},\omega) = 1-\frac{4\pi e^2}{q^2}\,\frac{1}{3\pi^2}k_F^3 q^2 m\omega^2 = 1-\frac{4\pi e^2 n}{m\omega^2} = 1-\frac{\omega_p^2}{\omega^2}, \tag{7.55}$$

where

$$\omega_p^2 = \left(\frac{4\pi e^2 n}{m}\right)^{1/2}, \tag{7.56}$$

and we have remembered that the density $n = N/V = k_F^3/3\pi^2$.

Exercise 7.10: (***) Expand further in powers of $\vec{q}$ (or alternatively, expand your previously derived formula for X_0, Eq. 7.22) to show that the plasmon dispersion

$$X_{\mathrm{RPA}}(\vec{q},\omega) \propto \frac{1}{1-\frac{\omega_p^2(|\vec{q}\,|)}{\omega^2}}, \tag{7.57}$$

is given by

$$\omega_p(q) = \left(\frac{4\pi ne^2}{m}\right)^{1/2}\left[1+\frac{3}{10}\left(\frac{qv_F}{\omega_p(0)}\right)^2+\dots\right]. \tag{7.58}$$

What we see therefore, is that $X_{\mathrm{RPA}}(\vec{q},\omega)$ has a *pole* at $\omega = \omega_p(\vec{q})$, where the position of the pole has a weak dispersion at small $\vec{q}$. This is in strong contrast to X_0 which has no poles, i.e. the interacting Fermi gas has a branch of coherent particle-hole exciations, which is known as *plasmons.* These are propagating waves of density oscillations.

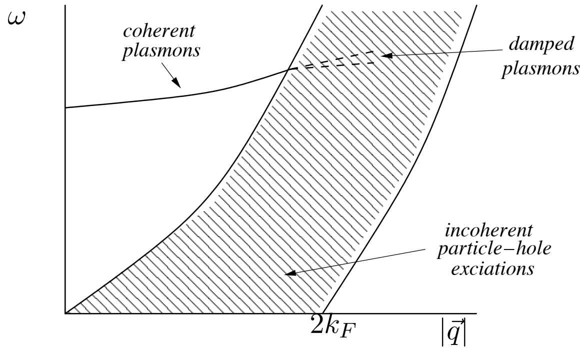


Figure 7.2.: The excitations of the Fermi Liquid. There is a coherent, weakly dispersive plasmon mode at small momenta and large energy, which becomes damped as it enters the incoherent particle-hole continuum.

Now, in this region of large ω and small $\vec{q}$, there is no finite imaginary part in the denominator of X_{RPA}, in other words, this branch of plasmon excitations is stable. However, if $\vec{q}$ becomes larger, eventually the excitation crosses the boundary of the incoherent particle-hole background. Here, the plasmon (which is a bound state of a particle and a hole) can decay into this background, so the plasmons acquire a finite lifetime. Technically, the poles are moved off the real axis. The excitations of the Fermi liquid are all put together and plotted in Fig. 7.2.

This has been a long chapter, but we have now, in my opinion, calculated all of the most important ground state properties of the Coulomb interacting free Fermi gas. There is of course an almost infinite number of further things one could calculate or discuss in this model, but I believe that having come this far, these can now be easily looked up in for example Mahan if and when they are needed. In the next chapter, we will mostly leave studying properties of the interacting Fermi gas, and return to learning how to extract meaningful experimental predictions from our expressions for causal Green functions.

8. Linear response theory and the fluctuation-dissipation theorem

There is a very strong link between correlation functions (fluctuations) and response functions to an external applied field (dissipation). For example, consider the expectation value

$$\langle GS|\hat{\rho}(\vec{x},t)\hat{\rho}(\vec{x}\,',t')|GS\rangle. \tag{8.1}$$

We have been thinking of this as a correlation function between two points and times. However, we can also think of it as applying some extra density at $\vec{x}\,', t'$ and seeing how it affects the density at x, t.

Time ordered correlation functions are what we have been learning to calculate using the diagrammatic technique. However, response functions are what experimentalists will measure - they will perturb the system in some way and see what it does in response. It is therefore very important for us to understand much better the relationship between response functions and correlation functions.

In fact, the fluctuation-dissipation theory in it's full glory can not be fully understood until we have looked at finite temperature Green functions - so we will revisit many of these concepts again later in Lecture 12. However, the importance of this topic means it is well worthwhile meeting it at least once before we leave the subject of zero temperature Green functions - which is the purpose of this lecture.

8.1. The theory behind response functions

Let us consider a system coupled to an external source field

$$\hat{H}_(t) = \hat{H}_0 + \hat{H}_s(t), \qquad \hat{H}_s(t) = -\hat{A}(t)f(t), \tag{8.2}$$

where $\hat{A}(t)$ is some operator of the system (i.e. can be written in terms of creation and annihilation operators of the system), and $f(t)$ is the strength of the source field.

Example 8.1: The operator $\hat{H}_s(t)$ could take the form

$$\hat{H}_s(t) = -\int d^3\vec{x}\; r\hat{h}o(\vec{x})\Phi(\vec{x},t). \tag{8.3}$$

In this case, $f(t) = \Phi$ is the external electrical potential, and $\hat{A}(t) = \hat{\rho}(t)$ is the particle density in the system.

The system will *respond* to the applied source field by a change in the expectation value of the operator $\hat{A}$.

It is worthwhile taking a minute to understand fully the notation in Eq. 8.2. The part of the Hamiltonian $\hat{H}_0$ is the Hamiltonian of the system before we start probing it with our source fields - however, the system is in general, interacting. Therefore in this chapter, $\hat{H}_0$ will be what up until this point we have always called $\hat{H}_0 + \hat{H}_{\text{int}}$. The perturbation to $\hat{H}_0$ is then the external field, and not the interaction. This all makes sense: as a theorist making a calculation, you want to split up the system into the solvable non-interacting part perturbed by something you can't solve exactly so you treat perturbativly. On the other hand, in the real physical world, it makes more sense to split the world into that intrinsic to the system, and that which we are probing it with.

We can therefore go into an "interaction" representation, where the time dependence of operators comes from the (interacting!) $\hat{H}_0$, and that of wavefunctions from the perturbation $\hat{H}_s$:

$$\hat{A}_H(t) = \hat{U}^\dagger(t)\hat{A}_I(t)\hat{U}(t), \qquad \hat{U}(t) = T\exp\left\{-i\int_{-\infty}^{t} \hat{H}_s(t')\,dt'\right\}. \tag{8.4}$$

Note that the interaction representation $\hat{A}_I$ actually just corresponds to the Heisenberg representation of the unperturbed (but interacting!) system, $\hat{H}_0$, so we will just write it as $\hat{A}(t)$ unless serious confusion may arise.

If we expand $\hat{U}(t)$ to first order in $\hat{H}_s$, which is equivalent to saying linear order in the external field $f(t)$, we see that

$$\hat{A}_H(t) = \hat{A}(t) - i\int_{\infty}^{t}\left[\hat{A}(t), \hat{H}_s(t')\right]\,dt' + O(\hat{H}_s^2). \tag{8.5}$$

If we take expectation values (and stop writing $O(\hat{H}_s^2)$ because we understand that everything we will do here is *linear response*):

$$\langle\hat{A}_H(t)\rangle = \langle\hat{A}(t)\rangle - i\int_{\infty}^{t}\langle\left[\hat{A}(t), \hat{H}_s(t')\right]\rangle\,dt'. \tag{8.6}$$

Therefore, the change $\langle\hat{A}_H - \hat{A}\rangle$, i.e. the *response* to the source field is given by

$$\begin{aligned}\langle\delta\hat{A}(t)\rangle &= -i\int_{\infty}^{t}\langle\left[\hat{A}(t), -\hat{A}(t')f(t')\right]\rangle\,dt' \\ &= \int_{-\infty}^{\infty}dt'\,\chi(t-t')f(t'). \end{aligned} \tag{8.7}$$

Here, $\chi(t-t')$ is known as a *generalized dynamical susceptibility*,[1] and is given by

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[1] For a number of specific operators $\hat{A}$, it has more specific names - we will meet a number of examples of these shortly.

$$\boxed{\chi(t-t') = i\langle GS| \left[\hat{A}(t), \hat{A}(t')\right] |GS\rangle \theta(t-t'). \qquad (8.8)}$$

Notice that Eq. 8.7 is in the form of a convolution, so if we take the Fourier transform and work in frequency space, then

$$\langle \delta\hat{A}(\omega)\rangle = \chi(\omega) f(\omega). \tag{8.9}$$

The operator $\hat{A}$ can in principle be anything, but there a number of important choices worth mentioning:

- $\hat{A} = \hat{\rho}_{\vec{q}}$ – which gives us *the dynamical susceptibility*, which is closely related to the dielectric function of the material in question - we'll see how this works shortly.
- $\hat{A} = \hat{S}^z$ – which gives us the *magnetic susceptibility.* We'll also see an example of this during this lecture.
- $\hat{A} = \hat{\jmath} = \frac{e\vec{q}}{m}\hat{\rho}_{\vec{q}}$ – i.e. the current operator. This gives us the *electrical conductivity* of the material. This particular form of linear response goes by the name of *Kubo formulae*, and has a few peculiarities that go with it. We will therefore defer a discussion of this until Lecture 12.

We now have an expression for the linear response of a system to some perturbing field, and knowledge of which generalized susceptibility to use in order to calculate which experimentally measurable quantity. However using diagrammatic perturbation theory, we can only evaluate time-ordered correlation functions. How can we use these to obtain χ?

If we go to the Lehmann representation of Eq. 8.8, we will see that χ is completely analogous to the retarded Green function introduced in Lecture 6. To be specific, let us take the example where we perturb by adding an external electric field - i.e. $\hat{A} = \hat{\rho}$. In this case, we will see that

$$\operatorname{Re}\chi(\omega) = \operatorname{Re} X_0(\omega), \tag{8.10}$$

however $\operatorname{Im}\chi(\omega)$ does not change sign when ω passes through the chemical potential. More concretely, we can see that for the non-interacting system,[2]

$$\chi(\vec{q},\omega) = -2\sum_{\vec{k}} \left[\frac{\theta(\xi_{\vec{k}+\vec{q}})\theta(-\xi_{\vec{k}})}{\omega - \xi_{\vec{k}+\vec{q}} + \xi_{\vec{k}} + i\delta} - \frac{\theta(-\xi_{\vec{k}+\vec{q}})\theta(\xi_{\vec{k}})}{\omega - \xi_{\vec{k}+\vec{q}} + \xi_{\vec{k}} + i\delta} \right], \tag{8.11}$$

which we should compare to the equivalent expression for X_0, Eq. 7.14, which is identical except for the sign of the $i\delta$ in the second term. We therefore see that $\chi_0(\vec{q},\omega) = X_0(\vec{q},\omega + i\delta)$, and in fact we can show in general that this is true:

$$\chi(\vec{q},\omega) = X(\vec{q},\omega + i\delta), \tag{8.12}$$

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[2] An equivalent expression can be derived for the interacting system using the Lehmann representation - the only difference being in the absence of matrix elements in the non-interacting case. See the books for more details.

but we must remember that diagrammatics can only be done with the time-ordered correlation functions, and the analytic continuation to obtain χ from X must only be done **after** all other integrals in the perturbation expansion (unless you wish for incorrect results). We will now look in more detail at some important examples of Eq. 8.8 at work.

8.2. Example: the dielectric function

Let us consider classical electrodynamics, and Coulomb's law:[3]

$$\phi(\vec{r}) = \frac{q}{4\pi\epsilon_0 r}. \tag{8.13}$$

This is modified in a dielectric medium, to

$$\phi(\vec{r}) = \frac{q}{4\pi\epsilon_0\ \epsilon\ r}, \tag{8.14}$$

where ϵ is the material specific dielectric constant. If we Fourier transform this into reciprocal space, we get

$$\phi(\vec{q}) = \frac{4\pi}{q^2}\frac{\rho_e(\vec{q})}{\epsilon(\vec{q})}, \tag{8.15}$$

where we have written ρ_e to explicitly represent that this is the *external* charge density, and we have allowed the dielectric constant to have $\vec{q}$ dependence (which generally from experimental measurements it does). We can also however calculate the potential as

$$\phi(\vec{q}) = \frac{4\pi}{q^2}[\ \underbrace{\rho_e(\vec{q})}_{\text{external}}\ +\ \underbrace{\rho_s(\vec{q})}_{\text{screening}}\ ], \tag{8.16}$$

i.e. forget the dielectric function, but include all of the charges, including the screening charges induced in the material. Comparing these two expressions, we see that

$$\frac{1}{\epsilon(\vec{q})} = \frac{\rho_e(\vec{q}) + \rho_s(\vec{q})}{\rho_e(\vec{q})} = 1 + \frac{\rho_s(\vec{q})}{\rho_e(\vec{q})}. \tag{8.17}$$

Now, the external charges alone generate an external potential

$$\phi_e(\vec{q}) = \frac{4\pi}{q^2}\rho_e(\vec{q}), \tag{8.18}$$

and as we learned earlier in this lecture, within linear response, this external potential generates a (static) screening charge[4]

$$\rho_s(\vec{q}) = -\chi(\vec{q}, \omega = 0)e^2\phi_e(\vec{q}) = -\frac{4\pi e^2}{q^2}\chi(\vec{q}, \omega = 0)\rho_e(\vec{q}). \tag{8.19}$$

Hence one has a microscopic calculation of the dielectric properties of materials:

$$\boxed{\frac{1}{\epsilon(\vec{q})} = 1 - U_{\vec{q}}\chi(\vec{q}, \omega = 0). \qquad (8.20)}$$

---

[3] As usual, $r = |\vec{r}|$. Also, in this section we will occasionally reinstate the factor of $1/4\pi\epsilon_0$ for clarity of formulae. We won't however put this factor in everywhere - so read with care!

[4] It is fairly obvious to see how the extension to dynamics (e.g. in order to calculate the propagation of light through the material) will work.

8.3. Example: magnetism and the Stoner criterion

Let us consider now the magnetic susceptibility of a material. First, we will consider the system macroscopically. Similar to the electric potential case, the magnetic response to an applied field is given by

$$\vec{M}(\vec{x}) = \int d^3\vec{x}\,\chi_M(x-x')\vec{B}(\vec{x}), \tag{8.21}$$

or if we work in momentum space

$$\vec{M}(\vec{q}) = \chi_M(\vec{q})\vec{B}(\vec{q}). \tag{8.22}$$

These equations are a definition of the magnetic susceptibility, $\chi_M(\vec{q})$, which is in general is a second order tensor. Let us consider for simplicity though that the magnetic field is in the z direction, i.e. $\vec{B} = (0, 0, B_z)$, and we are looking at the response in the same direction (i.e. we are calculating χ_M^{zz}.

Now let us consider the system microscopically. The term added to the Hamiltonian when we apply a magnetic field in the z direction is the Zeeman term:[5]

$$\hat{H}_s = -\mu_B^2 \hat{S}_z(\vec{x})B_z(\vec{x}). \tag{8.23}$$

Therefore by the general theory of linear response, Eq. 8.8, the magnetic susceptibility is given by

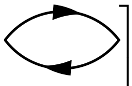
$$\chi_M^{zz}(\vec{q},\omega) = i\mu_B^2 \int dt\, e^{i\omega t} \int d^3\vec{x}\, e^{i\vec{q}.\vec{x}}\, \underbrace{\langle GS|\left[\hat{S}_z(\vec{x},t), \hat{S}_z(0,0)\right]|GS\rangle}_{}. \tag{8.24}$$

8.3.1. Pauli Susceptibility

Now $\hat{S}_z = (\hat{n}_\uparrow - \hat{n}_\downarrow)/2$, analogous to $\hat{\rho} = \hat{n}_\uparrow + \hat{n}_\downarrow$. Hence

$$\langle \hat{S}_z \hat{S}_z \rangle = \frac{1}{4}\left(\langle \hat{n}_\uparrow \hat{n}_\uparrow \rangle + \langle \hat{n}_\downarrow \hat{n}_\downarrow \rangle \underbrace{- \langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle - \hat{n}_\downarrow \hat{n}_\uparrow \rangle}_{\text{these terms give zero}} \right) /4 \tag{8.25}$$

$$= \frac{1}{4}\left[2 \times \right.$$



$$\left. \right] \sim X_0(\vec{q},\omega)/4.$$

Hence for the non-interacting Fermi gas,

$$\chi_M^{zz}(\vec{q},\omega) = \frac{\mu_B^2}{4} X_0(\vec{q},\omega + i\delta). \tag{8.26}$$

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[5] To be precise, there will also be an orbital term which is responsible for possible diamagnetism - but let us ignore this term.

If we take the static case $\omega = 0$, then $\operatorname{Im} X_0 = 0$ so we can just use the Lindhard function, Eq. 7.20:

$$\chi_M^{zz}(\vec{q}) = -\frac{\mu_B^2}{2}\int \frac{d^3\vec{k}}{(2\pi)^3}\,\frac{n^0(\vec{k}+\vec{q})}{\xi_{\vec{k}+\vec{q}} - \xi_{\vec{k}}}. \tag{8.27}$$

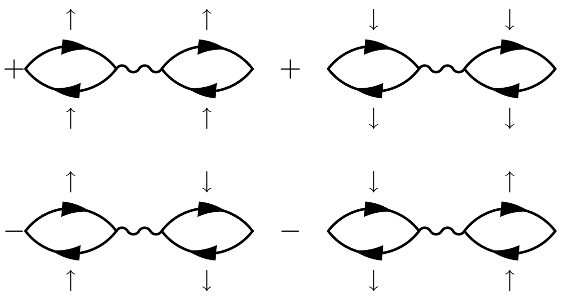
If we furthermore go to the uniform limit $\vec{q} \to 0$, we obtain the Pauli susceptibility

$$\chi = -\frac{\mu_B^2}{2}\int \frac{d^3\vec{k}}{(2\pi)^3}\,\frac{\partial n_0}{\partial \xi}. \tag{8.28}$$

Remembering that $n_0(\xi_{\vec{k}}) = \theta(-\xi_{\vec{k}})$, we finally get

$$\chi = -\frac{\mu_B^2}{2}\int \frac{d^3\vec{k}}{(2\pi)^3}\,\delta(\xi_{\vec{k}}) = \frac{\mu_B^2 N_F}{2}. \tag{8.29}$$

It is worthwhile observing that if we add the Coulomb interaction and try to calculate $\langle \hat{S}^z \hat{S}^z \rangle$ within the RPA, all diagrams cancel - for example if we look at the first order diagrams:



(8.30)

As the bubble itself is independent of spin, these diagrams all have the same contribution, therefore cancel. It is not difficult to see that this is true at every order in the RPA.

In order to see how interactions modify magnetic properties of the material, one needs to work harder to single out the *exchange* part of the Hamiltonian - i.e. the part which depends on the relative signs of the spin.[6] Let us therefore turn away from the Coulomb interacting Fermi gas and look at a different model where the interaction is explicitly spin dependent, where this physics can be easily demonstrated.

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[6] In itinerant systems, this leads us towards Hertz-Millis theory, which is unfortunately beyond the scope of this course.

8.3.2. Stoner theory of Ferromagnetism in the Hubbard model

Let us consider the Hubbard model, which is a model on a lattice with an on-site interaction:

$$\begin{aligned}\hat{H}_{\text{Hubbard}} &= \hat{H}_0 + \hat{H}_U \\ \hat{H}_0 &= \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma}, \\ \hat{H}_U &= \frac{U}{2} \sum_i \hat{n}_{i\downarrow} \hat{n}_{i\uparrow}. \end{aligned} \qquad (8.31)$$

where $\epsilon_{\vec{k}}$ is the tight binding spectrum

$$\epsilon_{\vec{k}} = -2t\left[\cos k_X + \cos k_y + \cos k_z\right], \qquad \text{in three dimensions,} \qquad (8.32)$$

and the sum over i in $\vec{H}_U$ is over all lattice sites. Notice that because the interaction is purely local, it's Fourier transform $U(\vec{q}) = U$, i.e. is a constant independent of $\vec{q}$ - but now dependent on the incoming and outgoing spins.

The interaction can be decomposed in a different way

$$\hat{H}_U = \frac{U}{4} \sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})^2 - \frac{U}{4} \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2. \qquad (8.33)$$

Exercise 8.1: (**) Draw the RPA diagrams for this model, to show that the electronic $X(\vec{q},\omega)$ and magnetic $X^M(\vec{q},\omega)$ pair correlation functions for the Hubbard model,

$$X \sim \langle T\, \hat{\rho}\hat{\rho} \rangle, \qquad X^M \sim \langle T\, \hat{S}^z \hat{S}^z \rangle \qquad (8.34)$$

are given (with the random phase approximation) by

$$X_{\text{RPA}} = \frac{X_0}{1 + \frac{U}{2} X_0}, \qquad X^M_{\text{RPA}} = \frac{X_0}{1 - \frac{U}{2} X_0}. \qquad (8.35)$$

Now, let us go to the static, uniform limit $\omega = 0, \vec{q} \to 0$, where we have seen previously that $X_0(\vec{q} \to 0, \omega = 0) = N_F$.[7] Then we see that if we start increasing the interaction strength U, until the point where

$$\frac{U_c}{2} N_F = 1, \qquad (8.36)$$

then there is a pole in X^M at zero frequency. This pole will lead to an infinite χ^M, which means that the system has an *infinite response to a static, uniform* field. This is

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[7] If we look back to Eq. 8.29, we derive this for the free Fermi gas - but notice at no point do we use the form of the spectrum, so in fact this result is true for any (non-interacting) model. In fact, it can be seen in some ways as the definition of the density of states at the Fermi level, N_F.

an indication of a *quantum phase transition* from a paramagnetic phase for $U < U_c$ to a ferromagnetic phase at $U > U_c$. Bear in mind the discussion in Lecture 4, where we showed that one cannot use perturbation theory through a phase transition - so while our perturbation expansion gives the presence of the ferromagnetic transition, we will need a different starting point if we want to actually calculate properties of the ferromagnetic phase.

Equation 8.36 is known as the Stoner criterion, and although we have studied it only by example, it should be obvious that the physics behind it can be easily generalized. As usual, for a more formal approach, see the textbooks. In general, the linear response theory means that a pole in any pair correlation function at $\omega = 0$ implies a large response to an infinitesimal perturbation and the system is unstable towards some other (ordered) phase. We have already seen a pole in $X^M(\vec{q} \to 0, \omega = 0)$ implies a ferromagnetic phase. If the pole is at a finite value of $\vec{q}$ (but always $\omega = 0$), this would be a transition to an antiferromagnetic ($\vec{q} = \pi$) or for general $\vec{q}$, a spin density wave (SDW). Similarly, if the pole is in the electronic X rather than the magnetic X^M, then the transition would be a charge density wave (CDW). Many others are possible.

9. Scattering potentials and disordered systems

While we now have a fair amount of experience in the Green function/diagrammatic expansion technique for many body physics, all of our examples so far have been limited to two-body interactions, and even more specifically almost exclusively the Coulomb interaction. We will now have two lectures on some different applications of diagrams within condensed matter physics.

9.1. Point scatterer

Consider a Hamiltonian

$$\hat{H} = \underbrace{\sum_{\vec{k}} \epsilon_{\vec{k}} \hat{c}^{\dagger}_{\vec{k}} \hat{c}_{\vec{k}}}_{=\hat{H}_0} + \hat{H}_{sc}, \tag{9.1}$$

where $\hat{H}_{sc}$ is a scattering potential

$$\hat{H}_{sc} = \int d^3\vec{x}\ \hat{\Psi}^{\dagger}(\vec{x})\hat{\Psi}(\vec{x})U(\vec{x}). \tag{9.2}$$

To be specific, we will later on be considering free electrons $\epsilon_{\vec{k}} = k^2/2m - \mu$ scattering off a point impurity $U(\vec{x}) = u_0\delta(\vec{x})$, but let us remain much more general for now.

We could also perform a Fourier transform to write $\hat{H}_sc$ in the momentum representation

$$\hat{H}_sc = \sum_{\vec{k},\vec{k}'} U_{\vec{k}-\vec{k}'} \hat{c}^{\dagger}_{\vec{k}} \hat{c}_{\vec{k}'}, \tag{9.3}$$

where

$$U_{\vec{q}} = \int d^3\vec{x}\ e^{i\vec{q}\cdot\vec{x}} U(\vec{x}). \tag{9.4}$$

Notice that the full Hamiltonian $\hat{H}$ is quadratic - but let us suppose it is nevertheless not easily solvable. For example, for a scattering potential which is not translationally invariant (which in general it isn't - if it was, it wouldn't be scattering), the the Fourier transform does not diagonalize the Hamiltonian. How can we use Feynman diagrams to help us solve this?

9.1.1. Disorder diagrams

The first thing we should note is that the Green function

$$-i\,\langle T\hat{\Psi}(\vec{x},t)\hat{\Psi}^\dagger(\vec{x}\,',t')\rangle = G(\vec{x},\vec{x}\,',t-t') \tag{9.5}$$

is no longer a function of just the difference $\vec{x}-\vec{x}\,'$ (although G_0 of course, still is) as translational symmetry has been broken.

We now need to derive the Feynman rules for this new sort of perturbation. As usual, we can write write the Green function for $\hat{H}$ as a perturbation theory about that of $\hat{H}_0$.

$$\begin{aligned} G(\vec{x},\vec{x}\,',t-t') &= -i\,\langle T\hat{\Psi}(\vec{x},t)\hat{\Psi}^\dagger(\vec{x}\,',t')\rangle \\ &= -i\,\frac{{}_0\langle T\hat{\Psi}(\vec{x},t)\hat{\Psi}^\dagger(\vec{x}\,',t')S(\infty,-\infty)\rangle_0}{{}_0\langle S(\infty,-\infty)\rangle_0}, \end{aligned} \tag{9.6}$$

where

$$\begin{aligned} S(\infty,-\infty) &= T\,\exp\left[-i\int_{-\infty}^{\infty}\hat{H}_{sc}(t_1)\,dt_1\right] \\ = \quad 1-iT\int_{-\infty}^{\infty}dt_1\,\hat{H}_{sc}(t_1) &+ \frac{(-i)^2}{2!}T\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2\,\hat{H}_{sc}(t_1)\hat{H}_{sc}(t_2)+\ldots \end{aligned} \tag{9.7}$$

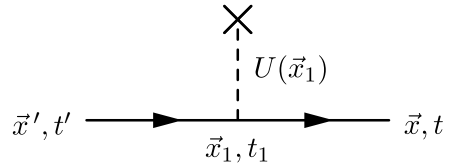
Let us look in more detail at the first order term

$$(-i)^2\int d^3\vec{x}_1\int dt_1\,{}_0\langle T\,\hat{\Psi}(\vec{x},t)\hat{\Psi}^\dagger(\vec{x}\,',t')\hat{\Psi}(\vec{x}_1,t_1)\hat{\Psi}^\dagger(\vec{x}_1,t_1)\rangle_0\,U(\vec{x}_1). \tag{9.8}$$

Note that the other possible Wick contraction would lead to a disconnected diagram (can you see this?), so it will be cancelled by the denominator, and we will worry about it no further. Therefore we obtain for the first order correction to G:

$$\begin{aligned} G^{(1)} &= (-1)(-i)^2\int d^3\vec{x}_1\int dt_1\,U(\vec{x}_1)\,{}_0\langle T\,\hat{\Psi}(\vec{x},t)\hat{\Psi}^\dagger(\vec{x}_1,t_1)\rangle_0\,{}_0\langle\hat{\Psi}^\dagger(\vec{x}_1,t_1)\hat{\Psi}(\vec{x}\,',t')\rangle_0 \\ &= \int d^3\vec{x}_1\int dt_1\,U(\vec{x}_1)G_0(\vec{x}-\vec{x}_1,t-t_1)G_0(\vec{x}_1-\vec{x}\,',t_1-t'). \end{aligned} \tag{9.9}$$

This can be represented diagrammatically as



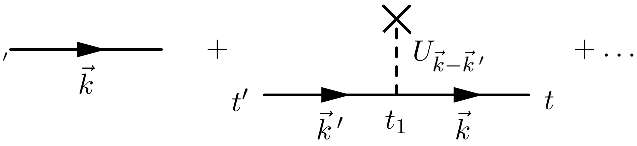
and interpreted as a particle travelling from $(\vec{x}\,',t')$ to $\vec{x},t$ via an intermediate scattering event at $(\vec{x}_1,t_1)$. In terms of the Feynman rules, the most important thing is that Eq. 9.9 contains no extraneous factors of i. We can therefore extrapolate and state the Feynman rules for Hamiltonian 9.1:

- To form a diagram of order n, draw a connected graph with $n+1$ Fermion lines and n disorder vertices (which link two Fermion lines) at positions $\vec{x}_i, t_i$.
- For each fermion line, associate a factor of G_0. For each disorder vertex, associate a factor $U(\vec{x}_i)$.
- Integrate over all intermediate positions and times.

Exercise 9.1: (**) Verify the rules (in particular, the absence of any extra factors of (-1) or i) explicitly to second order by expanding the S matrix to this order. Convince yourself that these rules are true to all orders.

One could equally well work in momentum space:

$$G(\vec{k},\vec{k}',t-t') = \delta_{\vec{k}\vec{k}'} \qquad (9.10)$$



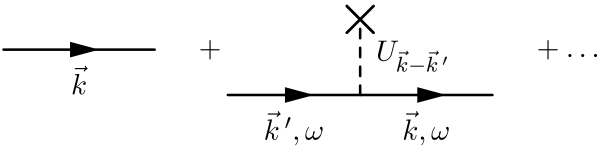
Notice here that the lack of translational invariance means that momentum is not conserved. The Green function

$$G(\vec{k},\vec{k}',t-t') = \int d^3\vec{x} \int d^3\vec{x}'\; e^{i\vec{k}\cdot\vec{x}} e^{-i\vec{k}'\cdot\vec{x}'} G(\vec{x},\vec{x}',t-t'), \qquad (9.11)$$

is therefore a function of two momenta, not just one.

Finally, one could work in $(\vec{k},\omega)$ space:

$$G(\vec{k},\vec{k}',\omega) = \delta_{\vec{k}\vec{k}'} \qquad (9.12)$$



where the static nature of the disorder potential means that a) energy is conserved at the scattering vertex, and b) the vertex is energy independent.

9.1.2. Friedel oscillations around the point impurity

Now, let us look at a specific important example: that of a point impurity at $\vec{x}=0$:

$$U(\vec{x}) = u_0\delta(\vec{x}), \qquad (9.13)$$

or if we Fourier transform into momentum space

$$U_{\vec{q}} = u_0, \qquad (9.14)$$

independent of momentum.

Let us look at the change in the density of electrons due to the presence of the impurity:

$$\delta\rho(\vec{x}) = \langle \hat{\Psi}^\dagger(\vec{x})\hat{\Psi}(\vec{x})\rangle - \rho_0, \tag{9.15}$$

which from the definition of the Green function we see can be written as

$$\delta\rho(\vec{x}) = iG(\vec{x},\vec{x},t=0^-) - \rho_0. \tag{9.16}$$

Let us calculate G to first order in perturbation theory. If we look at the expansion 9.1.1 and write down the corresponding expression, we get

$$G(\vec{k},\vec{k}\,',\omega) = \delta_{\vec{k}\vec{k}'}G_0(\vec{k},\omega) + \underbrace{u_0 G_0(\vec{k},\omega)G_0(\vec{k}\,',\omega)}_{\delta G}. \tag{9.17}$$

The zeroth order contribution will of course give us the background density, to get $\delta\rho$, we just need to consider δG. Putting this all together gives us

$$\begin{aligned}\delta\rho(\vec{x}) &= iu_0 \sum_{\vec{k},\vec{k}\,'} e^{i(\vec{k}-\vec{k}\,')\cdot\vec{x}} \int \frac{d\omega}{2\pi}\, e^{i\omega 0^-} G_0(\vec{k},\omega)G_0(\vec{k}\,',\omega)\\ &= iu_0 \sum_{\vec{k},\vec{k}\,'} e^{i(\vec{k}-\vec{k}\,')\cdot\vec{x}} \int \frac{d\omega}{2\pi}\, e^{i\omega 0^-} \frac{1}{\omega - \xi_{\vec{k}} + i\delta\,\mathrm{sign}\,\xi_{\vec{k}}}\;\frac{1}{\omega - \xi_{\vec{k}'} + i\delta\,\mathrm{sign}\,\xi_{\vec{k}'}}.\end{aligned} \tag{9.18}$$

Exercise 9.2: (***) Show that evaluating the integrals in Eq. 9.18 gives the final result

$$\delta\rho(\vec{r}) \sim u_0 \frac{\cos 2k_F r}{r^3}, \qquad r = |\vec{r}|. \tag{9.19}$$

Hint: First do the energy integral by contour integration, where the factor $e^{i\omega 0^-}$ means you must evaluate the integral in the lower half plane. You can then turn the momentum sums into integrals and evaluate with contour integral or otherwise to obtain the result.

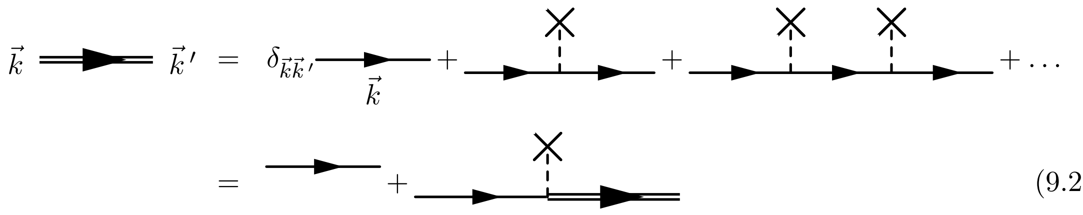
The result 9.19 tells us that if we put an impurity at the origin, then the free electron gas will rearrange itself to give density oscillations around this impurity, of wavevector $2k_F$ and decaying as one over distance cubed (in three dimensions).[1] These are known as *Friedel* oscillations, after the guy who first studied them.

---

[1] What about one dimension? What about d dimensions?

9.2. The T-matrix expansion

We can in fact sum over all diagrams exactly (which is an immediate consequence of the Hamiltonian being quadratic). Let us write down the full expansion:

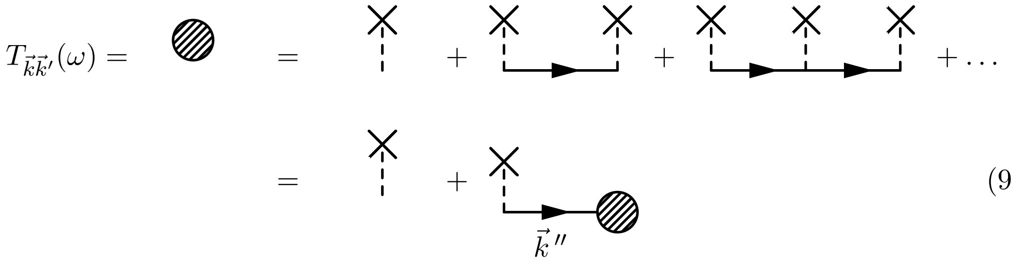


(9.20)

This second line is a Dyson series for the Green function, switching from pictures to equations, we see that

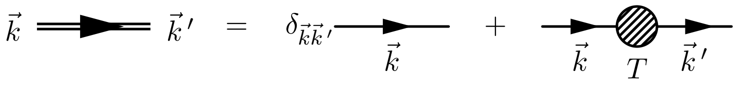
$$G(\vec{k},\vec{k}\,',\omega)=\delta_{\vec{k}\vec{k}\,'}G_0(\vec{k},\omega)+\sum_{\vec{k}\,''}G_0(\vec{k},\omega)U_{\vec{k}-\vec{k}\,''}G(\vec{k}\,',\vec{k}\,'',\omega). \tag{9.21}$$

This is more usually written by employing a function known (for reasons that have always eluded me) as the T-matrix. This object plays in potential scattering diagrams the same role as the self energy plays in two-body interaction diagrams. It can be represented diagramatically as



(9.22)

One can then write the Green function as



(9.23)

i.e.

$$G(\vec{k},\vec{k}\,',\omega)=\delta_{\vec{k}\vec{k}\,'}G_0(\vec{k},\omega)+G_0(\vec{k},\omega)T_{\vec{k},\vec{k}\,'}(\omega)G_0(\vec{k}\,',\omega). \tag{9.24}$$

We see that the T matrix is something like a renormalized scattering, including not just a single scattering event, but also summing up over all possible multiple scattering events. One can see from the diagrammatic expansion 9.2 that T is given by the Dyson equation

$$T_{\vec{k},\vec{k}\,'}(\omega)=U(\vec{k}-\vec{k}\,')+\sum_{\vec{k}\,''}U(\vec{k}-\vec{k}\,'')G_0(\vec{k}\,'',\omega)T_{\vec{k}\,'',\vec{k}\,'}(\omega). \tag{9.25}$$

Let us now look at an example of the T-matrix in use. We will take the same example we used earlier - a point scatterer at $\vec{x} = 0$, so $U_{\vec{q}} = u_0$ independent of $\vec{q}$. The Dyson equation for T then becomes

$$T_{\vec{k},\vec{k}'}(\omega) = U(\vec{k} - \vec{k}') + u_0 \sum_{\vec{k}''} G_0(\vec{k}'', \omega) T_{\vec{k}'',\vec{k}'}(\omega). \tag{9.26}$$

It is not difficult to see that in this case, T can not depend on $\vec{k}$ or $\vec{k}'$.

Exercise 9.3: (*) See this.

Therefore the equation becomes particular simple

$$T(\omega) = u_0 + u_0 F(\omega) T(\omega), \qquad \text{where } F(\omega) = \sum_{\vec{k}''} G_0(\vec{k}'', \omega), \tag{9.27}$$

which is easily solved to give

$$T(\omega) = \frac{u_0}{1 - u_0 F(\omega)}. \tag{9.28}$$

Now,

$$F(\omega) = \int \frac{d^d\vec{k}}{(2\pi)^d} \frac{1}{\omega - \xi_{\vec{k}} + i \,\mathrm{sign}\, \xi_{\vec{k}}}, \tag{9.29}$$

where we have written the expression for a general d-dimensions. Now, for any spherically symmetric spectrum $\epsilon(\vec{k}) = \epsilon(|\vec{k}|)$, one can rewrite this multi-dimensional integral as

$$F(\omega) \int d\epsilon \, \frac{N(\epsilon)}{\omega - \epsilon + i\delta \,\mathrm{sign}\, \epsilon}, \tag{9.30}$$

where $N(\epsilon)$ is the density of states.

Let us consider a fun example of single-particle behavior - i.e. the chemical potential $\mu = 0$. Therefore

$$F(\omega) = \int_0^{\Lambda} d\epsilon \, \frac{N(\epsilon)}{\omega - \epsilon + i\delta}, \tag{9.31}$$

where Λ is a high energy cut off.[2]

The density of states in d-dimensions looks like

$$N(\epsilon) \sim \epsilon^{d/2-1}, \tag{9.32}$$

---

[2] Occasionally we come across integrals which don't converge at high energy. This is known in field theory as an ultra-violet divergence (as opposed to an infra-red divergence which is one which happens at low energy). Now, in condensed matter these ultra-violet divergences don't matter too much (except when we start discussing universality - which we will not), as there is a natural high energy cut-off to the integrals anyway - the bandwidth. For a much more in-depth discussion of such divergences in quantum field theory in condensed matter, I highly recommend reading the Nobel acceptance speech by Wilson (or find any book about renormalization group).

which means that for small ω, we see that

$$F(\omega) \sim -\omega^{d/2-1}, \tag{9.33}$$

which diverges for $d \leq 2$. We therefore see that in dimensions less than two,

$$T(\omega) \sim \frac{u_0}{1 + u_0\, \omega^{d/2-1}} \tag{9.34}$$

has a pole for arbitrarily small attractive (negative) u_0. In other words, a delta-function potential well will have at least one bound state for arbitrarily small potential in dimensions less than two, whereas in three a finite critical u_0 is needed before a bound state is formed.

9.3. Disorder averaging

While the analysis we have carried out above is perfectly fine and makes sense for a single impurity, suppose we have a finite density of impurities (which although may be small - but it still means we have *a lot* of impurities).[3] The perturbation series, and therefore the Green function depends on the exact position of each of these impurities, in other words the exact microscopic properties depend on the exact *realization of disorder*.

Now, the typical macroscopic properties do not depend on this level of detail,[4] so we would like to find a way to *average over disorder realizations*, to find out what a typical lump of impure material will do. To make the problem more concrete, let

$$\hat{H} = \underbrace{\sum_{\vec{k}} \epsilon_{\vec{k}} \hat{c}^\dagger_{\vec{k}} \hat{c}_{\vec{k}}}_{=\hat{H}_0} + \hat{H}_{\text{disorder}}, \tag{9.35}$$

where $\hat{H}_{\text{disorder}}$ is of the same form as the scattering potential in the previous section:

$$\hat{H}_{\text{disorder}} = \int d^3\vec{x}\; U(\vec{x}) \hat{\Psi}^\dagger(\vec{x}) \hat{\Psi}(\vec{x}), \tag{9.36}$$

but we will now consider the scattering potential to have the specific form

$$U(\vec{x}) = \sum_{j=0}^{N_I} V(\vec{x} - \vec{R}_j). \tag{9.37}$$

---

[3] For example a crystal may be pure to one part in a billion (10^9). However, if we have a typical macroscopic amount of material, the mole $\approx 10^{24}$ atoms, this still means 10^{15} impurities. Which I would say is a lot. Of course in the thermodynamic limit which is so useful for calculations, $N \to \infty$ means an infinite number of impurities at any finite density.

[4] Although in mesoscopic systems, one can measure and calculate some things which do, such as universal conductance fluctuations - but this is another story.

Here, $V(\vec{x}-\vec{R}_j)$ is the atomic potential around each impurity, and $\vec{R}_j$ is the position of the impurity. The important point is that N_I is a macroscopic quantity, and the expectation value of some operator

$$\langle\hat{A}\rangle = A(\{\vec{R}_j\}) \tag{9.38}$$

in general depends on the position of all of the impurities. What we actually want to calculate is the *quenched average* of $\langle\hat{A}\rangle$:

$$\overline{\langle\hat{A}\rangle} = \int\prod_j \frac{d^3\vec{R}_j}{V}\langle\hat{A}(\{\vec{R}_j\})\rangle. \tag{9.39}$$

Be careful not to confuse the V in the denominator of this expression (which is the volume of the system - a normalization factor), with the atomic potential $V(\vec{R}_j)$.

9.3.1. Quenched averages and white noise potential

Let us first consider averages of the potential itself. Now, the average potential $\overline{U(\vec{x})}$ can just be absorbed into the definition of the chemical potential - so we will assume $\overline{U(\vec{x})}=0$. We will be far more interested in fluctuations around this average:

$$\overline{U(\vec{x})U(\vec{x}\,')} = \int\prod_j \frac{d^3\vec{R}_j}{V}\sum_i V(\vec{x}-\vec{R}_i)\sum_l V(\vec{x}\,'-\vec{R}_l). \tag{9.40}$$

Now, remembering that we have defined V in such a way that $\overline{U(\vec{x})}=0$, we see that the sum over l will give zero unless $l=i$. Hence

$$\begin{aligned}\overline{U(\vec{x})U(\vec{x}\,')} &= \sum_i\int\prod_j \frac{d^3\vec{R}_j}{V}\, V(\vec{x}-\vec{R}_j)V(\vec{x}\,'-\vec{R}_j)\\ &= \frac{N_I}{V}\int d^3\vec{R}\, V(\vec{x}-\vec{R})V(\vec{x}\,'-\vec{R}).\end{aligned} \tag{9.41}$$

Notice the prefactor $N_I/V = n_i$ is the density of impurities.

Now, suppose we have point impurities, $V(\vec{x}-\vec{R}) = u_0\delta(\vec{x}-\vec{R})$, then we see the fluctuations are white noise like

$$\overline{U(\vec{x})U(\vec{x}\,')} = n_i u_0^2\delta(\vec{x}-\vec{x}\,'). \tag{9.42}$$

Let us neglect any possible higher moments of the average disorder potential, and we will work assuming Eq. 9.42, along with $\overline{U(\vec{x})}=0$ defines our disorder potential.

For calculations, it is usually more convenient to work in momentum space, so let us take the Fourier transform of some of these expressions. The disorder potential

$$\begin{aligned} U(\vec{q}) &= \int d^3\vec{x}\; e^{-i\vec{q}\cdot\vec{x})} U(\vec{x}) \\ &= \sum_j e^{-i\vec{q}\cdot\vec{R}_j} \underbrace{\int d^3\vec{x}\; e^{-i\vec{q}\cdot(\vec{x}-\vec{R}_j)} V(\vec{x}-\vec{R}_j)}_{=V(\vec{q})} \\ &= V(\vec{q}) \sum_j e^{-i\vec{q}\cdot\vec{R}_j}. \end{aligned} \tag{9.43}$$

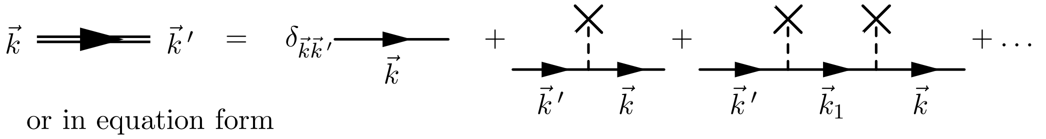
Obviously, $\overline{U(\vec{q})} = 0$. Let us now look at the correlations:

$$\begin{aligned} \overline{U(\vec{q})U(\vec{q}\,')} &= n_i u_0^2 \int d^3\vec{x} \int d^3\vec{x}\,'\; e^{-i\vec{x}\cdot\vec{q}} e^{-i\vec{x}\,'\cdot\vec{q}\,'} \delta(\vec{x}-\vec{x}\,') \\ &= n_i u_0^2 \int d^3\vec{x} e^{-i(\vec{q}+\vec{q}\,')\cdot\vec{x}} \\ &= n_i u_0^2\, \delta_{\vec{q}+\vec{q}\,'}. \end{aligned} \tag{9.44}$$

Now we have seen the properties of the averaged disorder, let us turn to the Green function.

9.3.2. Disorder averaging the Green function

As the perturbation is of the same form as the previous section, we can use the same diagrammatic expansion:



(9.45)

or in equation form

$$\begin{aligned} G(\vec{k},\vec{k}\,',\omega) = \delta_{\vec{k}\vec{k}\,'} G_0(\vec{k},\omega) + G_0(\vec{k}\,',\omega) U(\vec{k}-\vec{k}\,') G_0(\vec{k},\omega) \\ + \sum_{\vec{k}_1} G_0(\vec{k}\,',\omega) U(\vec{k}-\vec{k}_1) G_0(\vec{k}_1,\omega) U(\vec{k}_1-\vec{k}) G_0(\vec{k},\omega) + \dots \end{aligned} \tag{9.46}$$

So we can calculate by the perturbation series G for any particular realization of the disorder - but what we actually want to calculate is the quenched average, $\overline{G(\vec{k},\vec{k}\,',\omega)}$.

The zeroth order Green function

$$\overline{G_0(\vec{k},\omega)} = G_0(\vec{k},\omega), \tag{9.47}$$

is obviously unaffected by the disorder average procedure. The single scattering event however

$$\overline{G_0(\vec{k}\,',\omega) U(\vec{k}-\vec{k}\,') G_0(\vec{k},\omega)} = G_0(\vec{k}\,',\omega) \overline{U(\vec{k}-\vec{k}\,')} G_0(\vec{k},\omega) = 0, \tag{9.48}$$

i.e. the first order contribution to G is zero after performing the disorder average. However, now let us look at the second order term - a double scattering event:

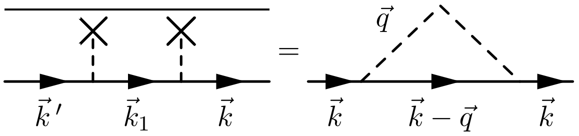
$$\begin{aligned}&\overline{G_0(\vec{k}\,',\omega)U(\vec{k}-\vec{k}_1)G_0(\vec{k}_1,\omega)U(\vec{k}_1-\vec{k})G_0(\vec{k},\omega)}\\ &\qquad\qquad = G_0(\vec{k}\,',\omega)G_0(\vec{k}_1,\omega)G_0(\vec{k},\omega)\,\underbrace{\overline{U(\vec{k}-\vec{k}_1)U(\vec{k}_1-\vec{k})}}_{}\,.\end{aligned} \tag{9.49}$$

Now, from our definition of the disorder average, Eq. 9.44, we see that

$$\overline{U(\vec{k}-\vec{k}_1)U(\vec{k}_1-\vec{k})} = n_i u_0^2 \delta(\vec{k}-\vec{k}_1+\vec{k}_1-\vec{k}\,') = n_i u_0^2 \delta(\vec{k}-\vec{k}\,'). \tag{9.50}$$

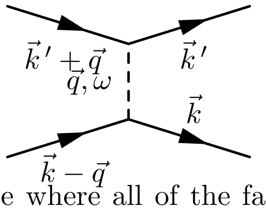
The most important consequence of this expression is the delta function - meaning momentum is *now conserved again.* In other words, while any particular realization of the disorder breaks translational invariance, the average over all realizations restores the translational invariance.

This restoration of momentum conservation can also be represented diagramatically (where the line above the first diagram indicates a disorder average):



(9.51)

In a higher order diagram, we see that the same thing will happen: to get a non-zero result, we have to pick pairs of disorder crosses to merge together (with a strength $n_i u_0^2$) giving momentum conservation for the resultant dashed-line which now links with fermions at both ends. This is exactly like an effective interaction:



$$V_{\text{eff}}(\vec{q},\omega) = -i\,n_i u_0^2 \delta(\omega = 0). \tag{9.52}$$

Let us see where all of the factors in Eq. 9.52 come from. The factor $n_i u_0^2$ should be obvious enough, so we look at the other two factors:

1. The factor $\delta(\omega = 0)$. In other words, the 'interaction' line can exchange no-energy. If we go back to the diagrams before disorder averaging, energy is conserved at each individual scattering cross. When we average over the disorder and pair up these crosses, we don't change this rule - if we look back to Eq. 9.49, we see that all Green functions are at the same energy.

   A better way to understand this is to go back to the time representation - we take two scattering events which can both happen at any time, not necessarily the same. The independence of the scattering on the relative times is what leads to the delta function in energy space.

   We call an interaction independent of the relative times (such as this one) an *infinitely retarded* (effective) interaction.

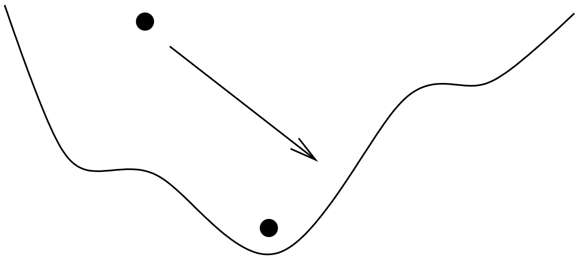


Figure 9.1.: Adding a second electron, it also wants to go into the lowest energy well - which could be viewed as an *attraction* to the first electron.

2. What about the factor $(-i)$? Technically, this is here so we can use the standard diagrammatic perturbation theory for interactions that we learned in Lecture 5. In the standard theory, we multiply an n^{th} order diagram by a factor i^n. However, we know from Eq. 9.49 that no such factors of i appear in the disorder diagrams, so we put a factor in the effective interaction to counteract this.

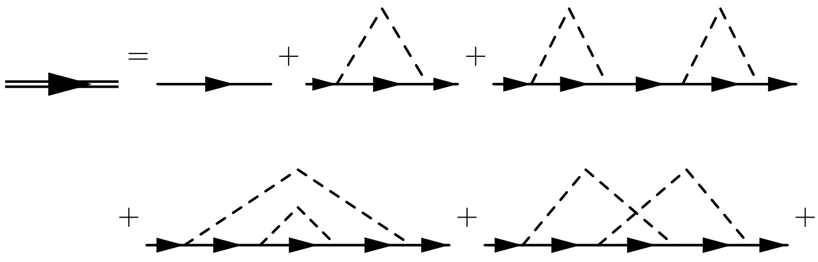
   So what does an imaginary effective interaction mean? Well, actually it is just an artifact of the perturbation theory (and doesn't appear if we do the calculation in imaginary time - see Lecture 11). In the standard perturbation theory, suppose instead of associating a factor of i^n with the order of the diagram, we simply associated a factor of i with each internal time integration. For the standard Coulomb interaction, this wouldn't make any difference - a diagram of order n has n internal times to integrate over. However, for this infinitely retarded effective interaction, we have two internal times rather than one, so in this language the factor of i goes into the second time integral and the only factor left in the effective interaction is -1, i.e. it is an effective attractive interaction.

Let us make a physical picture for this *effective attractive infinitely retarded interaction.* Consider a small region of the disordered potential as shown in Fig. 9.1. When one electron is added, it goes into the lowest energy state, which will be, roughly speaking, around the region where the disorder potential is lowest. Now suppose a second electron is added. It wants to go into the lowest energy state remaining, which is also around the same region as the first electron - in other words it is *attracted* to the first. Notice that in this effective attraction, it doesn't matter if the first electron is still there when we add the second electron - hence the infinite retardation.

9.3.3. Disorder diagrams

Now that we have derived that a disordered system, after disorder averaging is equivalent to an effective interaction, we can use the same diagrammatic expansions we learned about earlier in the course. For example, the Green function

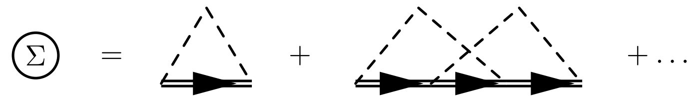
$\overline{G(\vec{k},\omega)} =$



(9.53)

We could write this in terms of the self-energy, $\Sigma(\vec{k},\omega)$:

$\overline{\Sigma(\vec{k},\omega)} =$



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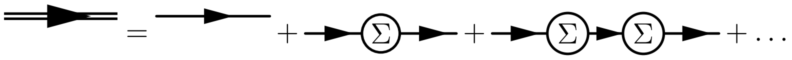
As usual, $G(\vec{k},\omega)$ is given in terms of the self-energy by the Dyson series:



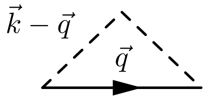
(9.55)

which is solved to give the usual form

$$G(\vec{k},\omega) = \frac{1}{\omega - \xi_{\vec{k}} - \Sigma(\vec{k},\omega) + i\delta \operatorname{sign} \xi_{\vec{k}}}. \tag{9.56}$$

Let us now calculate the self-energy, Σ, to lowest order, for the same case we have been dealing with - a collection of point scatterers. As we worked out previously for this case, $V_{\text{eff}} \sim -i n_i u_0^2$, which is independent of momentum. It is not hard to see therefore that the self energy $\Sigma = \Sigma(\omega)$ only:

$\Sigma(\omega) =$



$$\begin{aligned}
&= n_i u_0^2 \int \frac{d^3\vec{q}}{(2\pi)^3} G_0(\vec{q},\omega) \\
&= n_i u_0^2 \int \frac{d^3\vec{q}}{(2\pi)^3} \frac{1}{\omega - \xi_{\vec{q}} + i\delta \operatorname{sign} \xi_{\vec{q}}} \\
&= n_i u_0^2 \int d\epsilon \frac{N(\epsilon)}{\omega - \epsilon + i\delta \operatorname{sign} \epsilon}.
\end{aligned} \tag{9.57}$$

Now we come to the question of how to actually do this integral. In general, this isn't easy. However, let us use two pieces of physical intuition to help us:

1. Let us assume the disorder is weak - so that only states near the Fermi surface will be able to scatter. In this case, we can approximate the factor $N(\epsilon)$ by it's value at the Fermi surface N_F. We can also stretch the limits of the integral over ϵ to $\pm\infty$, again because we know anything physical is happening at the Fermi surface and not at these far away energies.
2. Let us bear in mind that after evaluating the integral, we will want to calculate a physically observable quantity, which will be related to retarded Green function $G_R(\vec{k},\omega) = G(\vec{k},\omega - i\delta)$. As there is no energy integrals in our expression, we can make this analytic continuation before evaluating the integral.[5] Therefore we will treat ω itself as a complex variable (with an imaginary part), which means we can ignore the $i\delta \operatorname{sign}\epsilon$.

We can now evaluate the integral:

$$\begin{aligned}\Sigma(\omega) &= n_i u_0^2 N_F \int_{-\infty}^{\infty} d\epsilon \, \frac{1}{\omega - \epsilon} \\ &= -niu_0^2 N_F \left[i\pi \operatorname{sign}(\operatorname{Im}\omega)\right] = -i\frac{1}{2\tau}\operatorname{sign}(\operatorname{Im}\omega),\end{aligned} \tag{9.58}$$

where the elastic scattering rate, τ is given by

$$\tau^{-1} = 2\pi n_i u_0^2 N_F. \tag{9.59}$$

Let me give without justification a few notes on the approximations we have made to achieve this result:[6]

- The extension of the limits of integration gives errors of the order $1/\epsilon_F\tau$, which is small for weak scattering.
- Replacing $N(\epsilon)$ by N_F will in practice affect only the real part of the integral. This can be absorbed into a change in the chemical potential, so isn't important anyway.

Therefore, we see that the Green function is given by

$$G(\vec{k},\omega) = \frac{1}{\omega - \xi_{\vec{k}} + i\frac{1}{2\tau}\operatorname{sign}\left[\operatorname{Im}\omega\right]}, \tag{9.60}$$

and from this, we can obtain the spectral function for the weakly disordered free Fermi gas

$$A(\vec{k},\omega) = -\frac{1}{\pi}\operatorname{Im} G(\vec{k},\omega - i\delta) = \frac{1}{\pi}\frac{(2\tau)^{-1}}{(\omega - \xi_{\vec{k}})^2 + (2\tau)^{-2}}. \tag{9.61}$$

---

[5] If there were internal energy integrals, we must remember that these integrals are strictly along the real axis - which is why these integrals and adding imaginary parts to external energies do not in general commute.

[6] As usual, for more details see the literature.

We see that the original delta function has been *broadened* - to a Lorentzian of width $1/\tau$. In other words, the electron now has a lifetime τ due to the disorder (hence the name *elastic scattering time*).

Let me finish our brief exploration into the world of disorder with a couple more comments about the result we have just derived.

- Suppose we substitute the Green function we have just derived, Eq. 9.60 into the equation for the self energy, Eq. 9.3.3, in other words, we want to calculate the self-consistent self-energy:

  $$\Sigma(\vec{k},\omega) =$$

  $$= n_i u_0^2 \int \frac{d^3\vec{q}}{(2\pi)^3} G(\vec{q},\omega) = -i\frac{1}{2\tau}\mathrm{sign}\,(\mathrm{Im}\,\omega). \tag{9.62}$$

  This is what we previously calculated as the self-energy, and most importantly, is the self-energy included in G in this calculation, i.e. our calculation of G is already self-consistent to this level of perturbation theory.

- If we evaluate the next self energy diagram, we will obtain

  $$\sim \left(\frac{1}{\tau}\right)^2 \times \frac{1}{\epsilon_F\tau}. \tag{9.63}$$

  This factor, which may also be written

  $$\frac{1}{\epsilon_F\tau} = \frac{1}{k_F l} \tag{9.64}$$

  where $l = v_F\tau$ is the mean free path, gives the size of the *quantum corrections* to classical conductivity. In other words, when we come to look at transport, we will see that the diagrams we have calculated will give the semi-classical Drude formula, this diagram whose size is controlled by the (hopefully) small parameter, $1/k_F l$, gives weak localization (quantum) corrections to the Drude formula.

There is a lot more I could say about disordered systems - one cannot do justice to this vast subject area in one lecture. However, I hope in this lecture I have given you a feel for how things work, so that the interested amongst you you can read more specialized textbooks with ease. I will return however to perhaps one of the most important applications of disorder diagrams which is in calculating transport properties. We will come back to this in Lecture 12, as it is something far easier done using finite-T Green functions (somewhat paradoxically, this is true, even at $T = 0$). Other than this though, I refer you to the literature for more information.

10. A little bit about phonons

So far, we have been dealing with just the electrons in the systems - the ions we have assumed are a static background, doing nothing more than canceling out the total charge of the electrons. However, the crystal lattice itself can have excitations - which we call *phonons*. In this lecture, we will first see how to make a quantum-field theory of phonons, then we will look at how phonons couple to the electronic degrees of freedom, making an effective interaction.[1] We then have a brief overview of how Feynman diagrams may be used in this context.

10.1. Normal modes and a quantized theory of phonons

Let us consider a model of one dimensional phonons. The atoms have equilibrium positions x_i - which is the minimum of the potential caused by the chemical bonds of the neighboring atoms. Around this equilibrium position, we can expand this potential, the lowest non-zero term will be the quadratic one, which gives a linear restoring force if the atom moves from it's equilibrium position. This is shown schematically in Fig. 10.1. We can therefore write down the Hamiltonian of the atoms

$$\hat{H} = \sum_i \frac{\hat{p}_i}{2M} + \frac{\kappa}{2} \sum_i (\hat{x}_i - \hat{x}_{i+1})^2, \tag{10.1}$$

where according to the usual rules of quantum mechanics, the momentum and the position operator do not commute:

$$[\hat{x}_n, \hat{p}_m] = i\delta_{nm}. \tag{10.2}$$

---

[1] Which was made famous by the BCS theory of superconductivity.

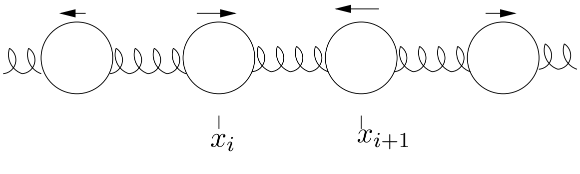


Figure 10.1.: A schematic of a model of a one-dimensional crystal lattice. The atoms can move from their equilibrium positions, but there is a harmonic restoring force, modeled by a spring between atoms.

We can diagonalize this Hamiltonian by going to the *normal modes*, which in this case are given simply by the Fourier series

$$\hat{x}_n = \frac{1}{N} e^{ikn} \hat{x}_k, \qquad \hat{x}_k = \sum_n e^{ikn} \hat{x}_n. \tag{10.3}$$

Then

$$\begin{aligned} \frac{\kappa}{2} \sum_i (\hat{x}_i - \hat{x}_{i+1})^2 &= \frac{\kappa}{2} \sum_k \hat{x}_k \hat{x}_{-k} \left(2 - e^{ika} - e^{-ika}\right) \\ &= \frac{M}{2} \sum_k \omega_k^2 \hat{x}_k \hat{x}_{-k}, \end{aligned} \tag{10.4}$$

where

$$\omega_k^2 = \frac{2\kappa}{M} \left(1 - \cos k\right). \tag{10.5}$$

In the k basis, the Hamiltonian now looks like

$$\hat{H} = \frac{1}{2M} \sum_k \hat{p}_k \hat{p}_{-k} + \frac{M}{2} \sum_k \omega_k^2 \hat{x}_k \hat{x}_{-k}. \tag{10.6}$$

with the commutation relations

$$[\hat{x}_k, \hat{x}_{k'}] = i\delta_{kk'}. \tag{10.7}$$

The astute amongst you will have noticed that this is now a sum over independent harmonic oscillators (labelled by different k's). We can therefore write the raising and lowering operators

$$\begin{aligned} \hat{a}_k &= \left(\frac{M\omega_k}{2}\right)^{1/2} \left(\hat{x}_k + \frac{i}{m\omega_k} \hat{p}_{-k}\right), \\ \hat{a}_k^\dagger &= \left(\frac{M\omega_k}{2}\right)^{1/2} \left(\hat{x}_{-k} - \frac{i}{m\omega_k} \hat{p}_k\right). \end{aligned} \tag{10.8}$$

which have the commutation relation

$$[\hat{a}_k, \hat{a}_{k'}^\dagger] = \delta_{kk'}. \tag{10.9}$$

These are also the commutation relations of bosons - so one can view phonons in two equivalent ways. One can view a phonon creation operator as a raising operator for one of the normal modes of the crystal lattice. On the other hand, one can view it as a creation operator for a bosonic particle. This duality between particles and normal modes is the very essence of quantum field theory.

Having written down these operators, we can then write the Hamiltonian in the form

$$\hat{H} = \sum_k (\hat{a}_k^\dagger \hat{a}_k + \underbrace{1/2}_{\text{zero point energy}}). \tag{10.10}$$

Exercise 10.1: (*) The above derivation has been somewhat succinct. Fill in the missing steps.

In general, when we are in three dimensions, and have the possibility of more than one atom per unit cell, the quantized phonon Hamiltonian is

$$\hat{H}_{ph} = \sum_{\vec{k}\lambda} \omega_{\vec{k}\lambda} \hat{a}^{\dagger}_{\vec{k}\lambda} \hat{a}_{\vec{k}\lambda}, \tag{10.11}$$

where we have omitted writing the (constant) zero point energy.

10.2. Electron-phonon coupling and the Fröhlich Hamiltonian

Having obtained the Hamiltonian for phonons, we can now turn our thoughts to how the phonons interact with the electrons. The general form of the Hamiltonian is

$$\hat{H} = \hat{H}_{ph} + \hat{H}_e + \hat{H}_{ep} \tag{10.12}$$

where $\hat{H}_{ph}$ is the phonon Hamiltonian we have just derived, $\hat{H}_e$ is the electronic Hamiltonian that we have spent most of this course looking at, and $\hat{H}_{ep}$ is the coupling between them. Without much thought, we see that we can write $\hat{H}_{ep}$ as

$$\hat{H}_{ep} = \sum_{\sigma} \int d^3\vec{r}\, \tilde{V}(\vec{r}) \hat{\Psi}^{\dagger}_{\sigma}(\vec{r}) \hat{\Psi}_{\sigma}(\vec{r}), \tag{10.13}$$

where $\hat{\Psi}^{\dagger}$ and $\hat{\Psi}$ are the usual electronic field operators and $\tilde{V}(\vec{r})$ is the difference in the potential between the current state and the ground state of the lattice. This can be written as

$$\begin{aligned} \tilde{V}(\vec{r}) &= \sum_i V\left(\vec{r} - (\vec{r}_i^{(0)} + \vec{x}_i)\right) - V(\vec{r} - \vec{r}_i^{(0)}) \\ &= \sum_i \vec{x}_i \nabla V(\vec{r} - \vec{r}_i^{(0)}), \end{aligned} \tag{10.14}$$

where x_i are the displacement of the atoms from the phonons as discussed in the previous section, $\vec{r}_i^{(0)}$ are the equilibrium positions of the atoms, and $V(\vec{r})$ is the atomic potential.[2]

---

[2] For an ionic crystal with an ionic charge of q,

$$V(\vec{r}) = \frac{4\pi e q}{r}, \tag{10.15}$$

for other sorts of chemistry, $V(\vec{r})$ will be different. For the general theory, we don't need to know the details of this, to estimate electron phonon couplings, we will of course have to know the details - which is usually the job for computational techniques such as Density Functional Theory (DFT). Analytically, one will usually treat the parameters $g_{\vec{k}\lambda}$ as empirical, and not worry about how to calculate them.

Now, one can write

$$V(\vec{r}) = \int \frac{d^3\vec{k}}{(2\pi)^3}\, V(\vec{k}) e^{i\vec{k}\cdot\vec{r}}, \tag{10.16}$$

so

$$\nabla V(\vec{r}) = i \int \frac{d^3\vec{k}}{(2\pi)^3}\, \vec{k}\, V(\vec{k}) e^{i\vec{k}\cdot\vec{r}}, \tag{10.17}$$

and therefore

$$\tilde{V}(\vec{r}) = i \int \frac{d^3\vec{k}}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, V(\vec{k})\, \vec{k} \cdot \left[\sum_i \vec{x}_i e^{-i\vec{k}\cdot\vec{r}_i^{(0)}} \right]. \tag{10.18}$$

Now, remembering that

$$\vec{x}_i = \frac{1}{N} \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}_i^{(0)}}\, \vec{x}_{\vec{q}}, \tag{10.19}$$

then we can write

$$\sum_i \vec{x}_i e^{-i\vec{k}\cdot\vec{r}_i^{(0)}} = \frac{1}{N} \sum_{\vec{q}} \vec{x}_{\vec{q}} \underbrace{\sum_i e^{i(\vec{q}-\vec{k})\cdot\vec{r}_i^{(0)}}}_{=N \sum_{\vec{G}} \delta(\vec{q}-\vec{k}-\vec{G})} \tag{10.20}$$

where $\sum_{\vec{G}}$ is the sum over all reciprocal lattice vectors. Hence

$$\tilde{V}(\vec{r}) = i \int \frac{d^3\vec{k}}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, V(\vec{k})\, \vec{k} \cdot \sum_{\vec{G}} \vec{x}_{\vec{k}+\vec{G}}. \tag{10.21}$$

If we assume that it is the long-wavelength (low energy) phonons that are most important, we can consider only the first Brioullin zone, and therefore extracting an expression for $\hat{x}$ from Eq. 10.8, we see that

$$\tilde{V}(\vec{r}) = \int \frac{d^3\vec{k}}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, \underbrace{g_{\vec{k}\lambda} \left(\hat{a}_{\vec{k}\lambda} + \hat{a}^\dagger_{\vec{k}\lambda} \right)}_{=\tilde{V}(\vec{q})}. \tag{10.22}$$

Exercise 10.2: (*) In terms of our previously defined objects, what is $g_{\vec{k}\lambda}$?

We can therefore write down the coupling between electrons and phonons:

$$\begin{aligned} \hat{H}_{ep} &= \sum_{\vec{q}\lambda} g_{\vec{q}\lambda} \hat{\rho}(\vec{q}) \left(\hat{a}_{\vec{q}\lambda} + \hat{a}^\dagger_{\vec{q}\lambda} \right) \\ &= \sum_{\vec{k}\vec{q}\lambda} g_{\vec{q}\lambda} \hat{c}^\dagger_{\vec{k}+\vec{q}} \hat{c}_{\vec{k}} \left(\hat{a}_{\vec{q}\lambda} + \hat{a}^\dagger_{\vec{q}\lambda} \right). \end{aligned} \tag{10.23}$$

The first term here corresponds to an electron absorbing momentum $\vec{q}$, and destroying a phonon in the process, in the second term the electron transfers a momentum $\vec{q}$ to a phonon.

We can now put all of this together to write the generic Hamiltonian for cohabiting electrons and phonons, known as the *Fröhlich Hamiltönian*:

$$\boxed{\begin{aligned} \hat{H} &= \hat{H}_e + \hat{H}_{ph} + \hat{H}_{ep} \\ \hat{H}_e &= \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}^\dagger_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma} \\ \hat{H}_{ph} &= \sum_{\vec{q}\lambda} \omega_{\vec{q}\lambda} \left(\hat{a}^\dagger_{\vec{q}\lambda} \hat{a}_{\vec{q}\lambda} + \frac{1}{2} \right) \\ \hat{H}_{ep} &= \sum_{\vec{k}\vec{q}\lambda} g_{\vec{q}\lambda} \hat{c}^\dagger_{\vec{k}+\vec{q}} \hat{c}_{\vec{k}} \left(\hat{a}_{\vec{q}\lambda} + \hat{a}^\dagger_{\vec{q}\lambda} \right). \qquad (10.24) \end{aligned}}$$

Just as a reminder, $\hat{c}^\dagger, \hat{c}$ are the electronic (fermion) creation and annihilation operators, $\hat{a}^\dagger, \hat{a}$ are the phononic (boson) creation and annihilation operators, $\epsilon_{\vec{k}}$ is the electronic free particle spectrum, $\omega_{\vec{q}\lambda}$ is the phonon spectrum and $g_{\vec{q}\lambda}$ are the electron phonon couplings.

10.3. Green functions for phonons

Having arrived at a Hamiltonian, we will now look at how we might go about solving it. We will start with an all to brief look at Green function for phonons. Now, in analogy with the electron Green function, we might be tempted to define the phononic one as

$$\langle T\, \hat{a}_{\vec{q}\lambda}(t) \hat{a}^\dagger_{\vec{q}\lambda} \rangle. \tag{10.25}$$

While there is nothing intrinsically wrong with this, let us remember that the vertex in the electron-phonon interaction is

$$\left(\hat{a}_{\vec{q}\lambda} + \hat{a}^\dagger_{\vec{q}\lambda} \right) = \hat{\phi}_{\vec{q}\lambda}, \tag{10.26}$$

where this equation serves as the definition of the vertex operator $\hat{\phi}$. Let us therefore, in anticipation of what will come shortly, define the phonon Green function $D_0(\vec{q}, t)$ as

$$D_0(\vec{q}, t) = -i \langle T\, \hat{\phi}_{\vec{q}}(t) \hat{\phi}_{-\vec{q}}(0) \rangle. \tag{10.27}$$

For clarity, we have dropped the phonon branch index, λ. In fact, in almost all problems involving phonons, only one branch will prove to be the most important, so one rarely has to include this index in calculations.

Exercise 10.3: (*) Completely identical to the calculation made for Fermions in Lecture 3, show that (within the Heisenberg representation)

$$\begin{aligned} \hat{a}_{\vec{q}}(t) &= e^{i\omega_{\vec{q}}t}\hat{a}_{\vec{q}}, \\ \hat{a}^{\dagger}_{\vec{q}}(t) &= e^{-i\omega_{\vec{q}}t}\hat{a}^{\dagger}_{\vec{q}}. \end{aligned} \tag{10.28}$$

One should also note that for most systems, $\omega_{\vec{q}} = \omega_{-\vec{q}}$.

For bosons without conserved particle number (such as phonons), the ground state is the state with no particles present, so

$$\langle \hat{a}_{\vec{q}}\hat{a}^{\dagger}_{\vec{q}}\rangle = 1, \qquad \langle \hat{a}^{\dagger}_{\vec{q}}\hat{a}_{\vec{q}}\rangle = 0. \tag{10.29}$$

Therefore, putting all of this together, we get the result

$$D_0(\vec{q},t) = -i\left[\theta(t)e^{-i\omega_{\vec{q}}t} + \theta(-t)e^{i\omega_{\vec{q}}t}\right]. \tag{10.30}$$

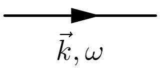
If we make the Fourier transform into energy space:

$$\begin{aligned} D_0(\vec{q},\omega) &= \int_{-\infty}^{\infty} dt\; D_0(\vec{q},t) \\ &= \int_0^{\infty} e^{i(\omega-\omega_{\vec{q}})t}dt + \int_{-\infty}^{0} e^{i(\omega+\omega_{\vec{q}})t}dt \\ &= \frac{1}{\omega-\omega_{\vec{q}}+i\delta} - \frac{1}{\omega+\omega_{\vec{q}}-i\delta} \\ &= \frac{2\omega_{\vec{q}}}{\omega^2-\omega_{\vec{q}}^2+i\delta}. \end{aligned} \tag{10.31}$$

10.4. Phonon diagrams

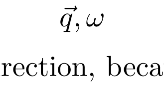
We can now treat $\hat{H}_0 = \hat{H}_e + \hat{H}_{ph}$ as the base non-interacting Hamiltonian, and $\hat{H}_{ep}$ as the perturbation in which we will perform the diagrammatic expansion. Going through the usual S-matrix expansion, we will see that our diagrams now have the following ingreedients:

- The electron propagator:



$$= G_0(\vec{k},\omega). \tag{10.32}$$

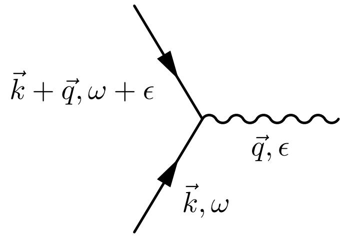
- The phonon propagator:



$$= D_0(\vec{q},\omega). \tag{10.33}$$

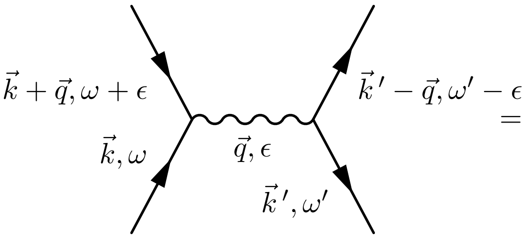
Note that this line has no direction, because $D_0(\vec{q},\omega) = D_0(-\vec{q},\omega) = D_0(\vec{q},-\omega)$.

- The vertex:



$$= -g_{\vec{q}\lambda}. \tag{10.34}$$

One could equally well imagine *integrating out the phonons* and leaving a model of just the electronic degrees of freedom, with an effective interaction:



$$= -g^2_{\vec{q}\lambda} D_0(\vec{q}, \epsilon) = -V_{\text{eff}}(\vec{q}, \epsilon). \tag{10.35}$$

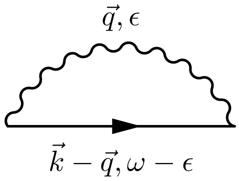
Let us make a few notes about the effective interaction V_{eff} arising from phonons:

- V_{eff} has a very strong frequency dependence. This shows the retarded nature of the effective interaction (c.f. the instantaneous Coulomb interaction which has no frequency dependence whatsoever, and the infinitely retarded effective interaction from disorder averaging - which has a delta function in it's frequency dependence). It is physically intuitive that the interaction should be retarded: phonons travel much slower than electrons, therefore interaction at a distance is far from instantaneous.
- There is only a weak dependence on momentum. This arises due to the spatially local nature (over only one or two lattice spacing) of the atomic potential, i.e. of the interaction between the phonons and the electrons.
- At a fixed frequency $\omega < \omega_D$ where ω_D is the Debye frequency of the phonons, $D_0(\vec{q}, \omega)$ changes sign as a function of $\vec{q}$. The residual low-energy attraction is usually *attractive*. This is responsible for Cooper pairing and the BCS theory of superconductivity.

Unfortunately, the scope of this course will not allow us to look at any examples of calculations in detail, so let us instead resort to drawing some of the diagrams which may be physically relevant.

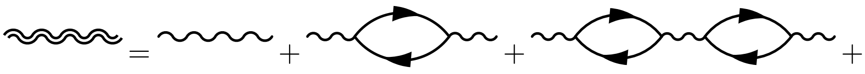
- First, let us note that as with every other sort of perturbation, one can look at the self energy of the electron:

$$\Sigma(\vec{k}, \omega) =$$



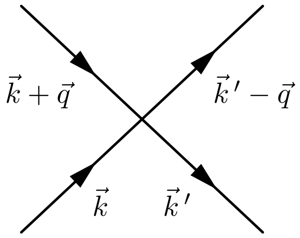
$$= \sum_{\vec{q}} \int \frac{d\epsilon}{2\pi}\, g^2_{\vec{q}} G_0(\vec{k} - \vec{q}, \omega - \epsilon) D_0(\vec{q}, \epsilon). \tag{10.36}$$

- One can also look at the screening of phonons:

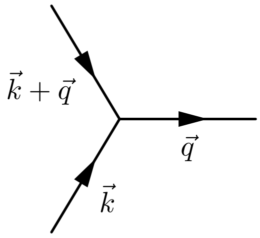


(10.37)

- Note that we described phonons using the harmonic approximation, where the restoring potential in the phonon Hamiltonian was $\propto (\hat{x}_i - \hat{x}_{i+1})^2$. Higher order terms will give a direct interaction between phonons, for example $(\hat{x}_i - \hat{x}_{i+1})^4$:



- This is even more interesting if the lattice is non-centrosymmetric, for example the Hexagonal lattice, when one can also get terms $(\hat{x}_i - \hat{x}_{i+1})^3$:



  In this case, one can have two phonons meeting and combing into one, or conversely, one phonon splitting itself into two.

In general, one can of course have both phonons and the Coulomb interaction, or both Coulomb and disorder - or any combination you want, in which case all of the Feynman rules may be combined. This can create some really quite artistic diagrams. However, this ends the first part of this course, and ends our discussion of zero temperature Green functions and diagrammatic expansions. We will now go on to have a brief look at how all of this is modified if we want to include the effects of finite temperature in our calculations.

11. Finte-T Green functions

So far, we have been dealing strictly with ground state properties of models, i.e. at zero temperature. Most experiments are not done at $T = 0$. In this lecture, we will learn how to generalize the theory to finite temperature. As a bonus, it will turn out that these finite-T Green functions are often easier to deal with than their zero temperature counterparts, even at $T = 0$.

11.1. Thermodynamic averaging

Let us define the thermodynamic average of an operator $\hat{A}$ as

$$\langle\langle \hat{A} \rangle\rangle = \frac{\operatorname{Tr} e^{-\beta \hat{H}} \hat{A}}{\operatorname{Tr} e^{-\beta \hat{H}}} = \frac{\sum_n e^{-\beta E_n} \langle n|\hat{A}|m\rangle}{\sum_n e^{-\beta E_n}}. \tag{11.1}$$

Here, $\beta = 1/T$ (note that the Boltzmann constant $k_B = 1$), and the trace (or equivalently, $\sum_n$) is over all eigenstates of the system. This is a double averaging procedure: first there is the quantum average $\langle \ldots \rangle$, and then there is the thermodynamic average $\operatorname{Tr} e^{-\beta \hat{H}}[\ldots]$.

Let me note a couple of important things before we proceed:

- $Z = \operatorname{Tr} e^{-\beta \hat{H}}$ is the partition function of the system.
- We will always be working in the grand canonical ensemble, i.e. let us replace

$$\hat{H} \to \hat{H} - \mu \hat{N}. \tag{11.2}$$

I haven't written this chapter yet.

12. Transport and the Kubo formulae

I haven't written this chapter yet.

13. Finale

While I hope this set of lectures has given you a pleasant introduction into the world of many body physics and diagrammatic perturbation theory, I must finally mention some of the important topics which did not get included. Within the methods side, the most significant subject for which I unfortunately did not have time is that of path integrals. On the applications side, I talked very little about phonons and did not mention superconductivity at all. This omission is not an oversight, but merely a factor of time, as my intention was always to introduce the subject area gently, and bring the student to a level where he or she will be able to read more specialized textbooks without difficulty.

A. Complex integration

This appendix serves as a reminder of the basic complex analysis that will be necessary to evaluate some of the integrals that arise in this course in quantum field theory. As it is expected the reader has already completed an undergraduate course in complex analysis, this appendix merely gives an overview of the necessary definitions and theorems followed by many exercises for the astute reader to work through. If none of this feels familiar, I recommend finding your favorite textbook on mathematics for physicists for further reading.

A.1. Analytic Functions

Consider a function $f(z) = u(x + \mathrm{i}y) + \mathrm{i}v(x + \mathrm{i}y)$. The derivative

$$f'(z) = \lim_{\delta z \to 0} \frac{f(z + \delta z) - f(z)}{\delta z} \tag{A.1}$$

must be independent of the path taken to approach $\delta z \to 0$. This gives rise to the Cauchy-Riemann conditions

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \; \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x} \tag{A.2}$$

If these conditions are satisfied, the function $f(z)$ is **analytic**.

Exercise A.1: Using the Cauchy-Riemann condition, demonstrate which of the following functions are analytic:

1. $f(z) = z^2$
2. $f(z) = |z|^2$
3. $f(z) = e^{\mathrm{i}z}$
4. $f(z) = 1/(z - a)$

A.2. The Residue Theorem

Cauchy's theorem states that

$$\oint_C f(z) dz = 0 \tag{A.3}$$

For any f(z) that is analytic on and inside the closed contour C. (Exercise: can you show this using Green's theorem in the plane and the Cauchy Riemann conditions?)

Suppose $f(z)$ has isolated singularites within the contour C (i.e. no branch cuts). These are called *poles* of the function. At such a point, the function can be expanded in a Laurent series as

$$f(z) = \frac{b_n}{(z-z_0)^n} + \frac{b_{n-1}}{(z-z_0)^{n-1}} + \ldots + \frac{b_1}{z-z_0} + a_0 + a_1(z-z_0) + a_2(z-z_0)^2 + \ldots \tag{A.4}$$

where n is the *order* of the pole. If $n = 1$, it is called a *simple pole.* If the singular part of the series does not terminate, i.e. $n \to \infty$, then z_0 is called an *essential* singularity, for example the point $z = 0$ in the function $f(z) = e^{-1/z^2}$. We will not deal with essential singularites.

The term b_1 is called the *residue* of the pole. This is important because of the following result. Suppose C is a circle of radius r centred on z_0, i.e. $z = z_0 + re^{\mathrm{i}\theta}$. Then

$$\oint_C \frac{dz}{(z-z_0)^n} = \int_0^{2\pi} \frac{\mathrm{i}re^{\mathrm{i}\theta}d\theta}{[re^{\mathrm{i}\theta}]^n} = \begin{cases} 2\pi\mathrm{i} & n = 1 \\ 0 & \text{otherwise} \end{cases} \tag{A.5}$$

The integral around C is always in the counterclockwise direction.

These results lead to the *Residue Theorem*:

$$\oint_C f(z)dz = 2\pi\mathrm{i} \cdot \text{sum of residues of } f(z) \text{ inside } C. \tag{A.6}$$

If z_0 is a simple pole, then the residue is given by

$$R(z) = \lim_{z \to z_0} (z - z_0) f(z). \tag{A.7}$$

If it is a multiple pole (of order n), the expression is a little more complicated

$$R(z) = \frac{1}{(n-1)!} \frac{d^{n-1}}{dz^{n-1}} \{(z-z_0)^n f(z)\} \tag{A.8}$$

Exercise A.2: 1. Determine the nature of the singularties and the residue at each one of the following functions

a) $\frac{1}{z^2+a^2}$

b) $\sin(z)/z^2$

c) $\cos(z)/z^2$

d) $\frac{e^{\mathrm{i}z}}{z^2-a^2}$

e) $1/\cos(2\pi z)$

2. Let C be the unit circle centred at the origin. Evaluate (assume $a > 0$)

a) $\oint \frac{dz}{z^2+a^2}$

b) $\oint \frac{e^{iz}dz}{z^2+a^2}$

c) $\oint \frac{zdz}{(z-1/2)^2-a^2}$

d) $\oint \frac{zdz}{(z-1/2)^2+a^2}$

e) $\oint \frac{dz}{\cos(2\pi z)}$

f) $\oint \frac{e^{iz}dz}{\cos(2\pi z)}$

A.3. Using the Residue theorem to evaluate definite integrals

There are a number of common ways one can evaluate definite integrals along the real axis by contour integration.

- To integrate some function $f(cos(\theta), sin(\theta)$ over a full period $0 < \theta < 2\pi$, one can make the substitution $z = e^{\mathrm{i}\theta}$ and integrate around a unit circle. In this case $dz = \mathrm{i}zd\theta$, $\cos\theta = (z + 1/z)/2$, $\sin\theta = (z - 1/z)/2\mathrm{i}$, and so on.
- To integrate a function $f(z)$ over the whole real line where $f(z) \to 0$ sufficiently fast as $|z| \to \infty$, then one can *complete the contour* in either the upper or lower half plane (it doesn't matter which). The part at infinity doesn't count towards anything so this contour integral is equivalent to the original one.
- Integrating a function $f(z)e^{\mathrm{i}az}$. If $a > 0$ this can be completed in the upper half plane. If $a < 0$, it can be completed in the lower half plane.
- Sometimes one has to be more inventive with contours. Consider as an example the function $f(z) = 1/\cosh(z)$ to be integrated (along the real line) from $-\infty < z < \infty$. Notice the symmetry $f(z + \mathrm{i}\pi) = -f(z)$, so integrating along a box shaped contour along the real axis, up to $\mathrm{i}\pi$, back along the line $\Im(z) = \pi$ and then down again to the real axis will be twice the integral we want because the sides won't count towards anything.

There is one last thing to be said, about if the path of the integral goes through one of the poles. For example, we know that

$$\int_{-\infty}^{\infty} \frac{dx}{x} = 0 \tag{A.9}$$

because the integrand is an odd function. However, this is the sum of two divergent parts, $\int_{-\infty}^{0} + \int_{0}^{\infty}$. This result is the *Principal value* of the integral.

Exercise A.3: 1. Evaluate

a)

$$I = \int_0^{2\pi} \frac{d\theta}{1 + acos\theta} \tag{A.10}$$

for $|a| < 1$.

b) What about $|a| > 1$ (be careful here in that the integral has poles on the line you are integrating. How about $a = 1$?

c) (Harder - do some other questions first): The following problem, which is Fourier transforming the Green's function of a tight-binding model in one-dimension is very similar (n is an integer):

$$G(\epsilon, n) = \int_{-\pi}^{\pi} \frac{e^{ikn}}{\epsilon - t\cos(k)} \frac{dk}{2\pi} \tag{A.11}$$

Suggestion: Write $a = -t/\epsilon$ so you have a question similar to the above problems. Think carefully about the symmetry $n \to -n$. Realize that if $n < 0$, then you are going to generate extra poles in your contour integral.

2. Calculate the following integrals (note: after you have done part a), the rest follow with very little extra work)

a)

$$I = \int_{-\infty}^{\infty} \frac{\cos(x)}{x^2 + a^2} dx \tag{A.12}$$

b)

$$I = \int_{-\infty}^{\infty} \frac{\sin(x)}{x^2 + a^2} dx \tag{A.13}$$

c)

$$I(k) = \int_{-\infty}^{\infty} \frac{\cos(kx)}{x^2 + a^2} dx \tag{A.14}$$

d)

$$I(k) = \int_{-\infty}^{\infty} \frac{e^{ikx}}{x^2 + a^2} dx \tag{A.15}$$

3. Assume $v > 0$, but remember that q and t could be positive or negative:

$$G(t, q) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{\mathrm{i}\omega t}}{\mathrm{i}\omega + vq} \tag{A.16}$$

4. Evaluate

a)

$$I = \int_{-\infty}^{\infty} \frac{dx}{\cosh x} \tag{A.17}$$

b) Hint: this next one is easy!

$$I = \int_{-\infty}^{\infty} \frac{dx}{\sinh x} \tag{A.18}$$

c) Hint: Think carefully about this before trying to do anything.

$$I = \int_{0}^{\infty} \frac{dx}{\sinh x} \tag{A.19}$$

5. In this one, consider very carefully the two cases $|p| > 1$ and $|p| < 1$:

$$I(p) = \int_{0}^{\infty} \frac{\sin t}{t} e^{ipt} dt \tag{A.20}$$

6. By making the substitution $z = e^t$ and then picking an appropriate contour, evalute

$$I = \int_{0}^{\infty} \frac{(\ln x)^2}{1+x^2} dx \tag{A.21}$$

Hint: You need to make use of the result of Q4 (a).

7. (Much harder). For $0 < a < 1$, evaluate

$$I = \int_{0}^{\infty} \frac{x^{-a}}{x+1} dx \tag{A.22}$$

Note that the function x^{-a} for a non-integer has a branch cut - which we will have to integrate around. In this case, it is best to take the branch cut along the positive real axis i.e. in polar coordinate $z = re^{i\theta}$, theta will vary from 0 to 2π. Then take a contour which bypasses the axis and you can relate the top contour and bottom contour to the integral in question.

8. (Also difficult - try for a few minutes yourself and then ask me which contour works best). Calculate

a)

$$I = \int_{0}^{\infty} \cos(t^2) dt \tag{A.23}$$

b)

$$I = \int_{0}^{\infty} \sin(t^2) dt \tag{A.24}$$

These are special cases of Fresnel integrals.

9. Again for this one, try for a little bit yourself and then ask me for the best contour. In this case, n is a positive integer:

$$I = \int_{0}^{\infty} \frac{dx}{1+x^n} \tag{A.25}$$

A.4. Notes: Dispersion relations

Suppose $f(z)$ is an analytic function in the upper half plane, with $|f(z)| \to 0$ as $|z| \to \infty$ in the upper half plane. Then a direct application of the residue theorem gives

$$f(x_0) = \frac{1}{i\pi} P \int_{-\infty}^{\infty} \frac{f(x)dx}{x - x_0}. \tag{A.26}$$

Now, let's decompose f into real and imaginary parts

$$f(x) = u(x) + iv(x) \tag{A.27}$$

where u, v are both real functions. Then substituting into (A.26) gives

$$\begin{aligned} u(x_0) &= \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{v(x_0)dx}{x - x_0} \\ v(x_0) &= \frac{-1}{\pi} P \int_{-\infty}^{\infty} \frac{u(x_0)dx}{x - x_0} \end{aligned} \tag{A.28}$$

Furthermore, if we assume $f(-x) = f^*(x)$, then we get the *dispersion relations*

$$\begin{aligned} u(x_0) &= \frac{2}{\pi} P \int_{0}^{\infty} \frac{xv(x_0)dx}{x^2 - x_0^2} \\ v(x_0) &= \frac{-2}{\pi} P \int_{0}^{\infty} \frac{x_0 u(x_0)dx}{x^2 - x_0^2} \end{aligned} \tag{A.29}$$

These were originally derived by Kramers and Kronig to relate the real and imaginary parts of the refractive index in optics. Applications in modern physics are now widespread, particularly in scattering theory.

B. Fourier Series and Transforms

Fourier theory is another topic that is covered extensively in undergraduate maths courses. However, because of it's importance in the calculations arising in this quantum field theory course, this appendix provides a short statement of the most important theorem's, and a number of exercises for the reader to refamiliarize his, or herself with the topic.

B.1. Fourier Series

Suppose we have a periodic function $f(x)$ such that $f(x+2\pi) = f(x)$. Then it can be represented as a Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{\mathrm{i}nx} \tag{B.1}$$

To calculate the coefficients c_n, multiply both sides of the equation by $e^{-\mathrm{i}mx}$ and integrate over one period

$$\int_{-\pi}^{\pi} f(x) e^{-\mathrm{i}mx} dx = \sum_{n=-\infty}^{\infty} c_n \int_{-\pi}^{\pi} e^{\mathrm{i}(n-m)x} dx \tag{B.2}$$

The integral on the RHS is 0 if $n \neq m$ and 2π if $n = m$. Hence

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-\mathrm{i}mx} dx \tag{B.3}$$

Exercise B.1: 1. Prove Parseval's theorem

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} |f(x)|^2 dx = \sum_{n=-\infty}^{\infty} |c_n|^2 \tag{B.4}$$

2. Show that if f(x) is real, then $c_n = c^*_{-n}$.
3. Show that if $f(x) = f^*(-x)$, then the c_n are purely real. Similarly, if $f(x) = -f^*(-x)$, then the c_n are purely imaginary.
4. Find the c_n for:
   a) $f(x) = 1$

   b) $f(x) = \cos ax$, a not necessarily an integer.
   c) $f(x) = a\delta(x)$ (the dirac delta function).

   All these functions are valid on the interval $[-\pi, \pi]$

5. Give the general form of the Fourier series for a function that is periodic on an interval L, i.e. $f(x + L) = f(x)$.

Note: In Condensed Matter Physics, this transformation usually runs backwards - when we are given some field c_n that is defined on a lattice and wish to Fourier transform into momentum space, which will be defined on an interval $(-\pi/a_0, \pi/a_0)$ where a_0 is the lattice spacing.

Suppose that $c(k)$ is the Fourier transform of c_n as defined above. Similar to Parseval's theorem, give an expression for the following in terms of $c(k)$

1. $\sum_n (c_n)^2$
2. $\sum_n c_n c_{n+1}$
3. $\sum_n (c_n^* c_{n+1} + h.c.)$
4. $\sum_n (c_n c_{n+1} + c_n c_{n+2})$
5. $\sum_n [c_n]^4$

B.2. Fourier Transforms

The Fourier transform of a function $f(x)$ defined on the whole real line is

$$f(k) = \int_{-\infty}^{\infty} dx e^{ikx} f(x) \tag{B.5}$$

The inverse transform is

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} f(k) \tag{B.6}$$

There are different conventions in the position of the factor $1/2\pi$. Sometimes it is nice to make the equations symmetric, and have a factor $1/\sqrt{2\pi}$ in front of each of them. In physics, the most common convention is to always associate an integral over momentum or frequency with the factor $1/2\pi$.

In more than one dimension, the transform is

$$f(\vec{k}) = \int d^{\vec{d}} x e^{i\vec{k}\cdot\vec{x}} f(\vec{x}) \tag{B.7}$$

Exercise B.2: 1. Let $f(k) = g_1(k) g_2(k)$. Show that

$$f(x) = \int_{-\infty}^{\infty} g_1(x-y) g_2(y) dy \tag{B.8}$$

2. Suppose $f(k) = dg/dk$. Relate $f(x)$ to $g(x)$.
3. Use Fourier transforms to solve the differential equation

$$a\frac{d^2f}{dx^2} + b\frac{df}{dx} + cf(x) = 0 \tag{B.9}$$

4. Calculate the Fourier transform of the Gaussian

$$\psi(x) = e^{-x^2/x_0^2} \tag{B.10}$$

   Use your result to verify the uncertainty relation $\Delta x \Delta k > 1$.

5. Fourier transform the following functions
   a) $f(x) = 1/a$ for $|x| < a$, and zero otherwise.
   b) $f(x) = 1/(x^2 + a^2)$
   c) $f(x) = 1/\cosh(x)$
6. Calculate the Fourier Transform of

$$\frac{1}{\vec{k}^2 + m^2} \tag{B.11}$$

   in three dimensions (hint: change the integral to spherical polar coordinates).

7. If you are bored, repeat the above question in two dimensions - again, change to polar coordinates. The angular integration is easy, the radial one is a standard integral for K_0, a Bessel function.
8. What about d dimensions?