Lecture Notes for Quantum Matter

MMathPhys

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Contents

Preface

This course covers interesting quantum states of matter (Superfluids, Superconductors, Fermi Liquids). This is where condensed matter really starts to get bizarre — and therefore even more fun (at least in my opinion).

However, I realize that possibly not everyone will have actually attended the official prerequisite courses (or possibly did attend, but didn't pay attention), so I will try to make this course as self-contained as possible, while still making contact with what has been taught in prior courses.

Lets get started!

At early points in one's career there is an inevitable tension between learning physics and learning mathematical formalism. While learning to manipulate commutation relations, and even learning the rules for green's function expansions can be fun — and indeed, by doing this one gets a feeling that one is actually learning something — the real hard part is learning to develop intuition for physics. Developing intuition is extremely hard, and it is something that professional physicists struggle with throughout their lives.

This course needs to strike a balance between the two tasks. For some we will not learn enough formalism. For others we will not learn enough physics. I hope we will be able to satisfy both factions, and I hope everyone will learn at least a bit of both.

Chapter 1

What we will study

1.1 Bose Superfluids (BECs, Superfluid He, Superconductors)

Much of the term will be focused on discussion of superfluids and superconductors.

We will discuss both Bose Einstein Condensates (BECs) and superfluids — the main example being superfluid Helium 4. The difference here is that a BEC is by definition a gas of noninteracting bosons, whereas Helium 4 is strongly interacting. In the modern era one calls a weakly interacting bose gas a BEC also – since it can be treated as a weak perturbation of the noninteracting case. Helium 4, however, is very far from noninteracting.

The tension between the physics of the interacting and noninteracting cases will be a theme.

We will then turn to study of superconductors. First we will view these as simply being a superfluid of charged bosons.

Of course superconductors are things like aluminum[1] are regular metals, where the charged objects are electrons, which are fermions of charge $-e$. However, as we will see later, these charged objects can pair into bosons of charge $-2e$.

Why are such pairs bosons? Recall that fermions accumulate a minus sign when they are exchanged. Exchanging a pair of fermions with another pair of fermions accumulates an even number of minus signs, hence a plus sign, so the pair of fermions is a boson.

This picture of electrons pairing into bosons is not entirely accurate and there are good reasons to believe that even using this as a cartoon picture is quite dangerous. However, in some other sense, this picture does make sense. In order to figure out how it makes sense we must first take a detour into a study of Fermions.

[1] Those using the british spelling and pronounciation "aluminium" will be ridiculed.

1.2 Theory of Fermi Liquids

Fermi liquids, metals and other systems of interacting fermions have some unusual properties — some of which you have probably studied in your introductory solid state or condensed matter courses[2]. However, in most of these treatments, the interaction between fermions is completely neglected. This is a terrible thing to do being that the interaction energy scale is usually just as a big (and sometimes even bigger) than the fermi energy — and both are immensely bigger than the temperature for usual metals at room tempertature. We will need to understand some of the properties of these fermi systems before we can go on to understand the more exotic physics of electron pairing.

1.3 BCS theory of superconductivity

This is not examinable

1.4 Special topics

also not examined. Subjects we may cover include:

Integer quantum Hall effect.

Topological Insulators.

Majoranas

[2]If you have not studied introductory solid state physics, you should do so. I can recommend a good book.

Chapter 2

Introduction to Superfluids

Superfluids and superconductors share the unusual property of zero dissipation. For example, we can imagine a toroidal pipe which we can fill with ^{4}He. If we start ^{4}He supefluid flowing around the torus it will continue essentially forever (with caveats that T must be low enough, the velocity must be small enough, and the system must be big enough). "Forever" here means an essentially unmeasurable long time.

Similarly with a superconductor. we can take a solid torus (a very thick loop of wire) and if we start a current flowing around the wire , it will conitnue with no loss essentially forever (again caveats, the temperature must be low enough, the current must be small enough and the the sample must be big enough). Experiments have measured that the decay time in certain superconducting wires exceeds 10^5 years. It is probably much longer, but it becomes very difficult to measure such tiny amounts of decay.

Insert story about crazy Gerrit Flim demonstrating persistant current flow in superconductors.

2.1 Some History and Basics of Superfluid Phenomena

In 1908 in Leiden, Heike Kamerlingh Onnes liquified helium for the first time allowing access to extremely low temperatures.

On April 8, 1911 Kamerlingh Onnes "discovered" both supercondctivity and superfluidity.

He noticed that below 4.2K the resistance of mercury (Hg) metal suddenly becomes unmeasurably small. He spent the next few years convincing himself that this is a real effect and not some error in the experiment. He also shows that many metals have the same superconducting behavior — each with its own critical temperature. There was no real explanation of the observed superconductivity until 1957 (the BCS theory). We will discuss superconductivity more in later chapters, but this chapter will focus on superfluidity.

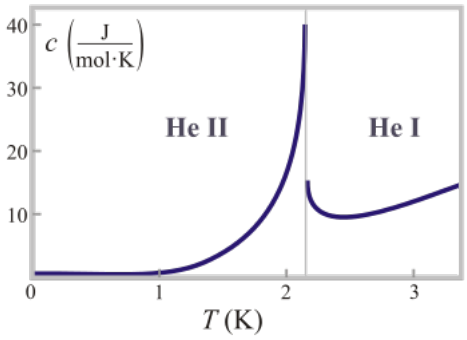


Figure 2.1: The Lambda transition in helium. The superfluid phase is known as He II.

On the very same day as the discovery of superconductivity, he notes in his lab book that something different is happening around 2K, but he didn't follow up on this for many years.

In 1913 Kamerlingh Onnes wins the Nobel prize.

In 1922-23 Onnes, along with some of his coworkers goes back to re-examine the "something strange" that happens around 2K. Looking at the heat capacity, they find something like Fig. 2.1. The diveregence in the heat capacity is a signal of a thermodynamic phase transition[1] The regular phase of helium is known as He I whereas[2] the superfluid phase is known as He II.

Onnes died in 1926, but the work in his lab continued on. With some exploration, they uncovered the full phase diagram shown in Fig. 2.2. The line separating the He I and He II phases is known as the Lambda-line.

Compared to other elements, helium is quite special in that it does not solidify at low temperature except when under pressure. This special feature is due to both its very light mass and its weak interactions (no chemical bonding). The light mass is important since $\Delta p \Delta x \geqslant \hbar/2$. If you try to localize x, you have a nonzero p. But since kinetic energy is $p^2/(2m)$ having a light mass means there is a very high energy cost to localizing the position of the atoms.

The most remarkable thing about superfluid helium is persistant flow (which Kamerlingh Onnes was never aware of). However, perhaps just as remarkable is the extremely good transport of heat in superfluids. In fact, going through the supefluid transition, thermal conductance can jump by a factor of 10^5 or more! Indeed, this was what Kamerlingh Onnes saw in 1911 when he said "something happens" at 2K). What is happening here

[1] For those who have studied phast transitions we have $C_v \sim |T - T_c|^{-\alpha}$ where the critical exponent matches that of the XY-universality class. When we study the order parameter in section 2.3 this might make more sense.

[2] This nomenclature is particularly confusing being that we also have ^{4}He and ^{3}He, indicating the number of nucleons. Everything in this chapter is in reference to phases of regular helium, ^{4}He, although we will also discuss ^{3}He in our chapter below on Fermi liquids.

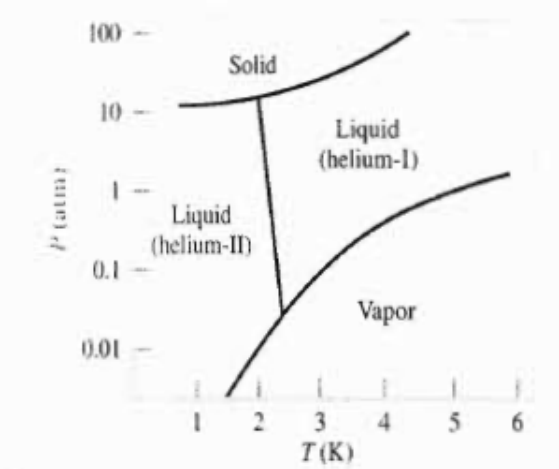


Figure 2.2: The Phase Diagram (P,T) of ^{4}He. The superfluid phase is known as He II. The nonsuperfluid phase is known as He I

is that the fluid suddenly goes from rapid boiling to no boiling at all in the superfluid phase. Boiling occurs when a small region of a system is at slightly higher temperature than the vaporization transition. This region turns into gas and then boils up to the top of the containier. In a superfluid, the thermal transport is so good that no region in the sample is at higher temperature than any other region. The system still has evaporation, but only directly from the surface.

The discovery of the superfluid properties of He II did not come until the mid 1930s. The next heros of our story are Peter (Pyotr) Kapitsa and John Allen.

Peter Kaptiza, having survived the flu epidimeic of 1918-19 in Russia which claimed half of his family, had moved to Cambridge to study with Rutherford. He was made a fellow of Trinity College Cambridge in 1925 two years after obtaining his PhD and he went on to build one of the world's finest low temperature physics labs at Cambridge. By the mid 1930s Kaptiza was earning what was considered a magnificent salary of 800 pounds per year.

By the early 1930s there were only four labs in the world that were able to liquidify helium and conduct low temperature experiments: Leiden, Oxford[3], Cambridge, and Berlin.

John Allen received his PhD from Toronto in their cryogenics lab, and moved to Cambridge to work with Kaptiza. Unfortunately, when he arrived there, he discovered that Kapitsa had been "detained" on a visit to the Soviet Union, and was told that he would not be allowed to return to Cambridge. This was the era of Stalin, and the Soviets wanted to have the great Kaptiza back in his native land.

[3]Oxford had liquid helium in 1933, one year before Cambridge did. Fredrick Lindemann, the first Viscount Cherwell, advertised Oxford's success in the Times and Nature. Nonetheless, the crucial discovery of superfluid flow was made at Cambridge

Kaptiza was well funded by the Soviets to set up a low temperature physics lab (they purchased much of his equipment from Cambridge).

John Allen, at Cambridge with no supervisor, had to work as an unsupervised postdoc. Rutherford, the head of the Cavendish lab at Cambridge, made the best of the situation — he used Kaptiza's salary to pay both Allen and a young theorist named Rudolf Peierls.

The cryogenic race was on: it was clear that there was plenty of interesting physics to be discovered to whoever got there first!

In 1938 both Kaptiza and Allen (with Misener, another student from the Toronto lab) simultaneously discovered the effect that gives superfluid helium its name — that superfluid helium flows with apparently no resistance through very thin capillaries.

Another very strange effect, now known as supercreep, was discovered the following year in Oxford by Sir Francis Simon (no relation that I know of) and Bernard Rollin: Superfluid helium in an open-topped container will creep up the walls of the container and eventually find its way to lower gravitational potential by siphoning itself onto the floor. This effect is often viewed as a combination of wetting and zero viscosity. Many liquids will form a layer an atom or two thick on the walls of their container all around the container — this is due to the attractive forces between the wall of the container and the fluid molecules. This phenomenon is known as wetting. Superfluid helium, with no viscosity, can flow readily through a layer which is atomically thin – whereas other fluids cannot. Thus superfluid helium can siphon itself out of a container onto the floor through this very thin layer.

However, the situation is more complicated than simply saying that the fluid has zero viscocity. Other experiments aiming the measure the viscocity of the liquid come up with finite results. For example, a vibrating wire, or rotating disk in the helium liquid will detect a finite viscous damping which only vanishes at zero temperature (Keesom and MacWood, Leiden Lab, 1938). This connundrum was one of the key points that led to the development of Landau's two fluid model.

2.2 Landau and the Two Fluid Model

2.2.1 More History and a bit of Physics

In 1938 just as Kapitsa was discovering superfluidity, the great theorist, Lev Landau was thrown in prison for publicly comparing Stalin to Hitler[4]. He remained imprisoned for a year until Kapitsa put his own head on the line — threatening to quit as a scientist unless Landau was released, and pleading that only Landau would be able to explain superfluidity.

[4]He was exceedingly lucky not to have been executed!

While Landau was in prison, the young Hungarian physicist Laszlo Tisza[5] working in Paris with Fritz London tried to explain superfluidity as a result of Bose-Einstein condensation[6]. Fritz and his brother Heinz London, several years earlier working with Lindemann in Oxford, had already tried to use a similar approach for understanding superconductors. While they had some success, Landau immediately realized what was wrong with their approach.

- Helium is *NOT* a noninteracting boson. It has extremely strong short range repulsive interactions.
- A noninteracting BEC does not have a diveregence in its specific heat
- A noninteracting BEC will *NOT* superflow. Interactions are crucial for obtaining this effect. (We will explain this in detail below in section 2.4)

At this point Landau gets into the game. He felt that BEC was not the right physics[7] — perhaps he even felt this more strongly than is actually warranted. Later Feynmann would clarify the importance of Bose physics for superfluidity (See below in chapter 5).

Landau made two major contributions to the theory of superfluidity.

- He develops the two-fluid model (an expansion on Tisza's work)
- He explains the criterion for superflow.

These contributions earned Landau a Nobel prize in 1962.[8]. Sadly a few months before the prize was annouced, Landau was in a car crash and coma. While he came out of the coma, he never fully recovered, he was never scientifically productive again, and he died in 1968, at age 60, from complications due to these injuries.

2.2.2 Landau's Two Fluid Model

The general idea of the two fluid model is that we should imagine two interpenetrating fluids which we call "super" and "normal"[9]. We write the total density of the fluid as the sum of the mass densities of the super and normal fractions.

$$\text{mass/volume} = \rho_{total} = \rho_S + \rho_N.$$

[5]Tisza moved to MIT in 1941 and lived in the US the remainder of his life. He passed away in 2009 at the age of 101.

[6]The prediction of BEC by Einstein was much earlier, in 1925.

[7]Apparently Landau also really hated Fritz London. It is unclear why this would be true, but Landau made a point never to cite London.

[8]There are many things that Landau could have been awarded a Nobel prize for!

[9]This is another terrible nomenclature. Above the critical temperature we have only normal fluid. But below the critical temperature we have both super and normal fluid. However, we also say that He II (below the critical temperature) is superfluid.

The normal fraction behaves like we should expect a fluid to behave. The superfluid fraction, however, has no viscosity, and carries no heat. At zero temperature we expect all of the fluid to be super, whereas above the critical temperature T_c, i.e., in the He I phase, we expect all of the fluid to be normal. At nonzero T but still in the He II phase, we expect to have a mixture of partially super and partially normal fluids.

$$\begin{array}{ccccc} T=0 & \rho_N=0 & \rho_S=\rho & & \\ T_c>T>0 & \rho_N(T) & \rho_S(T)=\rho_{total}-\rho_N(T) & & \text{interpolates} \\ T>T_c & \rho_N=\rho & \rho_S=0 & & \end{array}$$

One way to think about the super-fraction is to think of it as being the "ground state" of the system, and the normal fluid being the excitations. For a moment let us think about the analogy with BEC. In that system we know that only at $T=0$ are all of the bosons in the same lowest energy eigenstate. At any finite T there will be some bosons in the lowest energy eigenstate (these we might call "super") and some will be in the excited eigenstaes (which we might call "normal"). Once we go above the critical temperature, there will a microscopic fraction of particles (essentially zero) in the lowest energy eigenstate, and the entire system will be normal.

The mass current will also be divided into a normal and super component

$$\mathbf{j}=\rho_S\mathbf{v}_S+\rho_N\mathbf{v}_N$$

with $\mathbf{v}_N$ being the normal fluid velocity and $\mathbf{v}_S$ being the superfluid velocity. Here the super part of the fluid will be free from viscosity but the normal part is not.

This two fluid model nicely "explains" the two different measurements of viscosity. With a vibrating wire or a rotating disk, the object moving through the fluid will have to push the normal fluid out of the way, and hence will measure the normal viscosity. However, when trying to push the fluid through a small capillary, no matter how thin the capillary, the super-fluid component will always flow through – whereas the normal fluid will stay behind. Since flow occurs through small capillaries one would measure a fluid with essentially zero viscosity.

From a technical standpoint the two fluid model actually imposes the curl-free constraint

$$\nabla\times\mathbf{v}_S=0 \tag{2.1}$$

We will justify this constraint later; for now let us just treat it as a conjecture. However, it is worth understanding why this is an appropriate conjecture for a fluid that shows no visosity.

One explanation is to realize that viscosity is a statement transferring force through shear. However, the curl-free constraint is the statement that the fluid cannot shear at all! (Expand on this! add picture).

Suppose for a moment that ρ_S is fixed (say we are at zero temperature). Then we have

$$\nabla\cdot\mathbf{v}_S=0$$

by current conservation. If we use our conjecture Eq. 2.1 we can use a vector identity to derive

$$\nabla^2 \mathbf{v}_S = \nabla(\nabla \cdot \mathbf{v}_S) - \nabla \times (\nabla \times \mathbf{v}_S) = 0$$

If we then recall the Navier-Stokes equation we have

$$\left[\frac{\partial}{\partial t} + (\mathbf{v} \cdot \nabla)\right] \mathbf{v} + \frac{1}{\rho}\nabla P = \frac{\eta}{\rho}\nabla^2 \mathbf{v}_S$$

where η is the coefficient of viscocity. By using the curl-free constraint the viscosity term always vanishes!

2.2.3 More Physical Effects and Their Two Fluid Pictures

Fountain Effect

Another strange effect observed by John Allen[10] is known as the "fountain effect", shown in the left of Fig. 2.3. A tube is inserted in the superfluid and plugged with cotton such that only the "super" fraction of the fluid can get through. Heating the cotton, will result in superfluid being sucked into the tube at a high rate such that it can fountain out the top. This effect was explained in 1939 by Heinz London[11] using the two-fluid model. In this picture we think of the motion of the fluid as being similar to osmosis. If in some region (such as in the tube) we increase the temperature from T to $T + \Delta T$, this increases the concentration of ρ_N. Using the usual principle of osmosis, this makes ρ_S flow into the hotter region to try to bring the normal fluid back ot the same concentration as that of the surrounding area. I.e., the superfluid flows into the hotter region to try to bring the temperature back down.

This physics may look like a violation of the 2nd law of thermodynamics since fluid is flowing from cold to hot. However, it is not a violation since the superfluid carries no heat.

The situation can be analyzed in more detail by using the experimental setup shown in the right of Fig. 2.3. Here the tube between the two containers is assumed to be plugged with cotton, or is such a thin capillary that only superfluid can flow through it (but not normal fluid). This is sometimes known as a "superleak."[12]

We can analyze the situation using simple thermodynamics. In particular, we use the Gibbs-Duheim relationship for the change in chemical potential which we set to zero

[10] In fact, the discovery of this effect was a fortuitous error in an experiment!

[11] The London brothers were Jewish refugees from Germany in 1933. Lindeman at Oxford found money to fund as many German scientists as he could, but his money soon ran out. Fritz moved to Paris and eventually ended up at Duke university in the states. Heinz moved to Bristol, but was declared a potentially "hostile foreigner" and interned for some time on the Isle of Man. He was released to work on the British nuclear program and was given British citizenship. In the 1950s Heinz invented the dilution refrigerator which is used heavily in physics research for cooling materials down to as low as a few millikelvin.

[12] The superleak is crucial for this experiment since an open tube cannot have a pressure difference across it!

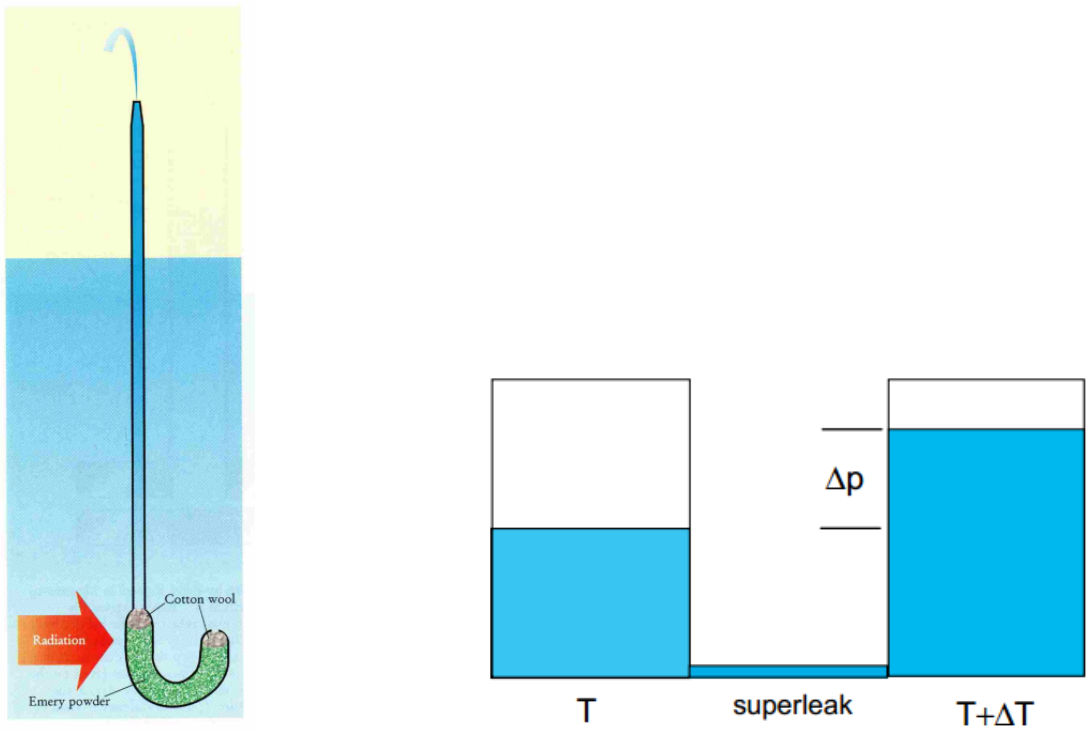


Figure 2.3: Left: The fountain effect. A tube is inserted in the superfluid and plugged with cotton such that only the "super" fraction of the fluid can get through. Heating the cotton, will result in superfluid being sucked into the tube at a high rate such that it can fountain out the top. Right: a similar experiment showing that a temperature difference implies a pressure difference.

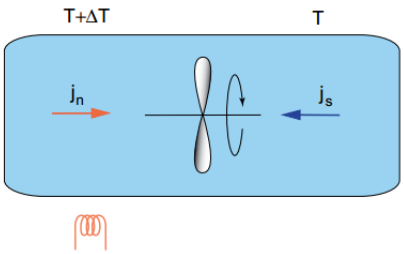


Figure 2.4: Thermomechanical Effect: The propeller turns as if fluid is flowing from hot to cold, even though there is no net tranport of mass.

in order to have equilibrium

$$d\mu = -\frac{S}{N}\,dT + \frac{V}{N}dP = 0$$

Rearranging this we can write

$$\frac{\Delta P}{\Delta T} = \frac{S}{V}$$

and the right hand side can be written in terms of

$$S(T) = \int_0^T dT' \frac{C_V(T')}{T'}$$

where C_V can be measured experimentally.

Thermomechanical Effect

In this experiment, a propeller is put in a container of helium. One side of the container is heated as shown in Fig. 2.4. No net current of fluid can flow due to the walls of the container. Nonetheless, the propeller turns as if fluid is flowing from hot to cold.

What is happening here is that the increased temperature (on the left in the figure) increases the density of normal fluid, and the normal fluid then tries to flow to the right. Similarly, by osmosis the superfluid tries to flow to the left to bring the two sides of the system into equilibrium where they have the same density of normal fluid (i.e., have the same temperature). Thus we have counter flow of normal and super fluid – with no net flow of mass.

Now the key is that the flow of the normal fluid pushes the propeller while the flow of the superfluid does not. The reason for this is that superfluid flow must not dissipate mechanical energy — otherwise superflow would not be dissipationless.

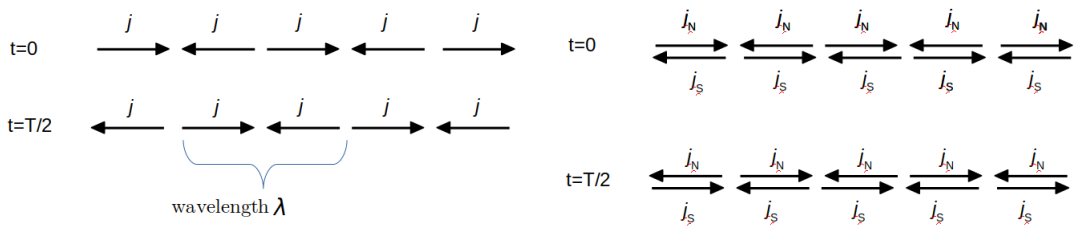


Figure 2.5: Left: Sound waves are density waves: mass sloshes back and forth. Right: Second sound waves involves counterflow. There is no mass transport, although heat is transported.

2.2.4 Second Sound

The idea of counter flow of normal and superfluids suggests the phenomenon of second sound[13].

First let us remind ourselves of how sound waves work. In the left of Fig. 2.5 we see the density flow in a sound wave — mass sloshes back and forth over the wavelength over the sound and with the period of the oscillation T. In the right of Fig. 2.5 we see second sound waves — the supercurrent is always counter-flowing the normal current so there is no net mass transport, $\mathbf{j}_{total} = 0$ everywhere. However, heat sloshes back and forth since only the normal current carries heat.

Such second sound waves provide extremely good thermal conduction — indeed, the best thermal conductance of any material since heat travels ballistically in second sound rather than diffusively. The heat transport can be over 100 times as efficient as heat transport in, say, copper.

Derivation of second sound

We now turn to do a more formal derivation of second sound. Since we are not interested in regular sound waves, we will assume that the pressure is constant and the density is constant (these approximations simplify quite a bit, but are not entirely necessary).

Since we have fixed density and fixed pressure, we will enforce

$$\mathbf{j}_{tot} = 0 = \rho_N \mathbf{v}_N + \rho_S \mathbf{v}_S$$

We now assume that there is an osmotic force from temperature imbalance. This is precisely the force that arises from the fountain effect. Usually we think of this as a force pushing the superfluid towards the heat, but since the total mass current is fixed to be zero, we can just as well think of this as a force pushing the normal fluid towards lower

[13] Second sound was first predicted by Tisza. The correct second sound velocity was predicted by Landau.

temperature regions

$$\dot{\mathbf{v}}_N = -\alpha \nabla T \tag{2.2}$$

with $\alpha > 0$. It is a homework exercise to estimate the value of the coefficient α.

We now write a continuity equation for entropy. Let us write s for the entropy density. We then have a conservation equation

$$\dot{s} = -\nabla(s\mathbf{v}_N) \tag{2.3}$$

since the entropy moves with the normal fluid only (the super fraction contains no entropy).

The entropy density is a function of the local temperature, which we can expand

$$s(T + \delta T) = s(T) + \kappa \delta T$$

where recalling that $c_V = Tds/dT|_V$. we must have

$$\kappa = c_V(T)/T$$

Here c_V is heat capacity per unit mass.

We can now put this expansion of the entropy into Eq. 2.3 to obtain

$$\kappa \dot{T} = -s(\nabla \cdot \mathbf{v}_N)$$

Here it may look like there should be another term on the right which would be $\mathbf{v}_N \cdot \nabla s$. However, we can throw this out since this is second order in "small" things. I.e, the gradient of the temperature is assumed small and the velocity is also assumed small.

Differentitating with respect to time we obtain

$$\ddot{T} = -\frac{s}{\kappa} \nabla \cdot \dot{\mathbf{v}}_N = \left(\frac{s}{\kappa}\alpha\right) \nabla^2 T$$

where we have again thrown away terms second order in "small", and we have also used Eq. 2.2. Thus we obtain the wave equation[14]

$$\ddot{T} = \gamma \nabla^2 T$$

with $\gamma > 0$ which tells us that heat propagates ballistically rather than diffusively as it usually does.

2.2.5 Big Questions Remaining

These questions will be addressed in the next sections.

1. What justifies the curl free constaint on the supercurrent $\nabla \times \mathbf{v}_S = 0$.

[14] Using the homework assignment where we estimate α as well as some results later about C_V and ρ_N we can get that the second sound velocity is independent of T at low enough T.

2. Why do we get dissipationless superflow? This is *NOT* only a result of item (1) the curl free constraint.

3. What do we expect the normal/super fluid density to be as a function of temperature $\rho_N(T)$ and $\rho_S(T)$?

2.3 Curl Free Constraint: Introducing the Superfluid Order Parameter

One of Landau's other great contributions to physics is the concept of an *order parameter*. (If you have studied the Landau theory of phase transitions you will know what this is.) Roughly, the order parameter describes the breaking of a symmetry in a physical system.

As a simpler example, let us reconsider a BEC. In this case, we take the the order parameter to be the complex wavefunction for the ground state, which we write as ψ, however, we normalize it so that it goes to zero at the phase transition — i.e., it's amplitude is proportional to the number of bosons in the ground state.

What symmetry has been broken when going from the normal state above the critical temperature to the superfluid state below the critical temperature? It is actually a gauge symmetry! When the order parameter ψ becomes nonzero it must choose a complex phase, which is a spontaneous breaking of a symmetry!

In the case where the bosons are not uniform in space, we generalize the uniform Landau order parameter to a Landau-Ginzburg order parameter and write it as a function of position $\psi(\mathbf{r})$.

For interacting bosons we do something quite similar, we define an order parameter as

$$\psi(\mathbf{r}) = \langle \hat{\psi}(\mathbf{r}) \rangle$$

where $\hat{\psi}(\mathbf{r})$ is a boson annihilation operator.

We will be more explicit about this approach in later chapters ***. For now it is acceptable to just think of this order parameter as being the complex wavefunction of a BEC with the one complication that we want to change the normalization so that

$$\int d\mathbf{r} |\psi(\mathbf{r})|^2 = N_S$$

rather than normalization to unity. Here N_S is the number of bosons in the superfluid condensate (i.e., in the super part of the fluid).

We can separate the phase degree of freedom from the magnitude by writing

$$\psi(\mathbf{r}) = \sqrt{n_S}\, e^{i\theta(\mathbf{r})} \tag{2.4}$$

where n_S is the superfluid density with $\rho_S = m n_S$ and m is the mass of the boson, and θ is a phase defined modulo 2π. Here we can think of $e^{i\theta}/\sqrt{V}$ as being the usual normalization of the wavefunction of a boson in its ground state.

Again thinking of ψ as a wavefunction for superfluid bosons, then we can write a superfluid boson current in the usual quantum mechanical way

$$\begin{aligned} \mathbf{j}_S &= \frac{1}{2}\left(\psi^* \hat{\mathbf{p}}\psi - (\hat{\mathbf{p}}\psi^*)\psi\right) \\ &= \frac{-i\hbar}{2}\left(\psi^* \nabla\psi - (\nabla\psi^*)\psi\right) \end{aligned} \tag{2.5}$$

where here the momenum operator $\hat{p}$ gives us a mass current.

Now using Eq. 2.4 we have

$$\nabla\psi = \left(\frac{\nabla n_S}{2n_S} + i\nabla\theta\right)\psi$$

which gives us a superfluid mass current of

$$\mathbf{j}_S = \hbar n_S \nabla\theta \tag{2.6}$$

We can write this current as a mass density times a supefluid velocity

$$\mathbf{j}_S = \rho_S \mathbf{v}_S$$

which, using $\rho_S = m n_S$ gives us an expression for the superfluid velocity

$$\mathbf{v}_S = \frac{\hbar}{m}\nabla\theta$$

which is a gradient. Which then implies the desired curl-free constraint

$$\nabla \times \mathbf{v}_S = 0$$

2.3.1 Vorticity Quantization

Circulation is defined as the line integral of a velocity around a closed contour. Choosing any given closed contour we have

$$\oint_C \mathbf{v}_S \cdot \mathbf{dl} = \frac{\hbar}{m}\oint_C \nabla\theta \cdot \mathbf{dl} = 2\pi p\hbar/m = ph/m \tag{2.7}$$

where p is an integer. Here we have used the fact that θ must be well defined only modulo 2π so going around a line integral, the value of θ needs to come back to the same value, but can change by integer multiples of 2π.

Thus we have shown that in a superfluid circulation is quantized in integer multiples of the circulation quantum h/m.

Suppose now that our contour surrounds only He fluid as shown in the left of Fig. 2.6. I.e, we have a big sample of He fluid [with nothing else in it but He fluid] and the contour can be continously contracted to a point. In this case we can use Stoke's theorem

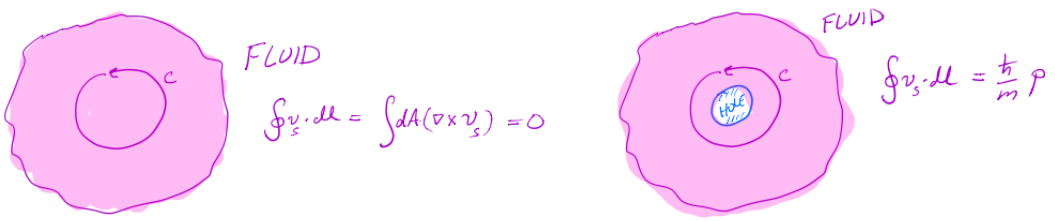


Figure 2.6: Left: A contour in fluid that can be contracted and therefore bounds a disk in the fluid. In this case the circulation must be zero. Right: A contour in fluid that cannot be contracted. In this case we can only say that the circulation is quantized in units of the elementary circulation quantum h/m.

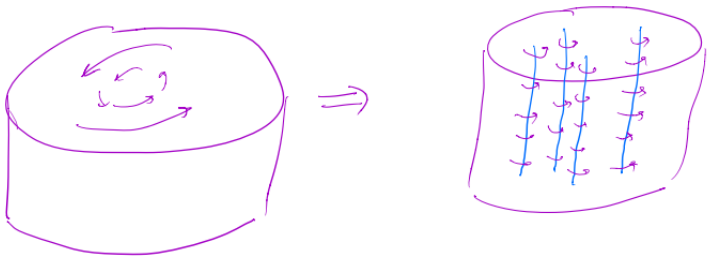


Figure 2.7: If we start a bucket of helium rotating above the critical temperature and then we cool it below the critical temperature, the circulation is accomodated by the introduction of many vortex lines.

$$\oint_{C=\partial D} \mathbf{v}_S \cdot \mathbf{dl} = \int_D dA \cdot (\nabla \times \mathbf{v}_S) = 0$$

where the area integration is over a disk D bounded by the contour C. Thus we would conclude that the circulation must be zero. However, this conclusion is only true if the entire disk lies within the fluid. If there is a hole within the fluid region which has no fluid in it (like a bundt cake, or a toroidal pipe) as shown in the right of Fig. 2.6, we cannot use Stoke's theorem and therefore we only know that the circulation is quantized in units of the elementary circulation quantum h/m.

In fact there is no constraint on the size of the hole — the hole in the fluid can be extremely small and this still consitutes a hole in the fluid. We only need a single point where the superfluid density goes to zero such that the phase is no longer defined at that one point. In this case we can have the phase θ wrap by any integer multiple of 2π as we go around this single point. This is known as a "vortex". The existence of vortices in superfluid helium was predicted by Feynmann in 1955[15].

Imagine a bucket of helium above the superfluid transition temperature. We start

[15] As we will discuss below, as similar prediction was made for superconductors somewhat earlier by Abrokosov, but he did not publish it until after Feymann convinced the world that the idea was reasonable.

the bucket rotating so that the circulation is very large

$$\oint \mathbf{v}_S \cdot \mathbf{dl} \gg 0$$

We now imagine cooling the system through the transition temperature T_c. Since the superfluid must be curl free, the only way we can accomodate the circulation is to have many point vortices, where there is quantized circulation around each such vortex. Looked at from far away, the velocity flow field is roughly the same in the superfluid phase as it was in the normal phase. As mentioned above, in the core of the vortex (here one dimensional lines) the superfluid density drops to zero. In actual superfluids He, the vortex core is only a few angstrom in diameter.

One often hears arguments that quantized circulation explains the persistant flow phenomenon observed in superfluids. Indeed, one can imagine starting a superfluid flowing around a toroidal pipe. Since the circulation is quantized, it can only decay in discrete steps. If there is some impediment, or activation barrier, to making sudden steps in circulation, one might imagine that this prevents the circulation from decaying at all.

While it is true that the circulation can be locked to a single value, this is actually not sufficient to explain dissipationless flow. The issue is not whether the circulation decays but whether energy is dissipated. Even without having a decay in the circulation (which is the line integral of the *velocity*) one can dissipate energy if some sort of friction heats the fluid. This would slowly reduce the superfluid fraction and increase the normal fraction, thus reducing the superfluid *current*, and eventually the system would have no superfluid left! So the question boils down to whether or not a particular superfluid will dissipate energy. In fact in noninteracting BECs, we will see below that, while circulation is quantized, they do dissipate energy to friction and therefore do not have persistent flow.

2.4 Landau Criterion for Superflow

Landau developed a brilliant argument to determine whether a fluid can flow without dissipating energy.

Let us assume that for a superfluid (and normal fluid) at rest there is some spectrum $\epsilon(\mathbf{p})$ for excitations which we will call "quasiparticles". In a BEC these are simply excitations of particles out of the ground state wavefunction. In an interacting superfluid, these are more complex collective excitations. We need only assume that such excitations exist.

We now imagine flowing the superfluid past a stationary wall at velocity $\mathbf{v}$ as in the right of Fig. 2.8, and we would like to ask whether energy can be dissipated. Another way to ask this is to ask wehether quasiparticles can be excited.

In order to answer this, the argument entirely boils down to figuring out the energy momentum relation *in the rest frame of the superfluid* and then asking whether energy and momentum can be conserved in a process that creates a quasiparticle excitation.

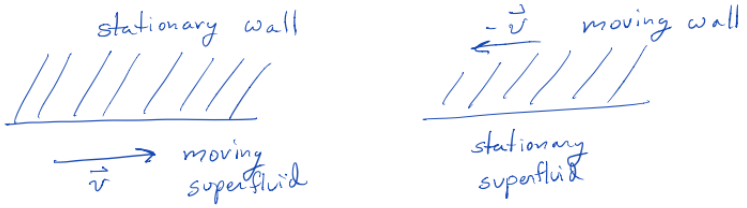


Figure 2.8: Left: Flowing a fluid past a wall. Right: In the fluid frame, the wall is moving.

Thus, let us switch to the fluid rest frame as in the right of Fig. 2.8. We know the dispersion $\epsilon_{fluid}(\mathbf{p}) = \epsilon(\mathbf{p})$ of excitations in this (the fluid) frame, and we would like to determine the dispersion relation in the lab frame. A classical Galilean transformation gives us

$$\epsilon_{lab}(\mathbf{p}) = \epsilon_{fluid}(\mathbf{p}) - \mathbf{p} \cdot \mathbf{v} \tag{2.8}$$

Note that here the quantum number $\mathbf{p}$ describes the momentum of the quasiparticle in the fluid frame.

To justify this Galilean transformation (Eq. 2.8) we should recall that in quantum mechanics the phase of the wavefunction oscillates as

$$\psi \sim e^{-i\epsilon t/\hbar}$$

So here we are claiming that a wavefunction for a particle with momentum $\mathbf{p}$ should oscillate as

$$\psi(\mathbf{p}) \sim e^{i\mathbf{p}\cdot\mathbf{x}/\hbar - i\epsilon t/\hbar}$$

If we transform into a moving frame we then have

$$\begin{aligned} \psi(\mathbf{p}) &\rightarrow e^{i\mathbf{p}\cdot(\mathbf{x}+\mathbf{v}t)/\hbar - i\epsilon t/\hbar} \\ &= e^{i\mathbf{p}\cdot\mathbf{x}/\hbar - i(\epsilon - \mathbf{p}\cdot\mathbf{v})t/\hbar} \end{aligned}$$

so we rederive Eq. 2.8.

A more familiar way of understanding this transformation is to think about frequencies $\omega = \epsilon/\hbar$ instead of energies. We then recognize Eq. 2.8 as being the usual Doppler shift of a frequency in a moving frame[16].

So given Eq. 2.8 our question is whether in the lab frame, the energy to create an excitation is ever negative. If so, excitaions are created spontaniously and energy is dissipated. So when does this happen? Obviously $\epsilon - \mathbf{v} \cdot \mathbf{p}$ is minimized when $\mathbf{v}$ and $\mathbf{p}$ are parallel. Thus we can get negative values of ϵ_{lab} only if

$$\frac{\epsilon(p)}{p} < v$$

[16]This argument is strictly correct for situations where the dispersion is linear — i.e., we have sound waves or phonons.

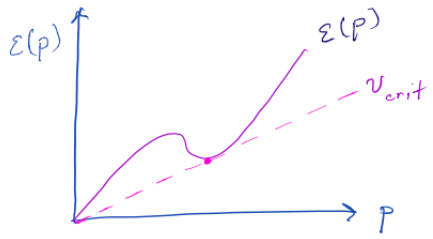


Figure 2.9: A spectrum $\epsilon(p)$ and the corresponding critical velocity for the superfluid.

Given a dispersion $\epsilon(p)$ (in the rest frame), there is thus a critical velocity

$$v_{crit} = \min_p \frac{\epsilon(p)}{p}$$

(see figure 2.9). Below this critical velocity, there is no way to create a quasiparticle while conserving energy and momentum. If the fluid flows at velocity greater than the critical velocity, quasiparticles are spontaneously generated and energy is dissipated from the superflow.

Note now that if one considers a BEC, the spectrum of excitations is simply $\mathbf{p}^2/(2m)$ i.e., just the spectrum of noninteracting particles. The critical velocity is then

$$v_{crit;BEC} = \min_p \frac{p^2/(2m)}{p} = 0 \quad (!)$$

We thus conclude (as Landau realized intuitively!) that *a noninteracting BEC does not superflow!*

When we add interacting between the bosons, the spectrum develops an acoustic wave (we will see this in more detail later!). In that case we have a low energy spectrum

$$\epsilon(p) = v_{sound}\, p + \dots$$

which then gives us a critical velocity

$$v_{crit} = v_{sound}$$

assuming the deviations hidden in the "$+\dots$" is positive. If it is a negative correction (as shown in Fig. 2.9) the critical velocity can be somewhat lower.

To be a bit more detailed about interacting bose systems, we recall what we have learned in other courses about the Bogoliubov approach to weakly interacting bose gases. In fact we will review this technique in section 4.5 below. We derived (and will derive again later in several ways), that for a weakly interacting bose gas with interaction

$$\frac{U}{2} \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}_j)$$

with U being weak, the excitation spectrum is given by

$$\epsilon(p) = \sqrt{(\frac{p^2}{2m} + nU)^2 - (nU)^2}$$

where n is the density of bosons. For small p this can be expanded as

$$\epsilon(p) \sim \frac{p}{\sqrt{2m}}\sqrt{\frac{p^2}{2m} + 2nU}$$

Thus we obtain a crtical velocity

$$\min_p \frac{\epsilon(p)}{p} = \min_p \frac{1}{\sqrt{2m}}\sqrt{\frac{p^2}{2m} + 2nU} = \sqrt{\frac{nU}{m}} = v_{acoustic} = v_{crit}$$

Note: about real experiments

While the Landau theory of critical velocity is quite beautiful and compelling, experiments do not often agree with the Landau estimate. In fact measured critical flow velocities can often be as much as 100 times smaller than the acoustic velocity — and furthermore the critical velocity often depends on the details of the geometry of the experiment.

In thin tubes of superfluid it is easy to qualitatively explain the physics of the critical velocity. This has to do with the physics of vortices and the quantization of circulation. As we mentioned above if we have a toroidal (but thin) tube of fluid, with a fixed circulation going around the tube, this circulation is quantized. This circulation can decay if a vortex is nucleated at one edge of the tube, flows perpendicular to the supefluid flow and then disintegrates at the other edge of the tube. This process can reduce the circulation in discrete steps.

Such a process begins to look much less likely in thick tubes of fluid — however, experiments seem to suggest that vortex physics is still involved.

2.5 Superfluid Density

Finally we turn to Landau's prediction of the superfluid density as a function of temperature $\rho_S(T)$.

2.5.1 The Andronikoshvili Experiment

Landau made a prediction for the superfluid density $\rho_S(T)$ then convinced a young experimentalist, Elephter Andronikoshvilli[17], to make careful measurements of the superfluid

[17] In my opinion, this is the coolest name of all physicists. The ending "vili" is Georgian meaning "descendant of". Thus, Elephter was part of a royal Georgian family that traces its ancestery back to Andronicos I of the Eastern Roman Empire in the 1100's. Andronikos seemed quite violent and fittingly met a violent end himself.

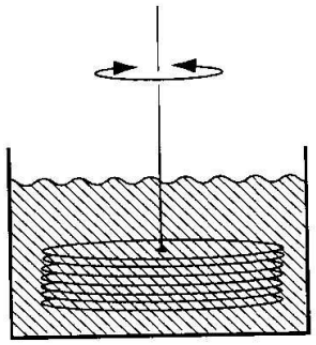


Figure 2.10: The Andronikoshvili experiment. Since normal fluid sticks between the closely spaced disks (but superfluid does not), the moment of inertia of the stack of disks, and hence frequency of oscillation of the disks tells us the fraction of fluid that is superfluid.

density in 1946, and the results supported his predictions (perhaps unsurprisingly since Landau was a genius!).

The experiment is shown in Fig. 2.10. A stack of closely spaced disks is hung in a container of helium by a thin wire which acts as a torsion oscillator. The idea is that when the stack of disks rotates, normal fluid, which is viscous will get stuck between the disks and must rotate with the stack. However superfluid, which has no viscosity slips through the closely spaced disks and does not rotate. The normal fluid thus contributes to the total moment of inertia of the stack, and hence changes the oscillation frequency of the torsion oscillator. By measuring the change in the oscillation frequency as a function of temperature, one can determine the fraction of helium that is superfluid as a function of temperature.

Andronikoshvili clearly measured that the normal fluid density is proportional to T^4 at low temperature.

$$\rho_N(T) \sim T^4$$

We should compare this result to a simple calculaton for a noninteracting BEC. We can write the mass of particles that are normal by simply counting the number of particles that are not in the condensate (i.e., not in $\mathbf{p} = 0$). We thus have

$$\rho_N(T) = \frac{m}{V} \sum_{\mathbf{p} \neq 0} n_B(\beta\epsilon(p)) = m \int \frac{d^3p}{(2\pi\hbar)^3} \; \frac{1}{e^{\beta p^2/(2m)} - 1} \tag{2.9}$$

where $\beta = 1/(k_B T)$ as usual, and we have used that

$$n_B(x) = \frac{1}{e^x - 1}$$

is the Bose factor and for the noninteracting Bose particles we have the dispersion $\epsilon(p) = p^2/(2m)$.

We can evaluate Eq. 2.9 by defining $q = \beta^{1/2} p$ giving us

$$\rho_N(T) = m(k_B T)^{3/2} \int \frac{d^3q}{(2\pi\hbar)^3} \frac{1}{e^{q^2/(2m)} - 1} \sim T^{3/2} \tag{2.10}$$

which differs markedly from the experimental result!

2.5.2 Landau's Calculation of Superfluid Density

Again this calculation relies on thinking about superfluids in both the lab and the moving superfluid frame as in Fig. 2.8. Here, however, we realize that the normal fluid is dragged by the wall and will have the same velocity as the wall, whereas the superfluid moves seperately (the fluid velocities drawn in Fig. 2.8 are for the super part of the fluid only).

Thus in the frame where the wall is moving but the super-fluid is still, the *normal* fluid current (which is the total fluid current) is given by

$$\mathbf{j}_{total} = \mathbf{j}_N = \rho_N \mathbf{v}_N \tag{2.11}$$

and we would like to calculate ρ_N.

As before, in the lab frame we have

$$\epsilon_{lab-frame} = \epsilon(\mathbf{p}) - \mathbf{v} \cdot \mathbf{p}$$

where $\epsilon(\mathbf{p})$ describes the excitation spectrum when the superfluid is in its rest frame. As mentioned in the above section where we calculated critical velocity, if $\epsilon_{lab-frame}$ becomes negative, then we get spontaneous generation of excitations and we get dissipation.

However, even if $\epsilon_{lab-frame}$ is positive, it can still be excited thermally. We expect that the density of such particles will be given by

$$n_B(\beta(\epsilon(\mathbf{p}) - \mathbf{v} \cdot \mathbf{p}))$$

and this gives the occupation probability of the state labeled $\mathbf{p}$ in the superfluid rest frame.

So, in the superfluid rest frame we have the momentum (i.e., the mass current) of the excitations (i.e., of the normal fluid) being given by

$$\mathbf{j}_N = \int \frac{d^3p}{(2\pi\hbar)^3} \, \mathbf{p} \, n_B(\beta(\epsilon(\mathbf{p}) - \mathbf{v} \cdot \mathbf{p}))$$

We can then expand for small $\mathbf{v}$ to obtain

$$\mathbf{j}_N = \int \frac{d^3p}{(2\pi\hbar)^3} \left[\mathbf{p} \, n_B(\beta\epsilon(\mathbf{p})) - \mathbf{p}\beta(\mathbf{v} \cdot \mathbf{p}) n_B'(\beta\epsilon(\mathbf{p}))\right]$$

The first term in the brackets vanishes by symmetry. To evaluate the second term, we can assume the velocity $\mathbf{v}$ is in the x direction. We then have

$$j_{N,x} = v_x \beta \int \frac{d^3p}{(2\pi\hbar)^3} p_x^2 \left[-n_B'(\beta\epsilon(\mathbf{p}))\right]$$

Referring back to Eq. 2.11 and realizing that the wall velocity v is the normal fluid velocity we obtain the result that

$$\rho_N = \beta \int \frac{d^3p}{(2\pi\hbar)^3} p_x^2 \left[-n_B'(\beta\epsilon(\mathbf{p}))\right] \tag{2.12}$$

Case 1: Noninteracting BEC

Let us try plugging in the dispersion $\epsilon(p) = p^2/(2m)$ for a noninteracting BEC. We can scale out the temperature by defining

$$\mathbf{q} = \beta^{1/2}\mathbf{p}$$

to obtain

$$\rho_N = \beta(\beta^{-5/2}) \int \frac{d^3q}{(2\pi\hbar)^3} q_x^2 \left[-n_B'(q^2/2m)\right] \sim T^{3/2} \tag{2.13}$$

which agrees with our prior calculation of the normal fluid density of a BEC in Eq. 2.10. (With some analytic work it can be shown that the two expressions in fact have the same prefactor too!).

Case 2: Interacting BEC / Superfluid

For an interacting BEC or superfluid, we expect a low energy acoustic mode so that

$$\epsilon(\mathbf{p}) = c|\mathbf{p}| + \dots$$

Again using Eq. 2.12 we can here instead define $\mathbf{q} = \beta\mathbf{p}$ so that

$$\rho_N = \beta\beta^{-5} \int \frac{d^3q}{(2\pi\hbar)^3} q_x^2 \left[-n_B'(c|q|)\right] \sim T^4 \tag{2.14}$$

in agreement with the results of Andronikoshvili! (Score one more for Landau!)

Heat capacity and a caution

It is correct to write the total internal energy of the bose system at finite temperature as

$$U = \int \frac{d^3p}{(2\pi\hbar)^3} \epsilon(p) n_B(\beta\epsilon(p))$$

Indeed, for a linear (phonon) spectrum this reproduces the usual T^3 Debye heat capacity of phonons at low temperature.

One might wonder whether we could calculate the normal fluid density by just writing

$$\tilde{\rho}_N \sim \int \frac{d^3p}{(2\pi\hbar)^3} n_B(\beta\epsilon(p))$$

While this redefinition of the normal fluid density worked in Eq. 2.10 for $\epsilon = p^2/(2m)$ (giving the same result as Eq. 2.13) it generally is not correct! Indeed, for $\epsilon = c|p|$ it fails to give the same result as Eq. 2.14.

The reason is simply that the quantity ρ_N is defined only by Eq. 2.11. One could also define the different quantity $\tilde{\rho}_N$ but this is in fact not a measurable quantity, whereas ρ_N is.

Chapter 3

Charged Superfluid ≈ Superconductor

To a large extent the phenomenology of a superconductor can be understood as just being a charged superfluid. This approach (roughly) is known as London theory, invented by Heinz and Fritz London when they were in Oxford in 1935. Historically this was before the discovery of the phenomenon of superfluidity! Indeed, much of the two fluid model was pioneered first in the context of superconductivity.

3.1 London Theory

As with the picture of superfluid Helium, we postulate both a normal and superfluid part of the charged fluid in a superconductor. We will ignore the normal component for now and focus on the motion of the super part — which flows with no dissipation.

A dissipationless fluid will display free acceleration when a force $\mathbf{F}$ is applied. We can thus write

$$\frac{\partial \mathbf{v}}{\partial t} = \frac{\mathbf{F}}{m^*} = \frac{-e^*\mathbf{E}}{m^*}$$

This is essentially Drude theory for a fluid with no scattering. We have written here a charge e^* and a mass m^* of the charge carrier. Note that here only the ratio e^*/m^* enters. This equation does not know whether the charge carrier is a single electron or a pair of electrons or quartets of electrons. However, $e^*/m^* = e/m$ in all cases.

The super current is then written as

$$\mathbf{j}_{super} = -e^* n_S^* \mathbf{v}$$

where n_S^* is the superfluid number density of the charge carriers. Note again that the combination $-e^* n_S^* = -e n_S$ does not know how big the individual particles are. It could be density n_S of particles of charge $-e$ or could be density $n_S/2$ of particles of charge $2e$

and so forth. The point here is that at level of this London theory, one has no way of knowing that the electrons might pair up into boson clusters.

Putting the last two equations together we derive the so-called First London Equation

$$\frac{\partial \mathbf{j}_{super}}{\partial t} = \frac{(e^*)^2 n_S^*}{m^*}\mathbf{E} \qquad \text{1st London Eq.} \tag{3.1}$$

Again, the charge cluster size here does not matter. Note that this equation is really nothing more than Drude theory with no scattering, and an assumption of a net charge density $-en_S$.

We can then take the curl of the first London equation and use Faraday's law to replace $\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial t$ to get

$$\nabla \times \frac{\partial \mathbf{j}_{super}}{\partial t} = \frac{(e^*)^2 n_S^*}{m^*}\nabla \times \mathbf{E} = \frac{-e^2 n_S}{m}\frac{\partial \mathbf{B}}{\partial t}$$

Then integrating both sides $\int dt$ starting at some initial time we get

$$\nabla \times \mathbf{j}_{super} = \frac{-e^{*2} n_S^*}{m^*}\mathbf{B} + \mathbf{C}(\mathbf{r}) \tag{3.2}$$

where $\mathbf{C}(\mathbf{r})$ is independent of time.

We now need to try to figure out what this integration constant $\mathbf{C}$ is. To do so, we imagine starting with a superconductor in $\mathbf{B} = 0$ in its ground state so that $\mathbf{j}_{super} = 0$. In this situation we can take $\mathbf{C}(\mathbf{r}) = \mathbf{0}$ everywhere, at least for this experimental protocol.

Next we imagine turning on $\mathbf{B}$ adiabatically. Then we have Ampere's law

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j}_{super} \tag{3.3}$$

Here we are ignoring the normal part of any current, since we are only concerned with current that is persistant. Further, since we are concerned with steady state we will ignore the contribution of $\partial \mathbf{E}/\partial t$. Taking the curl of Amperes' law we get

$$\begin{aligned} \nabla \times (\nabla \times \mathbf{B}) &= \mu_0 (\nabla \times \mathbf{j}_{super}) \\ \nabla(\nabla \cdot \mathbf{B}) - \nabla^2 \mathbf{B} &= \mu_0 \left(\frac{-e^{*2} n_S^*}{m^*}\mathbf{B} + \mathbf{C}(\mathbf{r}) \right) \\ \nabla^2 \mathbf{B} &= \frac{\mu_0 e^{*2} n_S^*}{m^*}\mathbf{B}(\mathbf{r}) \end{aligned} \tag{3.4}$$

This last equation has solutions of the form (for example)

$$\mathbf{B}(x) = \mathbf{B}_0 \; e^{\pm x/\lambda} \tag{3.5}$$

where λ is known as the *penetration depth*, and is given by

$$\lambda = \left(\frac{m^*}{\mu_0 n_S^* e^{*2}} \right)^{1/2} \tag{3.6}$$

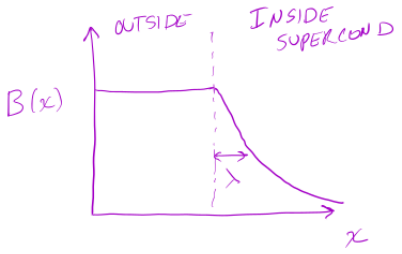


Figure 3.1: Depiction of magentic field decaying exponentially.

Once again we emphasize that this quantity does not know the size of the charged particle, but only knows the charge to mass ratio e/m and the total superfluid charge density en_S.

For most superconductors the penetration depth at zero temperature is somewhere between tens and hundreds of nanometers. Note, however, that as T gets very close to the critical temperature from below the superfluid density n_S^* gets very small (and eventually vanishes at T_c as the superfluid fraction goes to zero) so that λ diverges at T_c.

The exponential decay we derived in Eqs. 3.4 and 3.5 is depicted in Fig. 3.1. The magnetic field outside of the superconductor is a constant, but going into the superconductor it decays expontially with a decay length given by λ.

The reason the magnetic field decays going into the superconductor is that the magnetic field is screened by persistant superfluid electric currents. This is similar to Lenz's law: We start with a superconductor in no magnetic field, then we turn on a magentic field and currents flow in the superconductor to prevent the change of the magnetic field and these currents persist indefinitely since there is no resistance to current flow.

However, as we will see next, it turns out that the screening of magnetic field in a superconductor is fundamentally *more* than just Lenz's law!

3.1.1 Meissner-Ochsenfeld Effect

The Meissner-Ochsenfeld Effect (or just "Meissner Effect")[1] demonstrates that the screening of magnetic field from superconductors is not just Lenz's laws.

To demonstrate the effect, see figure 3.2. On the left we have a material in a magnetic field above its superconducting critical temperture. Then we cool the system down until it becomes a superconductor. While Lenz's law would predict that currents would flow so as to prevent any changes in the magnetic field, what is observed instead is that the magnetic field is completely expelled from the superconductor! So it is not just that the

[1] Walther Meissner had established in 1922 one of the world's only helium liquifiers in Berlin. In 1933, Meissner's student, Robert Oschsenfeld discovered that the magnetic field outside fo the superconductor changed when the superconductor is cooled through the critical tempertaure. Meissner got excited by this result and took over the experiment to the large extent.

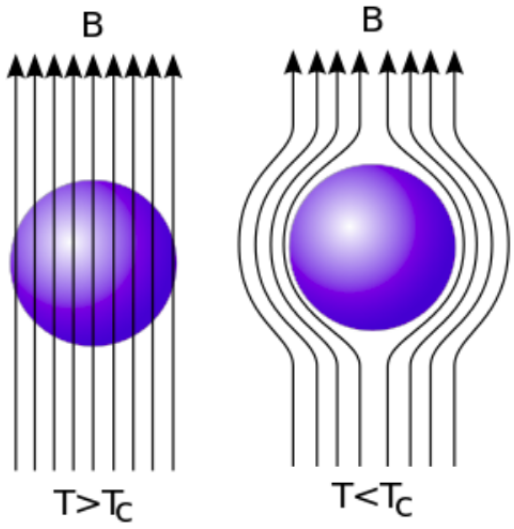


Figure 3.2: The Meissner Effect

superconductor is a perfect conductor: the superconductor is a perfect diamagnet! The ground state of the total system of superconductor and magnetic field has the magnetic field expelled from the superconductor. Thus the Meissner effect is thermodynamical not dynamical (i.e., Lenz's laws cares about the dynamics of how you get to a situation, the thermodynamic ground state does not).

To explain the Meissner effect the Londons postulated that the integration constant $C(\mathbf{r})$ in Eq. 3.2 is always zero, independent of the initial conditions. Thus we instead write

$$\nabla \times \mathbf{j}_{super} = \frac{-e^{*2} n_S^*}{m^*} \mathbf{B} \qquad \text{2nd London Equation} \tag{3.7}$$

which is known as the Second London equation. We should compare this equation to the curl free condition on superfluid helium, Eq. 2.1. This would be equivalent if we set the charge on the superfluid to zero (set $e^* = 0$).

London Gauge

Both London equations can be summarized with a single equation in terms of the vector potential by writing

$$\mathbf{j}_{super} = \frac{-e^{*2} n_S^*}{m^*} \mathbf{A} \tag{3.8}$$

if we take the curl of this equation, using $\nabla \times \mathbf{A} = \mathbf{B}$ we immediately recover the second London equation Eq. 3.7, whereas if we take the time derivative of this equation, using $\dot{\mathbf{A}} = -\mathbf{E}$ we obtain the first London equation Eq. 3.1. However we note that in order for Eq. 3.8 to make sense we have to work in so-called "London gauge" (or Coulomb Gauge)

where

$$\nabla \cdot \mathbf{A} = 0$$

This guarantees that $\nabla \cdot \mathbf{j}_{super} = 0$ which is what we need for a steady state current flow. Further, we must also choose the gauge

$$A_0 = 0$$

so that we have $\mathbf{E} = -\dot{\mathbf{A}}$ (which we already used) rather than $\mathbf{E} = -\dot{\mathbf{A}} - \nabla A_0$ which we would have otherwise.

3.1.2 Quantum Input and Superfluid Order Parameter

At this point we are going to rederive the London equations using input from quantum physics. This particular approach is beyond what the London brothers knew. We have a bit of advantage over the Londons' in that we have most of a century of experience with quantum physics, whereas in the 1930s when they were first introducing these ideas quantum mechanics was quite new[2].

Again let us we write an "order parameter" for the superconductor, which is basically a wavefunction for the superfluid (compare to the discussion of section 2.3). Given such a wavefunction ψ, we can write the superfluid current in the usual way we write a current in terms of a wavefunction

$$\mathbf{j}_{super} = \frac{e^*}{2m^*}\left[\psi^*(\mathbf{p} - e^*\mathbf{A})\psi - [(\mathbf{p} + e^*\mathbf{A})\psi^*]\psi\right]$$

A few things to note about this equation. First, it is obviously analogous to Eq. 2.5. We have included a prefactor of e^*/m^* because here we are interested in charge current rather than mass current. (Note, as we have mentioned a number of times, this ratio does not know how big the charge carrier is, it just knows the charge-to-mass ratio). Secondly we have minimally coupled the momentum to the vector potential in the usual way charged particles couple to a vector potential.

As in section 2.3 we rewrite the order parameter in terms of a magnitude and a phase

$$\psi(\mathbf{r}) = \sqrt{n_S^*}e^{i\theta(\mathbf{r})}$$

where here n_S^* is the density of superfluid charge carriers, so that the total charge density associated with the superfluid is[3]

$$\rho_S = n_S^* e^*.$$

Using $\mathbf{p} = -i\hbar\nabla$ and plugging in this form of ψ into our expresion for the superfluid current we obtain

$$\mathbf{j}_{super} = \frac{e^*}{m^*}n_S^*\hbar\nabla\theta - \frac{e^{*2}n_S^*}{m^*}\mathbf{A}$$

[2]We have another advantage over the Londons — we are alive and they are dead.

[3]In the previous chapter we used the symbol ρ_S as total *mass* density. I hope this does not cause confusion!

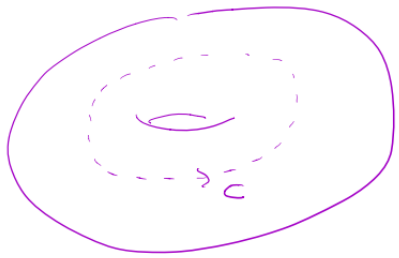


Figure 3.3: A superconducting torus. We are considering the path C as drawn.

The first term we identify as being analogous to Eq. 2.6.

We now insert a bit of physical intuition —in the ground state we expect the phase θ of the wavefunction will be a constant. We will prove this later, but for now let us just assume it is true. In this case we immediately recover the London equations in the vector potential form[4]as in Eq. 3.8

$$\mathbf{j}_{super} = \frac{-e^{*2}n_S^*}{m^*}\mathbf{A} \tag{3.9}$$

3.1.3 Superconducting Vortices

In the case of superfluid helium, we derived vorticity quantization in section 2.3.1 above. Here we would like to do something similar.

Let us consider a thick solid torus of the superconducting substance as shown in Fig. 3.3. We then consider the superconducting current cirulation around the handle of the torus

$$\oint_C \mathbf{j}_{super}\cdot\mathbf{dl} = \frac{e^*n_S^*\hbar}{m^*}\oint_C \nabla\theta\cdot\mathbf{dl} - \frac{e^{*2}n_S^*}{m^*}\oint_C \mathbf{A}\cdot\mathbf{dl} \tag{3.10}$$

For the first term on the right, just like in Eq. 2.7, the integral must be 2π times an integer. In the second term on the right, we use Stokes' theorem to give us

$$\oint_{C=\partial D} \mathbf{A}\cdot = \int_D dS\cdot(\nabla\times\mathbf{A}) = \int_D dS\cdot\mathbf{B} = \Phi$$

where here Φ is the magnetic flux enclosed by the path C. Thus Eq. 3.10 can be rewritten as

$$\oint_C \mathbf{j}_{super}\cdot\mathbf{dl} = \frac{e^*n_S^*\hbar}{m^*}2\pi p - \frac{e^{*2}n_S^*}{m^*}\Phi \tag{3.11}$$

[4]We have gotten something that seems to make sense only in London gauge. If we choose another gauge we must then not have $\nabla^2\theta \neq 0$ in order to preserve current conservation. This then destroys our intuition of thinking of θ as being similar to the phase in the Helium supefluid where $\nabla^2\theta = 0$.

where p is an integer. Rearranging this we have

$$\Phi + \frac{m^*}{e^{*2} n_S^*} \oint_C \mathbf{j}_{super} \cdot \mathbf{dl} = \frac{h}{e^*} p \tag{3.12}$$

The combination on the right hand side is often called the *fluxoid* since it is some modification to the flux. And it is this combination which is quantized. Note also the analogue of this equation to our equation for circulation quantization Eq. 2.7.

If we choose our path C to be deep inside a superconductor, we generally expect the current should be zero (any currents should run mostly on the surface, given the Meissner effect which expells any magnetic field — which currents would produce) in which case we obtain flux quantized in units of a fundamental flux quantum h/e^*.

$$\Phi = \frac{h}{e^*} p \tag{3.13}$$

Note that here it is now crucial that we know how big the charge carrying cluster e^* is! In fact we now know that the "boson" which forms the superconducting superfluid is a charge $2e$ cluster, so we have the elementary superconducting flux quantum given by[5]

$$\Phi_0 = \frac{h}{2e} = 2.067\ldots \times 10^{-15}\,\mathrm{Wb}$$

As with a superfluid, we can take the size of the hole down to zero size. This is known as a superconducting vortex. As with a superfluid, the superconducting particle density n_S must vanish at the center of the vortex and the phase twists around this point[6]. However unlike superfluid helium the rotation of the fluid is screened by the magnetic field. (Compare the 2nd London Equation, Eq. 3.7 to Eq. 2.1). Thus, the magnetic field penetrates the superconductor within a distance λ of the vortex core and screens the rotation of the fluid. Outside of this region no current flows, and there is no magnetic field.

At whatever distance we draw our path C, we will always have quantized fluxoid. If the path is far away from the vortex core, then there will be no current, and the flux enclosed is quantized. If the path is close to the vortex core, there is very little flux enclosed (let us approximate it as zero) so that the circulation is quantized.

[5] Quantization of flux through superconducting rings was first observed experimentally in 1961 by Deaver and Fairbank in Stanford and by Doll and Naubauer in Germany. Critical theory support was provided by Nina Byers and C. N. Yang. Yang had recently won a Nobel prize (in 1957) for his prediction of parity breaking in weak nuclear decays. Nina Byers was a fellow of Somerville college Oxford but remained in superposition between Oxford and California for a decade. She eventually converged in California. However, late in life she told me personally that she really had always regretted leaving Oxford. She passed away in 2014.

[6] The prediction of superconducting vortices was first made by Alexei Abrikosov of the Landau School in 1953. However, Landau didn't believe the result and prevented Abrikosov from publishing (Landau was a genius, but he was not always right!). In 1955 Feynman predicted vortices in superfluid Helium and eventually Landau was convinced of the result. Abrikosov's work was published in 1957. He won a Nobel prize for this work in 2003.

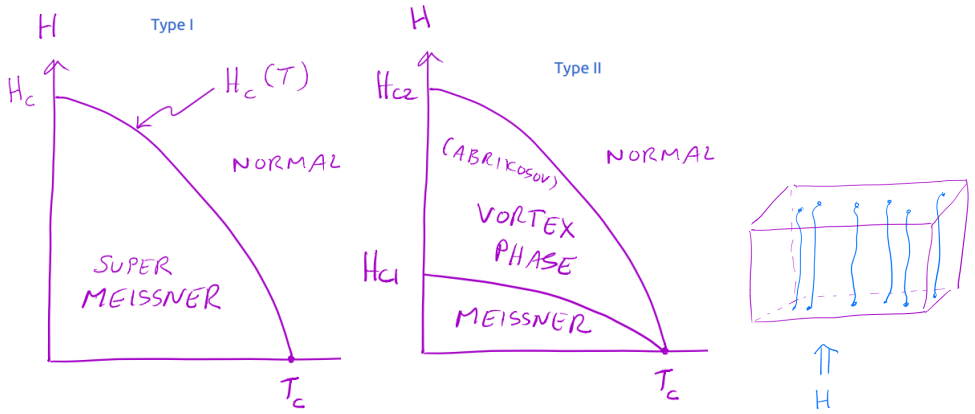


Figure 3.4: The phase diagram of Type I and Type II superconductors. Left: Type I superconductor. Magnetic field is always completely expelled whenever the material is superconducting (i.e, for fields lower than $H_c(T)$. Middle: Type II superconductor. For fields less than $H_{c1}(T)$ the magnetic field is completely expelled. However for fields between $H_{c1}(T)$ and $H_{c2}(T)$, the material is superconducting, and the magnetic field penetrates the material in discrete vortex lines. Right: A depiction of vortices penetrating a sample.

3.1.4 Type I and Type II superconductors

It turns out that there are two types of superconductors, creatively called Type I and Type II. In Type I, magnetic field does not penentrate the superconductor at all – it is completely expelled. This is known as the Meissner phase. Another way of thinking of this is that it is a perfect diamagnet[7] with susceptibility $\chi = -1$, the induced magnetization is exactly enough to precisely cancel the applied magentic field.

If enough magnetic field is applied, the superconductivity is destroyed. At temperature T, the field at which the superconductivity is destroyed is known as $H_c(T)$. This quantity goes to zero at the zero-field critical temperature T_c. (See left of Fig. 3.4) Note that although individual vortices are not stable in type I superconductors, one must still have a quantized magnetic flux through any hole in the superconductor.

The situation is different for type II superconductors. For small enough magnetic fields (below $H_{c1}(T)$, see middle of Fig. 3.4), the magnetic field is completely expelled from the superconductor giving a Meissner phase, similar to type I superconductors. However, for stronger magnetic fields $H_{c1}(T) < H < H_{c2}(T)$ the magnetic field penetrates the superconductor in individual vortex lines. This is known as the vortex phase or Abrikosov phase. (See right of Fig. 3.4). At strong enough fields, above $H_{c2}(T)$, the superconductivity is completley destroyed.

[7] To remind you $\mathbf{M} = \chi\mathbf{H}$ defines the susceptibility.

Vortex Pinning

Note that in the vortex phase, if vortices move, then the flux moves with it. This then generates a voltage via the Faraday effect

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} .$$

Thus, in the vortex phase, voltage (and hence resistance) is zero *only* if the vortices are not allowed to move.

The way one arranges for vortices to not move is to have them stick to pieces of disorder. Indeed, there is good reason that vortices stick to disorder. If some disorder kills superconductivity locally, a vortex that sits at this position costs no energy locally, because there is no superconductivity to kill. Hence vortices will try to stick to regions where superconductivity is already killed.

This phenomenon of vortex pinning being necessary in order to have a true zero resistance state is very similar to our experience with ferromagnets, where domain walls must be pinned by disorder in order to have a true ferromagnet that retains magnetization even in zero field.

3.1.5 How big is H_c

The size of the various critical fields depends on the particular superconductor. Some superconductors have critical fields in the milli-Tesla range, and others have critical fields that are tens of Telsa. Typically the more "robust" superconductors — meaning those with higher critical temperature — also have higher critical fields. Both temperature and magnetic field are perturbations that destroy superconductivity, and it is typically the case that a material that is stongly resistant to one is also strongly resistant to the other.

We can understand the critical fields with more detailed thermodynamics. We start by writing a Gibbs free energy, and consider changing the applied magnetic field $\mathbf{H}$, we have

$$dG = -\mu_0 \mathbf{M} \cdot \mathbf{H} V$$

where V is the volume of the system, and $\mathbf{M}$ is the magnetization (which is magnetic moment per unit volume). For simplicity let us assume that both $\mathbf{H}$ and $\mathbf{M}$ are aligned along the z-axis. We then integrate to obtain

$$G(H,T) - G(H=0,T) = -\mu_0 V \int_0^H dH' \; M(H') \tag{3.14}$$

The magnetization is typically given in terms of a magnetic susceptibility

$$M = \chi H'$$

Let us start by focusing on **type-I superconductors**. Type-I superconductors completely expell the magnetic field, meaning $\chi = -1$ as discussed above. Thus we can substitute into Eq. 3.14 and integrate to obtain

$$G_{super}(H,T) - G_{super}(H=0,T) = \mu_0 V H^2/2 \tag{3.15}$$

whereas for the normal state of a material, typically $\chi \ll 1$ and we have instead

$$G_{normal}(H,T) - G_{normal}(H=0,T) \approx 0$$

Now at the transition into the normal state (H_c) the free energy of the normal state and the free energy of the superconducting state must be the same (hence the transition), so we have

$$G_{super}(H_c,T) = G_{normal}(H_c,T) \approx G_{normal}(0,T)$$

Now substituting into Eq. 3.15 at $H = H_c$ we obtain

$$G_{normal}(H=0,T) - G_{super}(H=0,T) = \mu_0 V H_c^2/2 \tag{3.16}$$

This quantity is known as the *condensation energy*, and it is the amount of energy saved by allowing the material to superconduct rather than remain in the normal state.

On the other hand we can consider the free energy of **type-II superconductors** in a magnetic field. Here, the magnetic field penentrates the superconductor, but guided into flux vortices as shown in the right of Fig. 3.4. We should thus expect that the free energy is given by

$$G_{super}(H) \approx G_{super}(H=0) + N\epsilon L$$

where N is the number of vortices, L is the length of the vortex (i.e., the thickness of the sample) and ϵ is some energy per unit length.

Since each vortex accounts for Φ_0 worth of flux (one flux quantum), we thus have

$$N = \text{number of vortices} = \frac{\text{Area } H\mu_0}{\Phi_0}$$

So that we can write

$$G_{super}(H) = G_{super}(H=0) + \frac{V\epsilon H\mu_0}{\Phi_0}$$

which is linear in magnetic field, compared to Eq. 3.15 for the type I superconductor where the free energy difference is quadratic in magnetic field. We thus obtain a picture like that shown in Fig. 3.5. For applied magnetic fields less than $H_{c1} \approx 2\epsilon/\Phi_0$ the complete expulsion of the magnetic field (i.e., the Meissner phase) is energetically favorable. On the other hand, if $H > H_{c1}$ the vortex phase is lower energy.

Now the actual value of H_{c1} depends on ϵ, the energy per unit length of the vortex line. If ϵ is small, then vortex lines are not energetically costly and correspondingly H_{c1} will be small. If on the other hand, ϵ is large, then H_{c1} will be large. In some cases H_{c1} can be greater than H_c, meaning that the energy per unit length of a vortex is so large that at the magnetic field necessary to force a vortex to penetrate the superconductor, the superconductivity is already destroyed. This is precisely the case of a type-I superconductor where there is no vortex phase.

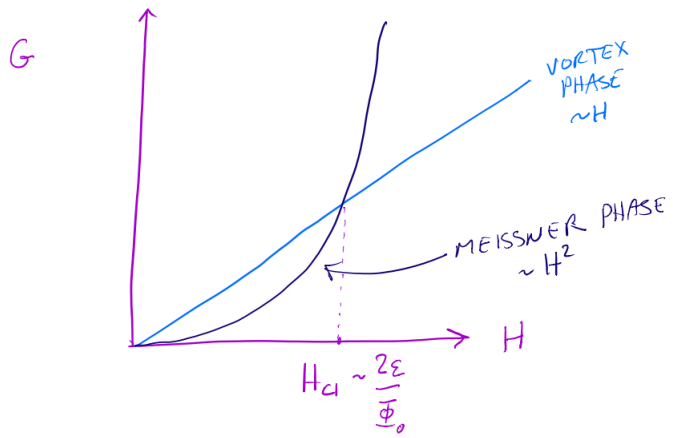


Figure 3.5: Gibbs free energy for the Meissner phase versus the vortex phase. For $H < H_{c1}$ the Meissner phase is the ground state, whereas for $H > H_{c1}$ the vortex phase is lower energy.

Chapter 4

Microscopic Theory of Bosons

We now try to derive some of the above discussed results on both bosonic superfluids and superconductors using a microscopic quantum mechanical picture.

4.1 Mathematical Preliminaries

We begin with some mathematical preliminaries on using second quantized operators. While many people will have seen this before, it is worth repeating because it is easy to get confused when it comes to some of the more complictated basis transformations and so forth[1].

4.1.1 Second quantization

We start with standard ladder operators for a harmonic oscillator

$$[a, a^\dagger] = 1.$$

The n^{th} mode of the harmonic oscillator, written in normalized form is

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$$

where $|0\rangle$ is the ground state. The states $|n\rangle$ with $n \geqslant 0$ form an orthonormal set.

The magic of second quantization is that it is entirely equivalent to say that $|n\rangle$ represents n bosons in an orbital!

We can write the number operator, which counts the number of bosons in this orbital as

$$\hat{n} = a^\dagger a = \text{number operator}$$

[1] I always get confused as to where the complex conjugations go.

4.1.2 Coherent States

We define a coherent state as

$$\begin{aligned} |\alpha\rangle_c = e^{\alpha a^\dagger}|0\rangle &= \left(1 + \alpha a^\dagger + \frac{\alpha^2 (a^\dagger)^2}{2} + \ldots\right)|0\rangle \\ &= \left(|0\rangle + \alpha|1\rangle + \frac{\alpha^2}{\sqrt{2!}}|2\rangle + \ldots\right) \end{aligned} \tag{4.1}$$

A few comments are in order here. First, we have put a subscript $_c$ on the ket $|\alpha\rangle_c$ to indicate that it is a coherent state. If no confusion will result, we may drop this subscript. Secondly, note that the coherent state $|\alpha\rangle_c$ is not normalized. In fact it is easy to show that[2]

$$_c\langle\alpha|\alpha\rangle_c = e^{|\alpha|^2} \neq 1$$

Similarly the coherent states are not orthogonal

$$_c\langle\alpha|\alpha'\rangle_c = e^{\alpha^*\alpha'}$$

Finally it is worth noting that if we examine the prefactors in Eq. 4.1 which are of the form $\alpha^n/\sqrt{n!}$ we will discover that this combination peaks at roughly $\sqrt{n} \approx |\alpha|$.

The point of using coherent states is that it allows us to turn creation and annihilation operators into numbers as we will now show.

Recall that

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

Applying this to Eq. 4.1 we obtain

$$\begin{aligned} a|\alpha\rangle_c &= \left(0 + \alpha|0\rangle + \frac{\alpha^2}{\sqrt{2!}}\sqrt{2}|1\rangle + \frac{\alpha^3}{\sqrt{3!}}\sqrt{3}|2\rangle + \ldots\right) \\ &= \alpha|\alpha\rangle_c \end{aligned}$$

Thus the coherent state $|\alpha\rangle_c$ is an eigenstate of the annihilation operator with eigenvalue α.

Thus, we can take a and replace it by α if the a operator is acting on the coherent state α. We then get the mapping

$$\begin{aligned} a &\to \alpha & a|\alpha\rangle_c &= \alpha|\alpha\rangle_c \\ a^\dagger &\to \alpha^* & _c\langle\alpha|a^\dagger &= {}_c\langle\alpha|\alpha^* \end{aligned}$$

So that a creation operator $a^\dagger$ acting to the left can also be replaced by α^*.

Let us use this principle to do some simple calculation. For example, let us calculate the expectation of the number operator $\hat{n}$ in the coherent state $|\alpha\rangle_c$.

[2] It is a simple excercise to show these! Try it!

We have (recalling that are working with non-normalized states)

$$\langle \hat{n} \rangle = \frac{{}_c\langle \alpha | a^\dagger a | \alpha \rangle_c}{{}_c\langle \alpha | \alpha \rangle_c}$$

Allowing the a to act to the right and the $a^\dagger$ to act to the left we obtain

$$\langle \hat{n} \rangle = \frac{|\alpha|^2 \; {}_c\langle \alpha | \alpha \rangle_c}{{}_c\langle \alpha | \alpha \rangle_c} = |\alpha|^2$$

Let us next try to calculate $\langle \hat{n}^2 \rangle$. Similarly we get

$$\langle \hat{n}^2 \rangle = \frac{{}_c\langle \alpha | a^\dagger a \, a^\dagger a | \alpha \rangle_c}{{}_c\langle \alpha | \alpha \rangle_c} = \frac{{}_c\langle \alpha | a^\dagger a^\dagger a \, a + a^\dagger a | \alpha \rangle_c}{{}_c\langle \alpha | \alpha \rangle_c} = |\alpha|^4 + |\alpha|^2$$

where we have used commutations to put the operators into normal order (all creation operators at the far left).

Using these two results we calcuate the variance of the number of bosons in the coherent state

$$\mathrm{Var}_N = \sqrt{\sigma_N^2} = \sqrt{\langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2} = \sqrt{|\alpha|^2} = \sqrt{\langle \hat{n} \rangle}$$

The important result here is that for large $\langle \hat{n} \rangle$ the fluctuations in particle number are much smaller than the mean – so it won't matter if we fix the particle number or we allow it to fluctuate. Given that the fluctuations are small, a system with a fixed particle number is not very different from a coherent state.

A comment for those who have not explored coherent states before: Laser light can be thought of as a coherent state of photon (which are, appropriately, bosons).

4.1.3 Multiple orbitals

Let us now consider the case of bosons which are allowed to reside in multiple orbitals. Let us assume we have an orthonormal set of orbitals which we will label $i, j, \ldots$. For each orbital i we have a corresponding creation operator $a_i^\dagger$ and annihilation operator a_i. These operators obey the commutations

$$[a_i, a_j^\dagger] = \delta_{ij} \tag{4.2}$$

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0 \tag{4.3}$$

In other words, the creation and annhilation operators in a given orbital are completely independent from the creation and annihilation operators from another orbital.

We also define a ket $|0\rangle$ to mean the vacuum of all the orbital; i.e., no bosons at all. Thus $a_1^\dagger |0\rangle$ means one boson in orbital 1, whereas $a_i^\dagger \frac{(a_2^\dagger)^2}{2!} |0\rangle$ means two bosons in orbital 2 and one boson in orbital 1, and so forth.

It is crucial that we are able to change basis for our orbitals. Suppose we have two seperate complete sets of orthonormal bases. Let us call the first set $\{|\phi_n\rangle\}$ and call the second set $\{\psi_m\}$. As an example we might imagine that one set is a set of plane waves, whereas maybe the other set is a set of harmonic oscillator wavefunctions. The conversion between the two corresponding sets of creation operators is given by

$$a^\dagger_{\phi_n} = \sum_m \langle \psi_m | \phi_n \rangle \, a^\dagger_{\psi_m} \tag{4.4}$$

A very importnat example is the case of particles hopping on a lattice. Here we have a natural tight binding basis where $\psi_{\mathbf{r_0}}(\mathbf{r}) = \delta_{\mathbf{r},\mathbf{r_0}}$ is a wavefunction of a particle localized at position $\mathbf{r}$ and the corresponding second quantized operator that creates a particle in this orbital is $a^\dagger_{\mathbf{r}}$. On the other hand, we also have the plane wave orbitals

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

with N the number of sites in the system. We write the corresponding second quantized operators that create a particle in these plane waves as

$$a_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} a^\dagger_{\mathbf{r}} \tag{4.5}$$

Any operator can be written in second quantized notation in any basis — this is done by representing it in terms of its matrix elements in that basis. For example, a one-body operator can be written as

$$\hat{O} = \sum_{n,m} \langle n | \hat{O} | m \rangle c^\dagger_n c_m$$

and so forth.

Continuum Limit

Very frequently we take the continuum limit where $\mathbf{r}$ lives not on a lattice, but in a continuum. In this case we conventionally replace the creation and annhilation operators $a^\dagger_{\mathbf{r}}$ and $a_{\mathbf{r}}$ with the continuum field operator $\hat{\psi}^\dagger(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$. The corresponding commutation relations are then given by

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$$

In terms of these field operators the plane wave creation operators are given by

$$a^\dagger_{\mathbf{k}} = \frac{1}{\sqrt{V}} \int d\mathbf{r} \, e^{i\mathbf{k}\cdot\mathbf{r}} \, \hat{\psi}^\dagger(\mathbf{r})$$

with V the volume of the system.

Indeed, any orbital basis $\{\phi_n\}$ can be written in terms of the continuum field operators as

$$a^\dagger_{\phi_n} = \int d\mathbf{r}\, \phi_n(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r})$$

The transformation in reverse, assuming we are working with a complete basis, is given by

$$\begin{aligned} \hat{\psi}^\dagger(\mathbf{r}) &= \sum_n \langle \phi_n | \mathbf{r} \rangle a^\dagger_{\phi_n} \\ &= \sum_n \phi^*_n(\mathbf{r}) a^\dagger_{\phi_n} \end{aligned} \tag{4.6}$$

4.2 BECs and the Gross-Pitaevskii Equation

We will now use second quantized operators to examine some of the physics of BECs and interacting bosons. We begin by considering noninteracting bosons.

4.2.1 Noninteracting BECs as Coherent States

The principle of a BEC is that we want to put many bosons in the same oribtal. Let us call this orbital ϕ_0, and write a creation operator $a^\dagger_{\phi_0}$ that creates a boson in this orbital. Now let us write a coherent state for many bosons in this orbital.

$$|\alpha; \phi_0\rangle \equiv e^{\alpha a^\dagger_{\phi_0}} |0\rangle$$

Enirely analogous to our above calculation we can calculate the expectatoin of the number of bosons in this orbital

$$\langle N_0 \rangle = \frac{\langle \alpha; \phi_0 | a^\dagger_{\phi_0} a_{\phi_0} | \alpha; \phi_0 \rangle}{\langle \alpha; \phi_0 | \alpha; \phi_0 \rangle} = |\alpha|^2$$

meaning that the coherent state puts (on average) $|\alpha|^2$ bosons into the orbital ϕ_0.

It is very useful to examine the effect of the field operator $\hat{\psi}(\mathbf{r})$ on the coherent state. To do this we use the decomposition given in Eq. 4.6 to give

$$\hat{\psi}(\mathbf{r}) |\alpha; \phi_0\rangle = \sum_n \phi_n(\mathbf{r}) a_{\phi_n} |\alpha; \phi_0\rangle \tag{4.7}$$

$$= \alpha \phi_0(\mathbf{r}) |\alpha; \phi_0\rangle \tag{4.8}$$

Thus, using a coherent state turns the field operator $\hat{\psi}(\mathbf{r})$ into a scalar

$$\hat{\psi}(\mathbf{r}) \to \psi(\mathbf{r}) = \alpha \phi_0(\mathbf{r}) = \sqrt{N_0}\ \phi_0(\mathbf{r})$$

where we assume the phase of α is real in the last step (although we did not have to make this assumption). Thus the field operator becomes $\psi(\mathbf{r})$ which is simply the ground state wavefunction ϕ_0 normalized to have N_0 particles.

4.3 Interacting Bosons and the Gross-Pitaevskii Equation

We now turn to consider interacting bosons. We write a first quantized Hamiltonian as

$$H = \sum_i \left[\frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_i) \right] + \frac{1}{2} \sum_{i \neq j} U(\mathbf{r}_i - \mathbf{r}_j) \tag{4.9}$$

Here, the term in bracket is a single paricle Hamiltonian, and we have included possibly a trapping potential $V(\mathbf{r})$. We can also include a chemical potential inside of V if we wish. The final term in the Hamiltonian is some intaction between the bosons.

We can now convert the first quantized Hamiltonian to second quantized form. This is a straightforward exercise[3] yielding

$$\begin{aligned} H &= \int d\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r}) \left[\frac{-\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) \\ &+ \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' : \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r})\ U(\mathbf{r} - \mathbf{r}')\ \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') : \end{aligned}$$

In the second line we have the density $\rho(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$ so that this term is an interaction between density at position $\mathbf{r}$ and position $\mathbf{r}'$. We have also included :'s around this term to indicate that the term should be interpreted as being normal ordered — i.e., all creation operators moved to the left. It is clear that this is necessary since applying this term to a state with a single boson should give a zero interaction energy (and this will not be the case unless the term is normal ordered)[4].

From here we will further specialize to a particularly simple delta-function interaction

$$U(\mathbf{r} - \mathbf{r}') = U\, \delta(\mathbf{r} - \mathbf{r}') \tag{4.10}$$

with U a scalar. Such a short range interaction is actually a very good respresentation of the interaction for many physical bosonic systems. For example, for superfluid helium, the Helium atoms are strongly repulsive only at very short distance, and so this is actually a fairly good approximation. Similarly for modern cold-atom BECs, it is often the case that the delta function interaction is actually very representative of the physical system.

This then simplifies our Hamiltonian to the form

$$H = \int d\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r}) \left[\frac{-\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{U}{2} \int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \tag{4.11}$$

Let us now consider a coherent state in an orbtial $\phi(\mathbf{r})$ as a trial wavefunction.

$$|\alpha; \phi\rangle = e^{\alpha a_\phi^\dagger} |0\rangle$$

[3] Try it! The trick is to convert terms to a convenient basis — position space or momentum space — as necessary.

[4] Note that leaving the term un-normal ordered will only make an order 1 error in an order N term, so for large numbers of particles it is not a bad mistake!

As discussed above, application of the field operator $\hat{\psi}(\mathbf{r})$ to this coherent state generates the number $\psi(\mathbf{r}) = \alpha\phi(\mathbf{r})$ with $|\alpha| = \sqrt{N}$.

We now calculate the expectation of the Hamiltonian in this coherent state

$$\begin{aligned}\langle H\rangle &= \frac{\langle\alpha;\phi|H|\alpha;\phi\rangle}{\langle\alpha;\phi|\alpha;\phi\rangle} \\ &= \int d\mathbf{r}\left(\psi^*(\mathbf{r})\left[\frac{-\hbar^2\nabla^2}{2m}+V(\mathbf{r})\right]\psi(\mathbf{r})+\frac{U}{2}|\psi(\mathbf{r})|^4\right)\end{aligned}$$

Finally integrating by parts to handle the derivative we get

$$\langle H\rangle = \int d\mathbf{r}\left(\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r})|^2+V(\mathbf{r})|\psi(\mathbf{r})|^2+\frac{U}{2}|\psi(\mathbf{r})|^4\right)$$

This expression is known as the Gross-Pitaevskii (or Ginzburg-Landau) form. This was first discussed by Vitali Ginzburg and Landau in 1950 in the context of superconductivity[5]. In 1960 it was rederived by both Gross (in the west) and Pitaevskii (in the USSR) in the context of superfluid Helium.

Minimizing the energy by taking a functional derivative and setting it to zero,

$$\frac{\delta\langle H\rangle}{\delta\psi^*(\mathbf{r})} = 0$$

we obtain

$$\left[\frac{-\hbar^2\nabla^2}{2m}+V(\mathbf{r})+U|\psi(\mathbf{r})|^2\right]\psi(\mathbf{r}) = 0 \tag{4.12}$$

which is known as the Gross-Pitaevskii equaiton, or non-linear-Schroedinger equation. We will study the solutions to this equation later.

4.3.1 Rederivation without Coherent States

Is there an easier way to get to the Gross-Pitaevskii equation? Do we need to work in a "grand-canonical ensemble" where the number of bosons is indefinite? Do we really have to work with second quantized operators?

The answer to these questions are: Yes, there is an easier way. We don't need any of these technical tools. In fact we can work with first quantized operators with a fixed number of particles.

Recall that a BEC wavefunction puts a macroscopic number of particles in a single orbital $\phi(\mathbf{r})$. So let us write a trial wavefunction for such a BEC as follows:

$$\Psi = \prod_{i=1}^{N}\phi(\mathbf{r}_i)$$

[5]Ginzburg won a Nobel prize for this work in 2003. It is worth reading Ginzburg's Nobel biography. It seems his early years, growing up in the Stalinist Soviet Union were somewhat harrowing!

Note that this wavefunction is properly antisymmetic under exchange of particle positions as a bosonic wavefunction should be.

We then find the expectation of our first quantized Hamiltonian Eq. 4.9 for our trial state

$$\langle\Psi|H|\Psi\rangle = N\int d\mathbf{r}\ \phi^*(\mathbf{r})\left[\frac{-\hbar^2\nabla^2}{2m}+V(\mathbf{r})\right]\phi(\mathbf{r})+\frac{N(N-1)}{2}\int d\mathbf{r}\int d\mathbf{r}' : |\phi(\mathbf{r})|^2\ U(\mathbf{r}-\mathbf{r}')\ |\phi(\mathbf{r}')|^2$$

making the substitution $\psi = \sqrt{N}\phi$ and neglecting the distinction between N and $N-1$ we get exactly the same result as when we used coherent states above. Minimizing the total energy in either approach will allow us to calculate the best single orbital $\phi(\mathbf{r})$, or equivalently ψ, which we should macroscopically occupy to form a BEC.

4.4 Order Parameter and Off-Diagonal Long Ranged Order

So if it is possible to derive everything with such a simple first quantized approach, why then did we go through the extra work of working with coherent states and using second quantization? The reason is that for an interacting BEC (particularly a strongly interacting BEC) it is in fact *not* correct to put all the bosons in a single orbital. A single orbital may be multipy occupied, but due to the interactions some bosons will be kicked out of this single orbital. We will discuss this physics in more detail later. However, despite this complication

$$\langle\hat{\psi}(\mathbf{r})\rangle \tag{4.13}$$

will remain a good order parameter and a good description, and a convenient description, of the condensate.

It is worth noting, however, that there are some who object to the use of such an object as an order paramter. The obvious objection is that it is perfectly possible to consider a system of bosons with a fixed number, in which case the order parameter Eq. 4.13 is strictly zero and one needs to think a bit harder[6]. It is enlightening to go through some extra work to try to understand in a bit more detail the physics of the superfluid order parameter for the case of fixed particle number.

Let us try to be a bit more precise with our definition of the order paramter for a system with strongly interacting bosons. We can here work with a fixed number of particles (a canonical ensemble). Let us write the folowing density operator

$$\rho_1(\mathbf{r}',\mathbf{r}) = \langle\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r})\rangle \tag{4.14}$$

This operator removes a particle from position $\mathbf{r}$ and puts a particle back in at position $\mathbf{r}'$. While this conserves total particle number, it does not *locally* conserve particle number if

[6]The Nobel Laureate Tony Leggett in particular has emphasized the shortcomings of a number non-conserving order parameter

$\mathbf{r}$ and $\mathbf{r}'$ are very different. In terms of the multi-particle wavefunction, this object can be written as

$$\rho_1(\mathbf{r}', \mathbf{r}) = \int d\mathbf{r}_2 \int d\mathbf{r}_3 \ldots \int d\mathbf{r}_N \;\; \Psi^*(\mathbf{r}', \mathbf{r}_2, \ldots, \mathbf{r}_N)\Psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

We can even write this quantity at finite temperature more generally as

$$\rho_1(\mathbf{r}', \mathbf{r}) = \sum_n e^{-\beta E_n} \int d\mathbf{r}_2 \int d\mathbf{r}_3 \ldots \int d\mathbf{r}_N \;\; \Psi_n^*(\mathbf{r}', \mathbf{r}_2, \ldots, \mathbf{r}_N)\Psi_n(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

Note also that $\rho_1(\mathbf{r}, \mathbf{r})$ is just the regular density at position $\mathbf{r}$, and if we wanted to, we could write even more complicated operators such as

$$\rho_2(\mathbf{r'}_1, \mathbf{r'}_2; \mathbf{r}_1, \mathbf{r}_2)$$

which would be an analogous expression with $N - 2$ integrals.

For a moment, let us think of positions $\mathbf{r}'$ and $\mathbf{r}$ as being discrete. In this case, we can think of $\rho_1(\mathbf{r}', \mathbf{r})$ as actually being a matrix (it has two indices, $\mathbf{r}'$ and $\mathbf{r}$). Since this matrix is hermitian it can be diagonalized and written in terms of its eigenvalues, which we call N_α and its eigenvectors which we call $\phi_\alpha(\mathbf{r})$. We thus have

$$\rho_1(\mathbf{r}', \mathbf{r}) = \sum_\alpha N_\alpha \, \phi_\alpha^*(\mathbf{r}')\phi_\alpha(\mathbf{r})$$

where the eigenvectors are normalized

$$\int d\mathbf{r} |\phi_\alpha(\mathbf{r})|^2 = 1$$

By convention we order the eigenvalues so that N_0 is the largest.

Noninteracting BEC at $T = 0$

For a noninteracting BEC at zero temperature, all of the bosons are in the same orbital. In this case it is easy to calculate that there is only one nonzero eigenvalue $N_0 = N$, the number of particles in the system, and ϕ_0 is the single macroscopically occupied orbital.

Let us consider this case in a bit more detail. For a noninteracting BEC without a trapping potential at $T = 0$, all of the bosons are in the single $\mathbf{k} = 0$ eigenstate, $\phi_0 = 1/\sqrt{V}$. We can then explicitly calculate the order parameter. The easiest way to calculate this is to go back to second quantized form of Eq. 4.14. We then have

$$\rho_1(\mathbf{r}', \mathbf{r}) = \langle \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}) \rangle = N\phi_0^*(\mathbf{r}')\phi_0(\mathbf{r}) = N/V$$

the particle density, for all $\mathbf{r}$ and $\mathbf{r}'$. See also the more detailed calculation in section 4.4.1 below.

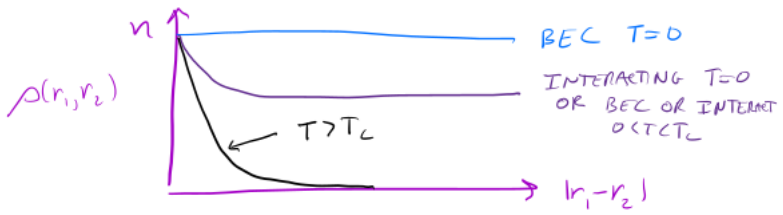


Figure 4.1: Measure of Off-Diagonal Long Range Order $\rho_1(\mathbf{r}_1, \mathbf{r}_2)$. For $\mathbf{r}_1 = \mathbf{r}_2$ we always have $\rho_1 = n = N/V$ the density. However, for $\mathbf{r}_1$ far from $\mathbf{r}_2$ a nonzero ρ_1 indicates the presence of a condensate. For a noninteracting BEC at $T = 0$ (top line) $\rho_1 = n$ for all $|\mathbf{r}_1 - \mathbf{r}_2|$. For a system in the normal phase, $T > T_c$, we have ρ_1 decaying to zero for large $|\mathbf{r}_1 - \mathbf{r}_2|$ as shown in the bottom line. The middle line shows that for a noninteracting BEC at $0 < T < T_c$ or for an interacting BEC at any $T < T_c$, then ρ_1 decays to a constant less than n but larger than zero.

More generally

However, we expect that even for a BEC for $0 < T < T_c$, there should be a single eigenvalue N_0 which will be smaller than N but still extensively large (we will demonstrate this below). Further, even for an interacting system, we can use N_0 being extensive as an indication of the existance of a condensate and ϕ_0 is the condensate wavefunction. Putting these two together into an order parameters, we have

$$\psi(\mathbf{r}) = \sqrt{N_0}\,\phi_0(\mathbf{r})$$

We can make a plot of ρ_1 for severeal different cases as shown in Fig. 4.1.

Recall that $\rho_1(\mathbf{r}_1, \mathbf{r}_2)$ is always just the density n for $\mathbf{r}_1 = \mathbf{r}_2$.

As shown in the figure (and we just discussed) for a noninteracting BEC at $T = 0$ we have $\rho_1(\mathbf{r}_1, \mathbf{r}_2)$ is constant as a function of distance $|\mathbf{r}_1 - \mathbf{r}_2|$. For a normal system without a condensate $T > T_c$, we have ρ_1 decaying to zero for large $|\mathbf{r}_1 - \mathbf{r}_2|$. We will prove this explicitly below.

Another case shown in the figure, that we will derive below is the case of a noninteracting BEC for $0 < T < T_c$. In this case ρ_1 decays to a constant larger than zero, but less than n for large $|\mathbf{r}_1 - \mathbf{r}_2|$.

More difficult to show, however, is the case of an *interacting* bose system below its critical temperature (possibly at $T = 0$, but possibly at $0 < T < T_c$). The behavior here is similar to that of a BEC at $0 < T < T_c$, that is ρ_1 decays to a constant larger than zero, but less than n for large $|\mathbf{r}_1 - \mathbf{r}_2|$. Qualitiatively this is again due to the fact that, similar to temperature, the interactions "kick" some of the bosons out of the single condensed state. For example, for superfluid Helium at $T = 0$ at large $|\mathbf{r}_1 - \mathbf{r}_2|$ the value of ρ_1 is less than 10% of the density.

The fact that the ρ_1 correlator becomes a constant for large $|\mathbf{r}_1 - \mathbf{r}_2|$ in the superfluid phase is known as *Off-Diagonal Long Ranged Order*[7]. It is sometimes abbreviated as ODLRO. The reason it is called 'off-diagonal" comes again from thinking about ρ_1 as a matrix with two indices, $\mathbf{r}_1$ and $\mathbf{r}_2$ which are taken different from each other (hence off-diagonal). The idea of using this quantity as an indicator of superfluid order is due to Oliver Penrose[8] in 1951 and the Nobel Laureate Lars Onsager in 1956.

4.4.1 non-interacting bosons at $T \geqslant 0$

It is easy enough to calculate ρ_1 explicitly for a noninteracting bose system at finite temperature (we will again assume no trapping potential so the single particle eigenstates are plane waves). It is again easiest to work with the second quantied definition of ρ_1 given in Eq. 4.14. We can also decompose the field operator into fourier modes

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{4.15}$$

We thus have

$$\rho_1(\mathbf{r}', \mathbf{r}) = \langle \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r})\rangle = \frac{1}{V} \sum_{\mathbf{k},\mathbf{k}'} \langle a^\dagger_{\mathbf{k}'} a_{\mathbf{k}}\rangle e^{i\mathbf{k}\cdot\mathbf{r} - i\mathbf{k}'\cdot\mathbf{r}'}$$

Where we can always write

$$\langle a^\dagger_{\mathbf{k}'} a_{\mathbf{k}}\rangle = \delta_{\mathbf{k},\mathbf{k}'} n_B(\epsilon_{\mathbf{k}})$$

where $\epsilon_{\mathbf{k}}$ is the energy of the boson in mode $\mathbf{k}$ and n_B is the bose factor.

Thus we have explicitly

$$\rho_1(\mathbf{r}', \mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}} n_B(\epsilon_{\mathbf{k}}) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$$

Now for $T > T_c$ we have n_B being a smooth function of $\mathbf{k}$. We can then freely convert the sum into an integral, and get the usual fourier transform. Since we are fourier transforming a smooth function the result ρ_1 is smooth and goes to zero for large $(\mathbf{r} - \mathbf{r}')$.

However, for $T < T_c$ we cannot convert the sum into an integral since a macroscopic number of particles are in the $k = 0$ state. In this case we need to separate $k = 0$ from the sum over $\mathbf{k}$, and then the remainder can be considered a smooth integral.

We then have instead

$$\langle a^\dagger_0 a_0\rangle = N_0(T)$$

[7] In comparison, *diagonal long range order* would be long range order in $\rho(\mathbf{r}, \mathbf{r})$ or the density — such as crystalization.

[8] Brother of Roger Penrose.

and correspondingly

$$\rho_1(\mathbf{r}', \mathbf{r}) = \frac{N_0}{V} + \frac{1}{V}\sum_{\mathbf{k}\neq 0} n_B(\epsilon_{\mathbf{k}}) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}$$

where the sum is again a smooth and decaying function.

4.5 Bogoliubov Theory for the Weakly Interacting Bose Gas

Above we mentioned that we would analyze the effect in more detail (We claimed that the interactions somehow "kick" bosons out of the condensate leaving ρ_1 at long distance less than the full physical density even at zero temperate.

The approach we follow here, so-called Bogoliubov Theory[9] is a controlled approximation accurate in the limit of weak, but non-zero interaction.

For simplicity let us consider the case where there is no external trapping potential $V(\mathbf{r}) = 0$ so that the single particle eigenstates are plane waves. We will further, for simplicity assume the inter-particle interaction is a delta function as in Eq. 4.10. Neither of these assumptions is required for the method to work, although both make the calculation easier.

The Hamiltonian in second quantized form, as in Eq. 4.11 is given by

$$H = \int d\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r}) \left[\frac{-\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right] \hat{\psi}(\mathbf{r}) + \frac{U}{2}\int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})$$

Since the single particle eigenstaetes are plane waves we can conveniently write the field operator $\hat{\psi}(\mathbf{r})$ in Fourier modes

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{4.16}$$

and rewrite the Hamiltonian in the form

$$H = \sum_{\mathbf{k}} \frac{\hbar^2\mathbf{k}^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{U}{2V}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} a^\dagger_{\mathbf{k}_1} a^\dagger_{\mathbf{k}_2} a_{\mathbf{k}_3} a_{\mathbf{k}_4}\ \delta_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4} \tag{4.17}$$

Now we expect that even when we turn on the interactions, the $\mathbf{k} = \mathbf{0}$ mode should be macroscopically occupied at zero temperateure as it is in BEC. However the commutator

$$[a^\dagger_{\mathbf{0}} a_{\mathbf{0}}, \text{Interaction}] \neq 0$$

which means that the interaction must kick some of the particles out of the $\mathbf{k} = \mathbf{0}$ state. Nonetheless, we still expect macroscopic occupancy of this orbital. Let us thus assume

[9] Nikolay Bogoliubov is probably more famous as a mathematician than a physicist. Nonetheless he also had several important contributions to the physics world, including being one of the B's in BBGKY from statistical physics.

that the $\mathbf{k} = \mathbf{0}$ orbital is in a coherent state with mean occupancy N_0 with $1 \ll N_0 < N$. At $T = 0$ if the interaction were zero, then $N_0 = N$. For sufficiently weak interaction, we might expect that

$$N - N_0 \ll N$$

Post-facto, we will verify that this is true for weak interaction.

Since we have a coherent state, as usual this allows us to replace operators $a_{\mathbf{0}}^\dagger$ and $a_{\mathbf{0}}$ with numbers via the usual substitution

$$a_{\mathbf{0}}^\dagger \to \sqrt{N_0} \qquad a_{\mathbf{0}} \to \sqrt{N_0}$$

Returning to our Hamiltonian, we now have a small parameter $1/N_0$ and we can organize the parts of the Hamiltonian Eq. 4.17 in terms of which has the most factors of N_0 (i.e., the most factors of $a_{\mathbf{0}}^\dagger$ or $a_{\mathbf{0}}$). In fact, the kinetic term has no factors of N_0 (since the kinetic energy of the $\mathbf{k} = \mathbf{0}$ state is zero). We thus turn to the interaction term and try to organize the pieces of the sum in order of which pieces have the most factors of N_0.

Looking at the sum over $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4$, the single term where

$$\mathbf{k}_1 = \mathbf{k}_2 = \mathbf{k}_3 = \mathbf{k}_4 = 0$$

is the largest term, giving us four factors of $\sqrt{N_0}$ Thus the value of this term in the sum is simply the constant

$$\frac{U}{2V} N_0^2 \tag{4.18}$$

At next order We look for a term where there are three factors of $\sqrt{N_0}$ meaning three of the $\mathbf{k}$'s are zero and one is nonzero. However, the delta function in the interaction term of Eq. 4.17 requires that if three of the $\mathbf{k}$'s are zero than the fourth one is too, so no such term exists.

At next order we look for a term where two of the $\mathbf{k}$'s are zero and two are nonzero. Necessarily the momenta on the remaining two $\mathbf{k}$'s must appropriately sum to zero. We can choose the two non-zero $\mathbf{k}$'s to be both creation, both annihilation, or one of each (which can be chosen in four different ways). Thus the sum of all these terms can be written as

$$\frac{UN_0}{2V} \sum_{\mathbf{k} \neq 0} \left[4\, a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{-\mathbf{k}} a_{\mathbf{k}} \right] \tag{4.19}$$

We can then look for terms where only one of the $\mathbf{k}$'s is zero. There are such terms, but these will be smaller by a factor of $1/\sqrt{N_0}$ so we throw these out. (In principle at the end of the calculation these terms can be considered as a small perturbation on top of what find).

We then assemble the terms we find. First, the kinetic term from the Hamiltonian Eq. 4.17, secondly, the zeroth order term Eq. 4.18 and the second order term Eq. 4.19.

Finally we use one additional trick, we write

$$N_0 = a_0^\dagger a_0 = N - \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$$

plugged inot the N_0 in Eq. 4.18 and we obtain the resulting Hamiltonian

$$H = \frac{U\rho}{2}N + \sum_{\mathbf{k}\neq 0}\left\{\left[\frac{\hbar^2\mathbf{k}^2}{2m} + U\rho\right]a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{U\rho}{2}\left(a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{-\mathbf{k}}a_{\mathbf{k}}\right)\right\}$$

where $\rho = N/V$. This Hamiltonian is quadratic (and therefore solvable), but it has so-called *anomolous* terms —those with two creation or two annihilation operators. These terms allow particles to scatter in or out of the condensate (the state with $\mathbf{k} = \mathbf{0}$). The scattering terms must conserve total momentum so you can only scatter two-in or two-out at a time.

4.5.1 Bogoliubov Transform

To solve the quadratic hamiltonian with anomolous terms, we invoke the so-called Bogoliubov transformation (invented 1947, by Bogoliubov). Let us write the following transformation

$$\begin{pmatrix} b_{\mathbf{k}} \\ b_{-\mathbf{k}}^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta_{\mathbf{k}} & \sinh\theta_{\mathbf{k}} \\ \sinh\theta_{\mathbf{k}} & \cosh\theta_{\mathbf{k}} \end{pmatrix}\begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{pmatrix} \tag{4.20}$$

It is easy to check given that the a's satistfy canonical commutations as in Eqs. 4.2 adn 4.3, then the b's similarly satisfy canonical commutations[10]

$$[b_{\mathbf{q}}, b_{\mathbf{p}}^\dagger] = \delta_{\mathbf{q},\mathbf{p}}$$
$$[b_{\mathbf{q}}, b_{\mathbf{p}}] = [b_{\mathbf{q}}^\dagger, b_{\mathbf{p}}^\dagger] = 0$$

Making this transformation (with a bit of algebra) the Hamiltonian becomes

$$\begin{aligned} H &= \text{const} + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\left[\left(\frac{\hbar^2\mathbf{k}^2}{2m} + U\rho\right)\cosh(2\theta_{\mathbf{k}}) - U\rho\sinh(2\theta_{\mathbf{k}})\right]\left[b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}\right] \\ &\quad - \left[\left(\frac{\hbar^2\mathbf{k}^2}{2m} + U\rho\right)\sinh(2\theta_{\mathbf{k}}) - U\rho\cosh(2\theta_{\mathbf{k}})\right]\left[b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + b_{-\mathbf{k}}b_{\mathbf{k}}\right] \end{aligned}$$

If we then choose

$$\tanh(2\theta_{\mathbf{k}}) = \frac{U\rho}{\frac{\hbar^2\mathbf{k}^2}{2m} + U\rho} \tag{4.21}$$

[10] (Sid's favorite comment): It may look very strange that the matrix in Eq. 4.20 is not a unitary matrix. We know we are allowed to make unitary changes of basis in quantum physics, but non-unitary transforms seem problematic. The reason that this is OK here is because we are making a change of basis on *operators*. If we work out what happens to the resulting *basis states* in the Fock space under this transformation, we will discover that this actually corresponds to a unitary transformation on the Fock space! The only thing we need for this to be true is that canonical commutations are preserved.

we eliminate the anomolous terms and we diagonalize the Hamiltonian, obtaining

$$H = \text{const} + \sum_{\mathbf{k}\neq 0} E_{\mathbf{k}}\, b^\dagger_{\mathbf{k}} b_{\mathbf{k}} \tag{4.22}$$

where

$$\begin{aligned} E_{\mathbf{k}} &= +\sqrt{\left(\frac{\hbar^2\mathbf{k}^2}{2m} + U\rho\right)^2 - (U\rho)^2} \\ &\sim \sqrt{\frac{U\rho}{m}}\hbar|\mathbf{k}| + \ldots \qquad \text{for small } \mathbf{k} \end{aligned}$$

Note that this spectrum of excitations in *linear* in $\mathbf{k}$ at low $\mathbf{k}$ and then curves to be quadratic at large $\mathbf{k}$. Because the dispersion is linear it satisfies the Landau criterion for superfluidity!

The excitations created by the $b^\dagger_{\mathbf{k}}$ operators are sometimes known as *bogoliubons*. The ground state is obviously given by the state with no bogololiubons present

$$b_{\mathbf{k}}|\text{ground state}\rangle = 0 \qquad \text{for all } \mathbf{k} \neq 0$$

Note however, that since we can invert Eq. 4.20, we can write this condition as

$$b_k = \cosh\theta_{\mathbf{k}} a_{\mathbf{k}} + \sinh\theta_{\mathbf{k}} a^\dagger_{-\mathbf{k}}$$

and thus,

$$a_{\mathbf{k}}|\text{ground state}\rangle \neq 0$$

meaning that in the ground state there is some occupation of bosons in $\mathbf{k} \neq 0$ orbitals. As we predicted previously, the interaction has pushed some of the bosons out of the $\mathbf{k} = 0$ orbital.

Occupancy of $\mathbf{k} = 0$: Depletion of Condensate

Let us try to calculate how many bosons are in the $\mathbf{k} = 0$ orbital. To do this we write as above

$$N_0 = N - \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$$

so that in the ground state we have

$$\frac{N_0}{N} = 1 - \frac{1}{N}\sum_{\mathbf{k}\neq 0}\langle GS|a^\dagger_{\mathbf{k}} a_{\mathbf{a}}|GS\rangle = 1 - \frac{1}{N}\sum_{\mathbf{k}\neq 0}\sinh^2\theta_{\mathbf{k}} \tag{4.23}$$

with a bit of nasty algebra it can be shown that

$$1 - \frac{N_0}{N} \sim U^{3/2}$$

Thus, as we claimed above, for weak interaction, only a few of the bosons are kicked out of the condensate. If U becomes large, then many bosons are kicked out of the condensate and we cannot use this expansion technique.

Appendix: Some nasty algebra

To show the previous result, we first note that from Eq. 4.21 we know $\tanh 2\theta$. We then have

$$\mathrm{sech}^2 2\theta = 1 - \tanh^2 2\theta$$

so

$$\frac{1}{\sqrt{1-\tanh^2 2\theta}} = \cosh 2\theta$$

Then we use

$$\frac{1}{2}(\cosh 2\theta - 1) = \sinh\theta$$

so that we obtain

$$\frac{N_0}{N} = 1 - \frac{1}{2N}\sum_{\mathbf{k}\neq 0}\left[\frac{1}{1-\tanh^2 2\theta_{\mathbf{k}}} - 1\right] = \frac{1}{2N}\sum_{\mathbf{k}\neq 0}\left[\frac{1}{1-\left(\frac{U\rho}{U\rho+\hbar^2k^2/2m}\right)^2} - 1\right]$$

Changing the sum to an integral

$$1-\frac{N_0}{N} = \frac{V}{2N}\int\frac{\mathbf{dk}}{(2\pi)^3}\left[\frac{1}{1-\left(\frac{U\rho}{U\rho+\hbar^2k^2/2m}\right)^2} - 1\right] = 1-\frac{4\pi V}{2N(2\pi)^3}\int_0 k^2dk\left[\frac{1}{1-\left(\frac{U\rho}{U\rho+\hbar^2k^2/2m}\right)^2} - 1\right]$$

where in the last step we have switched to spherical coordinates. Finally, we rescale variables by defining $k = \sqrt{2mU\rho/\hbar^2}z$ such that we have

$$1 - \frac{N_0}{N} = (\sqrt{2mU\rho/\hbar^2})^3\frac{4\pi V}{2N(2\pi)^3}\int_0 z^2dz\left[\frac{1}{1-\left(\frac{1}{1+z^2}\right)^2} - 1\right] \sim U^{3/2}$$

as claimed.

Chapter 5

Feynman Theory of Helium-4

For a strongly interacting bose gas, the Bogoliubov theory fails to be quantitatively accurate, and we need another approach. Feynman came up with a truly ingenious approach[1] for understanding strongly interacting bose system, with the particular application of superfluid Helium-4 in mind. We will follow this method[2] in order to elucidate the physics of superfluidity further. The question we would like to answer is "what do the low energy excitations of a strongly interacting bose gas look like?".

5.1 Ground State and Low Energy Excitations

First let us consider the ground state for the superfluid at rest in first quantized wavefunction form. we can write it as

$$\Phi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

This is some very complicated function of the arguments $\mathbf{r}_1, \ldots, \mathbf{r}_N$ since, due to interactions between the bosons, there will be significant correlations between the positions of the particles. Note however, that the wavefunction must be symmetric in exchange of any two particle coordinates by bosonic symmetry.

[1] Most people agree that Feynman could easily have been given a Nobel prize for his work on superfluidity, had he not won the prize for quantum electrodynamics.

[2] The Nobel Laureate Murray Gell-Mann joked that Feynman's method consisted of three steps:

1. Write down the problem
2. Think very hard
3. Write down the solution

While obviously he was joking, this does characterize much of Feynman's work. Feynman (similar to Landau) used physical arguments to simply argue what the answer has to be, rather than having to perform lengthy calculations (although apparently in private, Feynmann did plenty of lengthy calculations that he then hid from the world to maintain the appearance of being a competely intuitive genius). The negative point of this type of approach is that while it is easy to teach a calculational method, it is hard to teach someone to come up with brilliant physical insights.

Figure 5.1: Compression Waves = Longitudinal Phonon

Even if we don't know the form of the function Φ_0 we can still construct from it a wavefunction for a superfluid flowing. This will take the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \Phi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \prod_{i=1}^{N} e^{i\theta(\mathbf{r}_i)} \tag{5.1}$$

where $\theta(\mathbf{r})$ is a function of position which must be well defined modulo 2π (and it must be single valued if the amplitude of Φ_0 nowhere vanishes).

For a uniformly flowing supefluid we can choose

$$\theta(\mathbf{r}) = \mathbf{v} \cdot \mathbf{r}$$

for some velocity $\mathbf{v}$.

We can check that the velocity of the fluid matches our expectation by looking at the current expectation

$$\mathbf{j} = \frac{1}{2} \left(\Psi^* \hat{\mathbf{p}} \Psi - (\hat{\mathbf{p}} \Psi^*) \Psi \right)$$

Being that Φ_0 is defined to be the fluid at rest, we must have

$$\mathbf{j}(\Phi_0) = 0$$

and thus one easily shows that

$$\mathbf{j}(\Psi) = \hbar n \nabla \theta$$

as expected.

Thus given a ground state wavefunction representing a stationary fluid we can write a wavefunction for a flowing superfluid. However, this is not the type of excitation we are interetsted in. So let us now consider low energy excitations given that there is no superflow.

Claim: *In absence of superflow, the only low energy excitations of an interacting bose gas are (longitudinal) phonons. i.e., compression waves.*

A depiction of compression waves is given in Fig.5.1

We will next argue why this claim is true. We constrast this situation with that of a system of fermions. For fermions (which we will discuss later) the ground state is a fermi

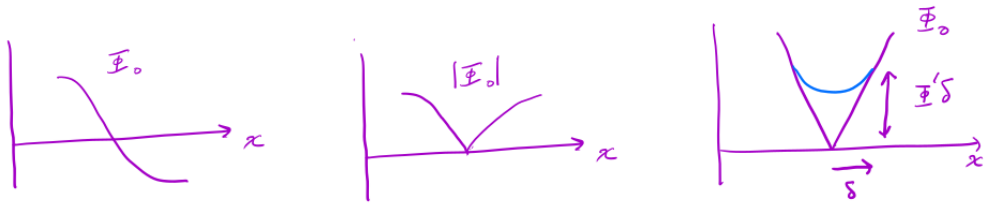


Figure 5.2: Left: A wavefunction Φ_0 which changes sign as a function of some coordinate written as x (but is meant to be some combinations of the positions $\{\mathbf{r}_i\}$. Middle: The absolute value of Φ_0. Except for (the set of measure zero) precisely at the cusp, this gives the same argument in Eq. 5.2 as Φ_0 itself. Right: Smoothing the wavefunction over a scale δ will always reduce the energy a little bit.

sea ($\mathbf{k}$ states filled up to some fermi surface). In this case we can have many different low energy excitation associated with exciting some fermion from slightly below the fermi surface to slightly above.

Point 1.1:. *The ground state wavefunction with no superflow, $\Phi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$, can be chosen real and positive everywhere.*

Firstly, since the Hamiltonian is time-reversal invariant ($H = H^*$), given that the ground state is unique, we must be able to take $\Phi_0 = \Phi_0^*$. Thus we have Φ_0 real. We would now like to show that Φ_0 does not change sign.

Since Φ_0 is assumed to be the ground state, it must minimize the energy

$$\begin{aligned} E &= \langle \Phi_0 | H | \Phi_0 \rangle \qquad (5.2) \\ &= \int \mathbf{dr}_1 \ldots \mathbf{dr}_N \left[\frac{\hbar^2}{2m} \sum_i |\nabla_i \Phi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 + \frac{1}{2} \sum_{i \neq j} U(\mathbf{r}_i - \mathbf{r}_j) |\Phi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 \right] \end{aligned}$$

We now want to show that Φ_0 for the ground state can always be taken everywhere positive. To show this we first note that if Φ_0 changes sign, then

$$E(\Phi_0) = E(|\Phi_0|)$$

The reason for this is that, as shown in Fig. 5.2, except for positions $\{\mathbf{r}_i\}$ that are a set of measure zero, both $|\Phi_0|^2$ and $|\nabla \Phi_0|^2$ are unchanged if you replace Φ_0 with $|\Phi_0|$. Thus the energy of Eq. 5.2 is unchanged.

Given that Φ_0 and $|\Phi_0|$ have the same energy, let us only consider $|\Phi_0|$ for the moment. Here, we can have a cusp where the wavefunction reaches zero. However, now we argue that we can always reduce the energy of the wavefunction by smoothing the cusp a little bit. Consider smoothing the cusp over a distance scale δ as shown in the right of Fig. 5.2. Let us estimate the energy change from doing this smoothing.

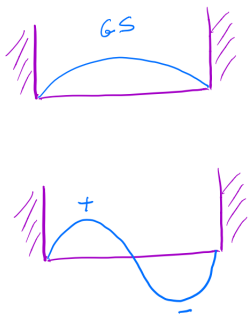


Figure 5.3: Particle in a box. Top: Ground state wavefunction is everywhere positive. Bottom: First excited state — the most positive point is far from the most negative point to minimize the gradient energy.

Roughly, the slope is reduced from $d\Phi_0/dx$ to (say for simplicity) zero, so the kinetic part of the energy (in 1d) (integrating over x) is changed decreased by roughly $\delta(d\Phi_0/dx)^2$. On the other hand, the magnitude of Φ_0 is increased from small (call it zero) to $\delta(d\Phi_0/dx)$. Thus the potential part of the energy is increased proportional to $\delta^3(d\Phi_0/dx)^2$. For small energy δ the decrease in kinetic energy always wins, and we conclude that the ground state Φ_0 can be taken everywhere strictly positive.

Point 1.2: *Any excited state must change sign so that it is orthogonal to the ground state. For a low energy excited state, one must keep gradients small, so the most positive configuration must be "far" from the most negative configuration.*

As a demonstration of this, let us consider the simple quantum mechanical problem of a single particle in a box as shown in Fig. 5.3. The ground state is everywhere postive. The first excited state must change signs to be orthogonal to the ground state. But to keep the gradient energy low, the most positive point (marked + in the figure) must be far from the most negative point (marked - in the figure).

What do these principles mean for a many-particle wavefunction? First, we realize that the first exctited wavefunction must change signs. But again we want to keep gradients small, so that the postive region should be "far" from the negative region. What do we mean by "far" in the case of a many particle wavefunction? This means "far" in the Nd dimensional parameter space $\{\mathbf{r}_i\}$ (with N the number of particles and d the spatial dimension). We might naively think that we should move all of the particles as far as possible. However, this isn't really correct, because the particles are indistinguishable. Suppose for example, we move all the particles to very far positions as in the left of Fig. 5.4. While this moves every particle "far" from its original position, it is equivalent to a different motion where each particle only moves a small distance, as shown on the right of Fig. 5.4 (due to the fact that the particles are indistinguishable). Thus we conclude that the "farthest" configuration from some initial configuration is actually a configuration where all particles move just a little bit (on order of the interparticle spacing) from their

Figure 5.4: Left: Moving particles "far" from their initial positions. Right: Since particles are indistinguishable, one can get to the same configuration by moving each particle only a little bit.

original position.

Thus we conclude that the lowest energy excitation should be some collective excitation where all particles should move a little bit. Further we know that any low energy excitation should not change the density of particles anywhere too much, since that would cost a lot of interaction energy. We claim that this will be consistent with our picture of small density waves on top of a uniform density background.

Point 2: *A good ansatz for making a low energy excited state from a ground state is to change a single quantum number (to make sure it is orthogonal to the ground state) and try to leave everything else unchanged.*

Suppose we know a ground state Φ_0. We would like to find the lowest energy excited state Ψ which minimizes

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

subject to the constraint of being orthogonal to the ground state

$$\langle \Psi | \Phi_0 \rangle = 0 \tag{5.3}$$

Let us try the approach of the approach proposed in Point 2 on the simple case of the Harmonic oscillator.

For a harmonic oscillator we know the ground state is $\Phi_0 \sim e^{-ax^2}$, and the ground state is even parity (reflects around $x = 0$). The simplest way we can change the parity quantum number if just by multiplying the wavefunction by the function x, giving a trial wavefunction $\Psi \sim x\Phi_0$. which has odd parity and then necessarily must satisfy the orthogonality condition Eq. 5.3 on account of having different parity from the ground state. This trial wavefunction is indeed very low energy because qualitatively it is as much like the ground state as it can possibly be, and yet is orthogonal to the ground state (Indeed, in this particular case we have actually guessed the exact first excited state wavefunction!).

Trial Excited State

We thus use the same general idea to write a trial wavefunction for the lowest energy excited state in an interacting bose gas. We propose the following

$$|\Psi_{\mathbf{k}}\rangle = \frac{1}{\sqrt{N}}\rho_{\mathbf{k}}|\Phi_0\rangle \tag{5.4}$$

where Φ_0 is the ground state and $\rho_{\mathbf{k}}$ is the density operator at wavevector $\mathbf{k}$ given explicitly by

$$\begin{aligned}\rho_{\mathbf{k}} &= \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = \rho^\dagger_{-\mathbf{k}} \\ &= \text{Fourier Transform}[\rho(\mathbf{r})]\end{aligned}$$

where

$$\rho(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i)$$

is the usual density operator.

Let us now list the reasons why this trial excited state wavefunction $|\Psi_{\mathbf{k}}\rangle$ is likely to be an accurate one

1. ρ is symmetric in exchanging particle (switch positions of particles i and j) so $\Psi_{\mathbf{k}}$ has the correct bosonic symmetry.

2. $\rho_{\mathbf{k}}$ changes the momentum quantum number. As described in Point 2 above, this means that the proposed excited state is necessarily orthogonal to the ground state for any $\mathbf{k} \neq \mathbf{0}$.

3. For small $\mathbf{k}$, the operator $\rho_{\mathbf{k}}$ is fairly smooth. This means that multiplying by $\rho_{\mathbf{k}}$ does not ruin any good correlations that are built into the ground state wavefunction Φ_0.

4. The operator $\rho_{\mathbf{k}}$ moves each particle just a little bit (it is a superposition of giving a small boost to each particle in turn). This matches with our disucssion in Point 1.2 that each particle should be moved only a bit.

5. The trial wavefunctiond does not correspond to a superflow (see Eq. 5.1).

6. The trial wavefunction does not change the local density much, so that it should not change the interaction energy much either.

7. Finally (to be shown below) this trial wavefunction matches up with the low energy excitations in Bogoliubov theory which is correct at least in the weak interaction limit.

Let us now confirm item 7, that we would get the same excited state wavefunction in Bogoliubov theory.

First, let us translate the density operator into second quantized notation. We can write

$$\rho(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$$

then fourier transform using the usual

$$\hat{\psi}^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} a^\dagger_{\mathbf{q}}$$

which allows us to write the fourier transformed density operator

$$\begin{aligned}\rho_{\mathbf{k}} &= \int \mathbf{dr}\; e^{i\mathbf{k}\cdot\mathbf{r}} \frac{1}{V}\sum_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{r}} a^\dagger_{\mathbf{q}'} a_{\mathbf{q}} \\ &= \sum_{\mathbf{q}} a^\dagger_{k+q} a_q\end{aligned}$$

Using the same principles we used in section 4.5 the largest terms are those that include the $\mathbf{q} = \mathbf{0}$ modes which are macroscopically occupied. With the usual replacement $a_0, a_0^\dagger \to \sqrt{N}$ we obtain

$$\rho_{\mathbf{k}} \sim \sqrt{N_0}\left(a^\dagger_{\mathbf{k}} + a_{-\mathbf{k}}\right)$$

Now from Eq. 4.22 we have that the effective hamiltonian can be written as

$$H = \text{const} + \sum_{\mathbf{k}\neq 0} E_{\mathbf{k}} b^\dagger_{\mathbf{k}} b_{\mathbf{k}}$$

so we can write the low energy excited states as

$$|\Psi_{\mathbf{k}}\rangle = b^\dagger_{\mathbf{k}}|\Phi_0\rangle$$

where Φ_0 is the ground state, meaning the Bogoliubon vacuum. We can, however, also use Eq. 4.20 to rewrite $b^\dagger$ in terms of $a^\dagger$ and a. For small $\mathbf{q}$ we have θ_q in Eq 4.20 being large which means $\sinh\theta \approx \cosh\theta$ and we have

$$b^\dagger_{\mathbf{k}} \sim a^\dagger_{\mathbf{k}} + a_{-\mathbf{k}}$$

Thus for the weakly interacting system, a single bogoliubon excitation is precisely the same as $\Psi_{\mathbf{k}}$ where we just apply the density operator to the ground state!

5.2 Single Mode Excitation Spectrum

So we have proposed a trial wavefunction Eq. 5.4 for the low energy excitations of our interacting bose gas in terms of the ground state Φ_0. Unfortunately, we do not actually

know the ground state Φ_0. Remarkably we can still make progress in calculating the energy of the excited state $\Psi_{\mathbf{k}}$. What we would like to calcualte is the energy of the excitation compared to the ground state which we write as

$$\Delta_{\mathbf{k}} = E_{\mathbf{k}} - E_0 = \frac{\langle \Psi_{\mathbf{k}} | H - E_0 | \Psi_{\mathbf{k}} \rangle}{\langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}} \rangle} \equiv \frac{f(k)}{S(k)} \tag{5.5}$$

where here we have defined the numerator to be called f and the denominator to be called S. Further, we have realized that these quantities will a function only of the magnitude $k = |\mathbf{k}|$.

Let us attack the denominator first. We have

$$S(\mathbf{k}) = \langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}} \rangle = \frac{1}{N} \langle \Phi_0 | \rho_{\mathbf{k}}^\dagger \rho_{\mathbf{k}} | \Phi_0 \rangle$$

this quantity is known as the *structure factor*, and it is directly measured by x-ray and neutron scattering[3]. We can simplify this result by using

$$\rho_{\mathbf{k}} = \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = \rho_{-\mathbf{k}}^\dagger \tag{5.6}$$

We then obtain[4]

$$\begin{aligned} S(\mathbf{k}) = \langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}} \rangle &= \frac{1}{N} \left\langle \Phi_0 \left| \textstyle\sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i} \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} \right| \Phi_0 \right\rangle \\ &= \frac{1}{N} \left\langle \Phi_0 \left| \textstyle\sum_{i,j} e^{-i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right| \Phi_0 \right\rangle \\ &= \text{Fourier Transform} \left[\left\langle \Phi_0 \left| \textstyle\sum_{i,j} \delta(\mathbf{r} - (\mathbf{r_i} - \mathbf{r_j})) \right| \Phi_0 \right\rangle \right] \end{aligned}$$

Experimental neutron diffraction measurements of the structure factor of Helium-4 are given in Fig. 5.5 The peak in the structure factor is roughly the analog of a Bragg peak for a crystal — it occurs at a wavevector of roughly $2\pi/a$ where a is the typical inter-particle spacing.

Let us now turn to the denominator of Eq. 5.5. We have

$$\begin{aligned} f(\mathbf{k}) &= \frac{1}{N} \left\langle \Phi_0 | \rho_{\mathbf{k}}^\dagger (H - E_0) \rho_{\mathbf{k}} | \Phi_0 \right\rangle \\ &= \frac{1}{N} \left[\left\langle \Phi_0 | \rho_{\mathbf{k}}^\dagger H \rho_{\mathbf{k}} | \Phi_0 \right\rangle - \left\langle \Phi_0 | \rho_{\mathbf{k}}^\dagger \rho_{\mathbf{k}} H | \Phi_0 \right\rangle \right] \\ &= \frac{1}{N} \left\langle \Phi_0 |, \rho_{\mathbf{k}}^\dagger \left[H, \rho_{\mathbf{k}} \right] | \Phi_0 \right\rangle \end{aligned} \tag{5.7}$$

[3] This is not quite the same structure factor we study in our elementary solid state courses when we study scattering from crystals, although it is very closely related. See next footnote

[4] In elementary solid state physics courses, we define the structure factor to be

$$\tilde{S}(\mathbf{k}) \sim \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j}$$

, and the scattering intensity is $\sim |\tilde{S}|^2$. However, in a fluid this $\tilde{S}(\mathbf{k})$ is zero for any $\mathbf{k} \neq 0$ since all positions are equally likely. Instead we are now calulating the expectation of the square of this quantity, with the average outside of the square.

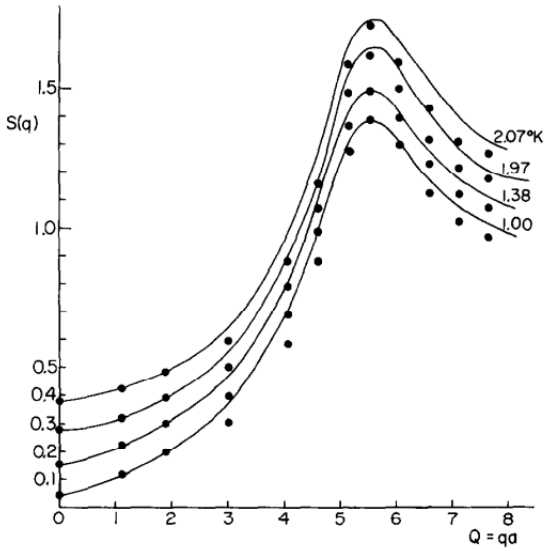


Fig. 1. Structure factor of liquid helium at various temperatures. The dots represent what Sears, Svensson, Woods and Martel have given [9].

Figure 5.5: The structure factor of superfluid Helium. Figure from A. Isihara, Physica 106B (1981) 161-164.

where in going to the second line used the fact that the Φ_0 is an eigenvalue with eigenenergy E_0.

On the other hand, we equivalently could have written

$$\begin{aligned} f(\mathbf{k}) &= \frac{1}{N}\left\langle \Phi_0|\rho_{\mathbf{k}}^\dagger(H-E_0)\rho_{\mathbf{k}}|\Phi_0\right\rangle \\ &= \frac{1}{N}\left[\left\langle \Phi_0|\rho_{\mathbf{k}}^\dagger H\rho_{\mathbf{k}}|\Phi_0\right\rangle - \left\langle \Phi_0|H\rho_{\mathbf{k}}^\dagger\rho_{\mathbf{k}}|\Phi_0\right\rangle\right] \\ &= \frac{-1}{N}\left\langle \Phi_0|[H,\rho_{\mathbf{k}}^\dagger]\,\rho_{\mathbf{k}}|\Phi_0\right\rangle \\ &= \frac{-1}{N}\left\langle \Phi_0|[H,\rho_{-\mathbf{k}}^\dagger]\,\rho_{-\mathbf{k}}|\Phi_0\right\rangle \\ &= \frac{-1}{N}\left\langle \Phi_0|[H,\rho_{\mathbf{k}}]\,\rho_{\mathbf{k}}^\dagger|\Phi_0\right\rangle \end{aligned} \tag{5.8}$$

where in going to second last line we have used the fact that, due to isotropy of the fluid we expect $f(\mathbf{k}) = f(-\mathbf{k})$ and in going to the last line we use that $\rho_{\mathbf{k}}^\dagger = \rho_{-\mathbf{k}}$.

Putting together Eq. 5.7 and 5.8 we obtain the double commutator form

$$f(\mathbf{k}) = \frac{1}{2N}\left\langle \Phi_0\left|\left[\rho_{\mathbf{k}}^\dagger,[H,\rho_{\mathbf{k}}]\right]\right|\Phi_0\right\rangle \tag{5.9}$$

We now must determine the double commutator, which will turn out to be a simple number rather than an operator! To do this we notice recall the Hamiltonian has three terms, a

kinetic term $\hat{K}$, a one body potential term $\hat{V}$ and a two body interaction term $\hat{U}$ (it would not matter if we had three or four body terms etc). We write

$$H = \hat{K} + \hat{V} + \hat{U}$$

where

$$\begin{aligned}
\hat{K} &= \sum_i \frac{-\hbar^2 \nabla_i^2}{2m} \\
\hat{V} &= \sum_i V(\mathbf{r}_i) \\
\hat{U} &= \frac{1}{2} \sum_{i,j} U(\mathbf{r}_i - \mathbf{r}_j)
\end{aligned}$$

And recall that

$$\rho_{\mathbf{k}} = \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = \rho^\dagger_{-\mathbf{k}} \tag{5.10}$$

We now want to calculate $[H, \rho_k]$. Here ρ only contains the operator $\mathbf{r}$ (not the conjugate operator ∇) and this then commutes with both U and V which also only contain $\mathbf{r}$ (and not ∇). However, ρ_k does not commute with the kinetic term, so we simplify

$$\begin{aligned}
[H, \rho_k] &= [\hat{K}, \rho_k] \\
&= \left[\sum_i \frac{-\hbar^2 \nabla_i^2}{2m} \, , \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j} \right] \\
&= \frac{-\hbar^2}{2m} \sum_j \left[\nabla_j^2 \, , \, e^{i\mathbf{k}\cdot\mathbf{r}_j} \right] \\
&= \frac{-\hbar^2}{2m} \sum_j \left(-\mathbf{k}^2 + 2i\mathbf{k}\cdot\nabla_j \right)
\end{aligned}$$

We then want to further calculate the double commutator

$$\left[\rho^\dagger_{\mathbf{k}} \, , [H, \rho_{\mathbf{k}}] \right] = \frac{-\hbar^2}{2m} \sum_j \left[\rho^\dagger_{\mathbf{k}} \, , \left(-\mathbf{k}^2 + 2i\mathbf{k}\cdot\nabla_j \right) \right]$$

The $-\mathbf{k^2}$ term is a scalar so it commutes and we have

$$\begin{aligned}
\left[\rho^\dagger_{\mathbf{k}} \, , [H, \rho_{\mathbf{k}}] \right] &= \frac{-\hbar^2}{m} \sum_j \left[\rho^\dagger_{\mathbf{k}} \, , (i\mathbf{k}\cdot\nabla_j) \right] \\
&= \frac{-\hbar^2}{m} \sum_j \left[\sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i} \, , (i\mathbf{k}\cdot\nabla_j) \right] \\
&= \frac{-\hbar^2 N}{m} \left[e^{-i\mathbf{k}\cdot\mathbf{r}} \, , (i\mathbf{k}\cdot\nabla) \right] \\
&= \frac{\hbar^2 \mathbf{k}^2 N}{m}
\end{aligned} \tag{5.11}$$

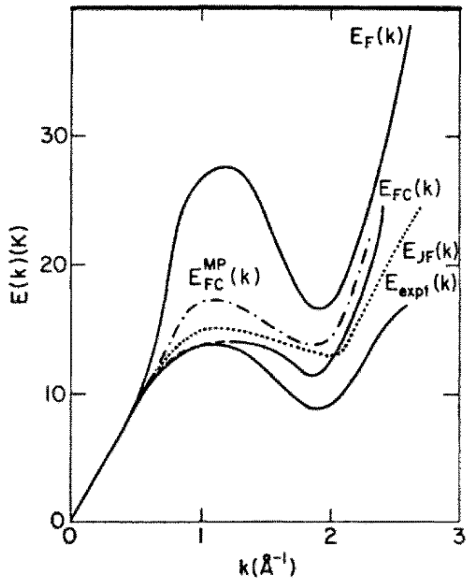


FIGURE 3.7. *Comparison of Jackson and Feenberg (1962) variational calculation of the excitation spectrum of liquid He II with prior calculations and with experiment.*

Figure 5.6: Feynman Theory and Low energy excitations of Helium. Figure from Pines and Nozieres. Top curve is prediction of Feynman theory. Bottom curve is experimental measurement of the excitation spectrum. Curves in between are modifications of the Feynman theory.

which is simply a scalar rather than an operator, as claimed. Thus plugging into Eq. 5.9 we obtain

$$f(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m}$$

We note that this double commutator calculation is used in several other common contexts, such as in the derivation of the well-known f-sum rule, and Kohn's theorem. (Don't worry if you don't know about these!).

Now plugging back into our original formula for the excitation energy, Eq. 5.5 we have

$$\Delta_{\mathbf{k}} = \frac{f(k)}{S(k)} = \frac{\hbar^2 k^2}{2mS(k)} \tag{5.12}$$

This is a rather remarkable result! In this approxiation[5], the low energy excitation spectrum is completely determined by the structure factor!

In Fig. 5.6 the top curve is the prediction of the Feynman theory using Eq. 5.12 with the experimentally measured structure factor $S(k)$ as input. The bottom curve is the

[5]It is an approximation here because we are using a trial wavefunction for the excited state.

experimentally measured excitation spectrum (using inelastic neutron scattering). The structure of the two curves is quite similar.

Note that in the long wavelength (small k) limit the Feynman theory matches the experimental results exactly. At higher k, the Feynman theory gives an excitation energy which is higher than the real excitation energy. This is to be expected. In fact, the Feynman theory can be taken to be a rigorous upper bound: What we have done is a variational calculation using $\rho_k|\Phi_0\rangle$ as the trial state — even though this isn't exactly the eigenstate (except in the long wavelength limit where it becomes exact). In the space of states orthogonal to the ground state, the exact state we are looking for is the lowest energy state, so our trial state is necessarily higher in energy than the exact state.

The minimum in energy at intermediate k is known as the *roton* minimum, and it corresponds (approximately) to the peak in the structure factor (See Fig. 5.5) at k roughly $2\pi/a$ with a the interparticle spacing.

In fact, Landau predicted this minimum before Feynman's theory. He based his prediction on specific heat data. Knowing that the spectrum is linear $E(k) = \hbar v k$ at small k, the usual Debye calculation gives a specific heat $C_v \sim T^3$ at low T. However, the experiments showed at higher T an additional contribution that appeared to turn on roughly as $\sim e^{-E_r/(k_b T)}$ for some constant E_r. Landau relized that a spectrum of the shape shown in Fig. 5.6 would give such a term where E_r is the energy of the roton minimum.

Chapter 6

Ginzburg-Landau Theory

6.1 Neutral Superfluids

Let us begin by recalling the Gross-Pitaevskii energy we derived earlier for weakly interacting (uncharged) bose gasses in Eq. 4.12 which we rewrite here

$$\langle H \rangle = \int d\mathbf{r} \left(\frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r})|^2 + V(\mathbf{r}) |\psi(\mathbf{r})|^2 + \frac{U}{2} |\psi(\mathbf{r})|^4 \right) \tag{6.1}$$

To anyone who has studied the Landau theory of phase transitions (and the associated Ginzburg-Landau[1] theory of fluctuations) this form is not surprising. Near a phase transition we typically expand a free energy order by order, writing down all terms that are allowed by symmetry. In the case of a neutral superfluid with a complex order parameter we generally expect a free energy functional of the form

$$F[\psi(\mathbf{r})] = \int d\mathbf{r} \left[\frac{\hbar^2}{2m} |\nabla \psi|^2 + \alpha_2 |\psi|^2 + \alpha_4 |\psi|^4 \right] \tag{6.2}$$

where $|\psi|^2$ is interpreted as the superfluid density[2]. Not only does this agree with Gross-Pitaevskii, but on symmetry grounds, this must be the form of the free energy near the phase transition.

[1] Vitali Ginzburg won a Nobel prize in 2003 for his eary work in the 1950s on what is now called the Ginzburg-Landau theory of superconductors. (We will come to this later in the current chapter). Ginzburg's Nobel biography is well worth a read — as a Jew in Stalin's USSR, he barely skirted death on several occassions!

[2] Generally we might have thought that the coefficient of the gradient term might have been an arbitrary fit parameter, but we fix it using the fact that if we write $\psi = |\psi| e^{i\mathbf{k}\cdot\mathbf{x}}$ we want $\hbar\mathbf{k}$ to represent a particle momentum.

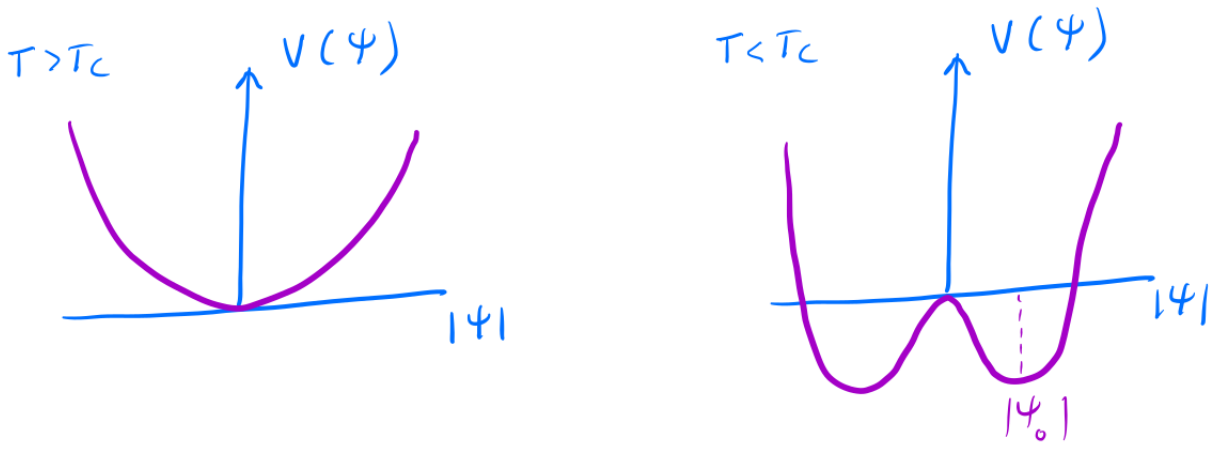


Figure 6.1: Left: The Ginzburg-Landau potential above T_c. Here the minimum is at $\psi = 0$ indicating no superfluid density. Right: The Ginzburg-Landau potential below T_c. Here the minimum is at a nonzero value of ψ indicating finite superfluid density.

6.1.1 Spatially Uniform Solution

To begin with, let us consider a uniform system — so that the gradient is zero. As in the usual theory of phase transitions we have

$$\alpha_2 = a(T - T_c)$$

with $a > 0$ and $\alpha_4 > 0$ as well for stability (i.e, so that for large enough ψ the free energy always increases.

Often we will think of the non-gradient terms of the potential as being a potential

$$\begin{aligned} V(\psi) &= \alpha_2|\psi|^2 + \alpha_4|\psi^4| \\ &= a(T - T_c)|\psi|^2 + \alpha_4|\psi^4| \end{aligned}$$

with $a > 0$.

For $T > T_c$ (so $\alpha_2 > 0$) the potential $V(\psi)$ looks like the left of Fig. 6.1, where the minimum is at $|\psi| = 0$ meaning that the ground state has no supefluid density.

On the other hand, for $T < T_c$ (so $\alpha_2 < 0$) the minimum is at some finite nonzero value of $|\psi|$ (which we label ψ_0) meaning there is a finite superfluid density ψ_0^2 in the ground state.

It is simple to minimize $V(|\psi|)$ to obtain

$$|\psi|^2 = \frac{|\alpha_2|}{2\alpha_4} = \psi_0^2 = n_s \tag{6.3}$$

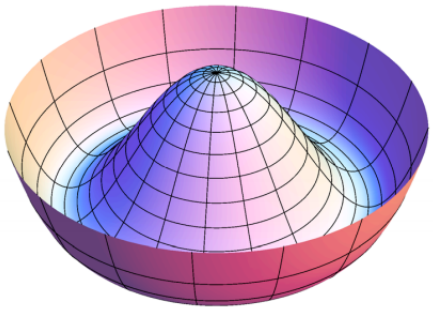


Figure 6.2: Left: The Ginzburg-Landau potential below T_c drawn as a function of the complex (2d) field ψ. The two orthogonal directions in the horizontal plane can be taken to be the real and imaginary parts of ψ. The minimum lies at the bottom of the trough (the bottom of the rim of the hat)

which is the density of the superfluid fraction.

Since ψ is actually a complex field, it should really be drawn as shown as shown as the so-called Mexican hat potential shown in Fig. 6.2. Note that the potential $V(\psi)$ is a function of $|\psi|$ only and is independent of the complex phase of ψ. This means that the ground state is degenerate — the ground state has magnitude ψ_0 but all possible complex phases have the same energy. In Fig. 6.2 we see this as the symmetry of the picture under rotation around the central z-axis. In particular, the minimum of the potential is a (degenerate) circle around the bottom of the rim of the mexican hat.

Whenever we have multiple global ground states related to each other by a contiuous symmetry (the result of spontaneously broken continous symmetry) we should have a Goldstone boson (or "Nambu-Goldstone" boson[3]). The boson in this case is the low energy excitation associated with the ground state locally reorienting this degree of freedom. In this case the Goldstone boson is nothing more than phase fluctuations of ψ (without changing the magnitude of ψ). These are the superfluid phonons, or bogoliubon excitations.

6.1.2 Spatial Dependence: Ginzburg Landau Theory

Let us now return to the free energy Eq. 6.2 and reintroduce the spatial derivative (i.e., no longer assume ψ has no spatial dependence). Here we will assume we are in the superfluid phase, i.e., $T < T_c$. To derive an equation for ψ we take the functional derivative of Eq. 6.2

[3]Named for Yoichiro Nambu, a Nobel Laureate, for his work on spontaneous symmetry breaking, and Jeffrey Goldstone, who generalized Nambu's discovery. Nambu joked that he won the Nobel prize mainly by outliving his enemies. He was 87 when he won the prize.

to minimize the free energy

$$\begin{aligned} \frac{\delta F}{\delta \psi^*} &= 0 \\ -\frac{\hbar^2}{2m}\nabla^2\psi + \alpha_2\psi + 2\alpha_4|\psi|^2\psi &= 0 \end{aligned}$$

which is a non-linear Schroedinger equation. Recalling that in a uniform system below T_c we have $|\psi_0|^2 = |\alpha_2|/(2\alpha_4)$, it is useful to define a new field

$$f = \psi/|\psi_0|$$

so that in the uniform system we just have $f = 1$.

Writing $\psi = f|\psi_0|$ and plugging into our nonlinear Schroedinger equation we obtain

$$-\frac{\hbar^2}{2m}\nabla^2 f + \alpha_2 f + 2\alpha_4|\psi_0|^2|f|^2 f = 0 \tag{6.4}$$

Dividing through by $-\alpha_2$ and using $|\psi_0|\alpha_4 = |\alpha_2|/2$ we obtain

$$\xi^2\nabla^2 f + f - f^3 = 0 \tag{6.5}$$

where

$$\xi = \sqrt{\frac{\hbar^2}{2m|\alpha_2|}} \tag{6.6}$$

is known as the Ginzburg-Landau coherence length. This is the natural length scale associated with the nonlinear Schroedinger equation. It is effectively a stiffness length for twising the phase or magnitude of the field ψ.

At low temperatures, the Ginzburg-Landau coherence length for superfluid ^{4}He is on the order of $\xi \approx 1$ Angstrom. However, note that at the critical temperature $\alpha_2 = a(T - T_c)$ changes sign (therefore going through zero) so as we approach T_c we must have ξ diverging as

$$\xi \sim |T - T_c|^{-1/2}$$

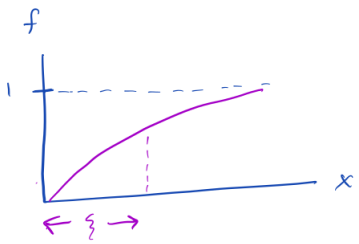
Note that Ginzburg-Landau theory is a mean field theory. A more accurate analysis of the problem will obtain a different exponent[4].

Despite the fact that our equation is nonlinear (and therefore hard to solve) some exact solutions are in fact possible.

Solution 1. Uniform solution:

$$f = 1 \quad \text{everywhere}$$

[4]This is 3d, XY universality class and $\nu = .671...$



(This one is obvious)

Solution 2. Hard wall boundary condition: We

$$f = \tanh\left(\frac{x}{\sqrt{2}\xi}\right) \tag{6.7}$$

This solution, shown roughly in Fig

$$\begin{aligned} f &\to 1 \qquad \text{at large } x \\ f &\to 0 \qquad \text{at } x \to 0 \end{aligned}$$

The proof that the tanh form in Eq. 6.7 satisfies the nonlinear Schroedinger equation 6.5 is a bit of an exercise in hypergeometric functions. We leave this to the reader.

Soltuion 3. A Single Vortex

We consider a vortex going along the z-axis. In cylindrical coordinates, we impose

$$f = |f(r)|e^{i\theta}$$

Plugging this into our nonlinear Schroedinger Equation 6.5, using

$$\nabla^2 f = \left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial}{\partial\theta}\right)\right] f$$

we obtain

$$\xi^2\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} - \frac{1}{r^2}\right]|f| + |f| - |f|^3 = 0$$

This leaves us with something that is unfortunately not analytically solvable. However, we can obtain two limits.

Small r: First, if we consider small r, we know that f needs to vanish as $r \to 0$. Thus we can throw out $|f|^3$ term. We then focus on the most singular terms which are those within the brackets. It is clear these can be made zero by using

$$|f| = \alpha r + \ldots$$

and a polynomial in r solution can be obtained. Thus we conclude that $|f| \sim r$ for small r

Large r: We know far from a vortex, we should get the bulk solution $|f| = 1$ so we look for a perturbation to this by substituting $|f| = 1 - y$. Keeping only terms linear in y and looking in the large r limit where the derivatives are suppresed we obtain

$$y = 1/(2\xi^2 r^2) + \ldots$$

so

$$|f| = 1 - 1/(2\xi^2 r^2) + \ldots$$

6.2 Charged Superfluids (i.e., Superconductors)

The same approach can be applied to charged superfluids with the additional complication being that we need to keep to keep track of the electromagnetic field. We can write a free energy function now in the form

$$\begin{aligned} F[\psi, \mathbf{E}, \mathbf{B}] &= \int d\mathbf{r} \left[\frac{1}{2m^*} |(-i\hbar\nabla - e^*\mathbf{A})\psi|^2 + \alpha_2 |\psi|^2 + \alpha_4 |\psi|^4 \right] \\ &\quad + \int' d\mathbf{r} \left[\frac{\mathbf{B}^2}{2\mu_0} + \epsilon_0 \frac{\mathbf{E}^2}{2} \right] \end{aligned} \tag{6.8}$$

and as usual $\alpha_4 > 0$ and $\alpha_2 = a(T - T_c)$ with $a > 0$. Here we have minimally coupled the momentum operator to the vector potential, and we have added the usual energy of an electromagnetic field (the second line). Note that the integral on the second line has a prime on it, this is to point out that integral of the electromagnetic field extends over all of space – the field energy still needs to be considered in regions outside of the physical sample, which may be finite.

As in the case of the neutral superfluid, below T_c we have

$$|\psi| = \psi_0 = \sqrt{\frac{|\alpha_2|}{2\alpha_4}} = \sqrt{n_s^*}$$

with n_s^* the number of particles in the superfluid (superconducting) fraction.

6.2.1 Anderson-Higgs Mechanism

As in the case of the neutral superfluid, one might expect that there would be a Goldstone mode associated with changing the phase of the order paramter — i.e., moving the field around the rim of the Mexican hat. But in fact, there is no such low energy mode of the

superfluid in a superconductor! This is precisely due to the so-called "Anderson-Higgs" mechanism[5] which we will now discuss.

It is perhaps more natural to discuss the Higgs Mechanisms in terms of Lagrangians rather than Free energies — since that makes it easier to keep track of dynamics[6]. However, so far we have been working in terms of free energies, and we will therefore continue using this approach since it is easier to compare to what we have done earlier.

First we note that the free energy is incariant under the gauge transform:

$$\begin{aligned} \psi &\rightarrow e^{i\alpha}\psi \\ e^*\mathbf{A} &\rightarrow e^*\mathbf{A} + \nabla\alpha/\hbar \end{aligned}$$

with α real. This gauge transform can be a function of both time and position $\alpha(t, \mathbf{r})$.

Recalling that for $T < T_c$ we have

$$|\Psi| = \psi_0 = \sqrt{\frac{|\alpha_2|}{2\alpha_4}}$$

which mininmize the potential $V(\psi)$. Here ψ_0 is the so-called Vacuum Expectation Value of the field, or VEV in high-energy language. Let us now consider fluctuations around this minimum.

We write

$$\psi = (\psi_0 + h)e^{i\chi} \tag{6.9}$$

where h and χ are both real. Here, h is the fluctuation of the magnitude of ψ, and χ is fluctuation of the angle around the "rim" of the Mexican hat. Near the bottom of the rim the energy should be quadratic in h describing, as

$$\alpha_2|\psi|^2 + \alpha_4|\psi|^4 = \alpha_2(\psi 0 + h)^2 + \alpha_4(\psi_0 + h)^4 = \text{const} + 2|\alpha_2|h^2 + \ldots$$

Now we would like to plug Eq. 6.9 into the free energy Eq. 6.8. However, before doing this, let us choose a gauge that absorbes the phase χ in Eq. 6.9. I.e., we gauge transform to make ψ real

$$\begin{aligned} \psi &\rightarrow \psi' = e^{-i\chi}\psi = \psi_0 + h \\ e^*\mathbf{A} &\rightarrow e^*\mathbf{A}' = e^*\mathbf{A} - \nabla\chi/\hbar \end{aligned} \tag{6.10}$$

[5]Perhaps the history of the Higgs mechanism starts with Nambu, who wrote a key paper in 1960 starting to understand the ideas of spontaneous breaking of a gauge symmetry. Then in 1962, Anderson fully described what we now call the Higgs mechanism in the context of superconductors. In 1964, in Higg's first paper (in the first paragraph) he credits Anderson saying (a) This is nothing more than extending what Anderson did to the electro-weak interactions and (b) Anderson himself suggested that a similar mechanism might exist in high energy. More detailed papers appeared the same year expanding further on the idea by Brout and Englert; and by Guralnik, Hagen, and Kibble.

[6]For those who want to write a Lagrangian, we simply consider F to be the Hamiltonian and write a Lagrangian density as $\mathcal{L} = i\hbar\psi^*\partial_t\psi - \mathcal{H}$ with $\mathcal{H}$ the Hamiltonian density.

With this transformation we have

$$\begin{aligned} F &= \int d\mathbf{r} \left[\frac{1}{2m^*} |(-i\hbar\nabla - e^*\mathbf{A}')(\psi_0 + h)|^2 + 2|\alpha_2|h^2 + \dots \right] \\ &\quad + \int' d\mathbf{r} \left[\frac{\mathbf{B}^2}{2\mu_0} + \epsilon_0 \frac{\mathbf{E}^2}{2} \right] \end{aligned} \tag{6.11}$$

Note that both the electric and magnetic fields corresponding to $\mathbf{A}'$ are the same as those corresponding to $\mathbf{A}$.

This free energy can be rewritten as

$$\begin{aligned} F &= \int d\mathbf{r} \left[\left(\frac{\hbar^2}{2m^*} |\nabla h|^2 + 2|\alpha_2|h^2 \right) + \frac{\psi_0^2 (e^*)^2}{2m^*} \mathbf{A}'^2 + \dots \right] \\ &\quad + \int' d\mathbf{r} \left[\frac{\mathbf{B}^2}{2\mu_0} + \epsilon_0 \frac{\mathbf{E}^2}{2} \right] \end{aligned} \tag{6.12}$$

One might naively expect there would have been terms $i\hbar(\nabla h) \cdot \mathbf{A}'$ but such terms have to cancel on account of being imaginary.

Let us first consider the terms involving h. this field is *massive*, meaning that there are no low energy excitation, the mass here being given by the α_2 term[7].

The term with $\mathbf{A}'^2$ represents a mass for the electromagnetic photon. Like the h^2 term, this term gives a finite energy to any nonzero value of the electromagentic field, and hence is a mass. We should compare this to the case of conventional electromagnetism where we have only the $\mathbf{B}^2$ and $\mathbf{E}^2$ terms.

$$\begin{aligned} \mathbf{B}^2 &= (\nabla \times \mathbf{A})^2 \\ \mathbf{E}^2 &= (-\nabla A_0 - \partial_t \mathbf{A})^2 \end{aligned}$$

Since both of these have derivatives, the energy of the electromagnetic field goes to zero at long wavelength (we should know this since the energy of a photon is $2\pi\hbar c/\lambda$). However, now with the $\mathbf{A}'$ term added the, energy of a photon is finite even at very long wavelenth.

What does it mean that the photon is massive? What is means is that even a long wavelength photon costs energy when it is inside a superconductor. If we imagine a photon outside a superconductor, when it tries to go into the superconductor it will experience an energetic barrier and will be repelled — this is precisely the Meissner effect, electromagnetism is expelled from superconductors!

What has happened here? The so-called Higgs mechanism is this process by which the Goldstone mode associated with the phase of the order parameter disappears (we got rid of it by absorbing the phase in Eq. 6.10), but in the process the photon becomes massive[8] Note also that where a massless photon has only two polarizations (due to the

[7] To see this, we see that any nonzero value of h gives a positive energy. The lowest energy we can get for a normalized function $h(\mathbf{r})$ is $2|\alpha_2|$ if h is uniform in space.

[8] The easy to remember catch phrase is that the gauge boson has become massive because it ate the goldstone boson... with the obvious reference being that one becomes massive when one eats. There may be other mechanisms by which the gauge boson gets some exercise and loses weight (that is a joke).

$T > T_c$		$T < T_c$
Oscillations of ψ in real and complex direciton		Oscillation of h in real direction only
2 polarizations of massless photon		3 polarizations of massive photon
4 total degrees of freedom	=	4 total degrees of freedom

Table 6.1: Conservation of total number of degrees of freedom in the Higgs mechanism.

fact that it moves at the speed of light), a massive photon which moves slower than the speed of light (like a phonon) has three possible polarizations — inlcuding a longitudinal mode. Thus, although we lose a degree of freedom from the oscillation of the field ψ, we gain a degree of freedom in a new oscillation mode of the photon. As shown in Table 6.1 the total number of degrees of freedom is the same above and below T_c.

One comment I feel compelled to add before leaving the discussion of Higgs mechanism: Particularly in the media, one often hears people say that the Higgs boson "gives" mass to particles. This is not true. The Anderson-Higgs boson in this case is the field h. However, it is the vacuum expectation value (VEV) ψ_0 that gives mass to photon. The Higgs boson represents the oscillations of the ψ field that remain once it has aquired a VEV (And further these oscillations become massive since the massless goldstone mode disappeared when we fixed the phase).

6.2.2 Energetics from Ginzburg-Landau theory: Type I and Type II superconductors revisited

From the Ginzburg-Landau potential

$$V(\psi) = \alpha_2|\psi|^2 + \alpha_4|\psi|^4$$

recall from Eq. 6.3 that we derived the minimum free energy occurs at

$$|\psi|^2 = \psi_0^2 = \frac{|\alpha_2|}{2\alpha_4} = n_s^*$$

where we have identified this quantity as the superfluid density (we have inserted the * as previously to again indicate that we do not know how many electrons might be bound together to form one boson).

Recall also from Eq. 3.6 the London penetration depth is given by

$$\lambda = \sqrt{\frac{m^*}{(e^*)^2 n_s^* \mu_0}} = \sqrt{\frac{2\alpha_4 m^*}{(e^*)^2 |\alpha_2| \mu_0}} \tag{6.13}$$

which gives us the decay length of a magnetic field when it penetrates into a superconductor.

On the other hand, we also derived in Eq. 6.6 a phase stiffness length (or coherence length)

$$\xi = \sqrt{\frac{\hbar^2}{2m^*|\alpha_2|}} \tag{6.14}$$

Note that both of these lengths as proportional

$$\xi \text{ and } \lambda \sim \frac{1}{\sqrt{|\alpha_2|}} \sim |T - T_c|^{-1/2} \tag{6.15}$$

when we are close to T_c.

Note that this exponent of $-1/2$ is a so-called *mean-field* exponent. A more careful renormalization group calculation will give a different exponent. However, it turns out that mean field theory tends to be extremely good for sueprconductors, except when one gets exceedingly close to the critical temperature[9].

The free energy density is given by

$$\begin{aligned} \min(F)/V = F[\psi_0]/V &= \alpha_2|\psi_0|^2 + \alpha_4|\psi_0|^4 \\ &= \frac{-\alpha_2^2}{4\alpha_4} \end{aligned} \tag{6.16}$$

This energy is the energy that is gained by allowing ψ_0 to become nonzero — i.e., it is the condensation energy per unit volume. Back in Eq. 3.16 we already calculated the condensation energy per unit volume and using thermodynamics we related it to the critical field H_c as

$$\text{condensation energy per volume} = \frac{mu_0 H_c^2}{2} = \frac{\alpha_2^2}{4\alpha_4}$$

Thus in terms of the Ginzburg-Landau parameters we obtain

$$H_c = |\alpha_2|\sqrt{\frac{1}{2\mu_0\alpha_4}} \sim (T - T_c) \tag{6.17}$$

as shown in Fig. 6.3

In Eq. 6.17 we have the combination $|\alpha_2|/\sqrt{\alpha_4}$ and it is useful to try to construct this combination out of the known quantities of the coherence length ξ in Eq. 6.14 and the penentration depth λ in Eq. 6.13. If we take the combination

$$\frac{1}{\xi\lambda} = \frac{|\alpha_2|}{\sqrt{\alpha_4}}\left(\frac{e^*}{\hbar}\right)\sqrt{\mu_0}$$

[9]The reason that mean field theory works so well is that that the coherence length ξ in a superconductor is extremely large compared to micscopic length scales. The typical flucations are of energy k_bT over a size ξ^D with D the dimensionality of space giving an energy density for the flucutations of $k_BT/\xi^D \sim\sim |T-T_c|^{D/2}$. We should compare this mean fluctuation energy to the mean field ground state energy density which is $\alpha_2^2/(4\alpha_4) \sim |T - T_c|^2$ (See Eq. 6.16). Close enough to T_c the fluctuation always becomes larger than the mean field energy (for $D < 4$) so mean field theory always fails. However, if the prefactor y in $\xi = y|T - T_c|^{-1/2}$ is extremely large, as it is in superconductors, then one must go very close to T_c before this failure happens.

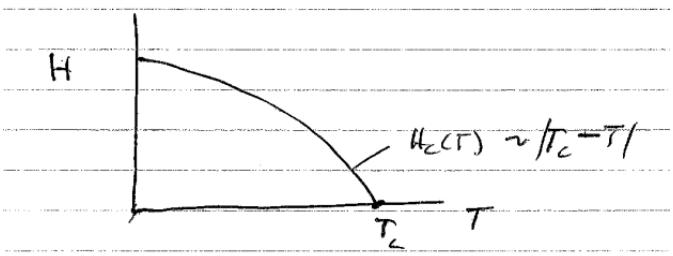


Figure 6.3: The critical field scales linearly with $T - T_c$ close to T_c, at least within a mean field theory calculation.

H_c H_{c1}

Figure 6.4: Pictoral Descriptions of Critical Fields. Left: H_c can be described as a field such that one flux quantum penetrates a box of size λ by ξ. Right: H_{c1} can be described as a field such that one flux quantum penetrates a box of size λ by λ.

where we note that a factor of $2m^*$ has cancelled here. Recalling that the superconducting flux quantum is $\phi_0 = 2\pi\hbar/(e^*)$ we can rearrange the prior two equations to get

$$H_c = \frac{1}{\xi\lambda} \frac{\phi_0}{2\pi\mu_0\sqrt{2}} \tag{6.18}$$

What this means is that if we draw a box of area λ on one side and ξ on the other side, H_c, the magnetic field necessary to completely destroy superconductivity, is the magnetic field where we have roughly one flux quantum penetrating this area as shown in the left of Fig. 6.4.

Now recall from the end of section 3.1.5 that the distinction between Type I and Type II superconductors depends on the energy per unit length ϵ, or "tension" of a vortex line. To remind you we have the lower critical field (where magnetic field first can penetrate a superconductor)

$$H_{c1} = \frac{\epsilon}{2\phi_0}$$

and if this quantity is lower than H_c then we have a Type II superconductor with a vortex (Abrikosov) phase for $H_{c1} < H < H_{c2}$, but if $H_{c1} > H_c$ then no vortex phase exists. It is thus useful to try to make an estimate of the vortex line tension ϵ, or energy per unit length of the vortex.

Roughly the energy of a vortex is due to the fact that the superconductivity is destroyed in the vortex core. Since the healing length of the order parameter is the coherence length, this means the core should be roughly size ξ. Thus the energy per unit length of the core is the condensation energy denstiy $H_c^2/(2\mu_0)$ times the area of the vortex core, $\pi\xi^2$. We thus have

$$\frac{\text{Energy}}{\text{Length}} = \epsilon = \frac{H_c^2}{2\mu_0}\pi\xi^2 \approx \frac{H_c^2}{\mu_0}\xi^2$$

where here we are dropping order unity factors (since we are not going to get them right anyway!). We thus have

$$H_{c1} = \frac{\epsilon}{2\phi_0} \approx \frac{\mu_0 H_c^2 \xi^2}{\phi_0} \approx \frac{\phi_0}{\lambda^2}\frac{1}{\mu_0} \tag{6.19}$$

where we are again dropping order one factors and in the last step we have used the expression Eq. 6.18 for H_c. The measning of this result is that H_{c1}, the lowest field where a vortex can penetrate a superconductor, is given by the magnetic field necessary such that a single flux quantum penetrates a square area of size λ by λ, as shown in the right of Fig. 6.4.

Comparing Eq. 6.18 to 6.19 we see that in order for H_{c1} to be less than H_c we must have

$$\frac{\lambda}{\xi} \gtrsim 1$$

which should be the necessary condition for a Type II superconductor. (We have dropped constants of order unity, so we should not expect to get the precise value correct.

Conventioanally one defines the dimensionless ratio known as the Ginzburg-Landau parameter

$$\kappa = \frac{\lambda(T)}{\xi(T)} = 2\sqrt{\frac{\alpha_4}{\mu_0}}\ \frac{m^*}{\hbar e^*}$$

which is temperature independent (at least whenever Ginzburg landau theory is valid).

A more precise calculation can be done to give the condition for a Type II superconductor is that $\kappa > \frac{1}{\sqrt{2}}$.

In order to have a vortex we must have a type II superconductor, meaning, $\kappa \gtrsim 1$. This means the London penetration depth, the screening length for magnetic fields, is longer than the coherence length, the healing length for the order parameter. Thus around a vortex core, the order parameter heals quickly whereas the magnetic field is screened slowly. This is roughly depicted in Fig. 6.5.

In fact a more precise calculation will show that the energy of an isolated vortex will have a $\log\kappa$ correction that we ignored. By caculating the energy of the vortex core, we found that the energy per unit length is (See Eq. 6.19)

$$\epsilon \approx 2\mu_0 H_c^2 \xi^2$$

However, the actual result includes a term of the form

$$\mu_0 H_c^2 \xi^2 \log(\lambda/\xi)$$

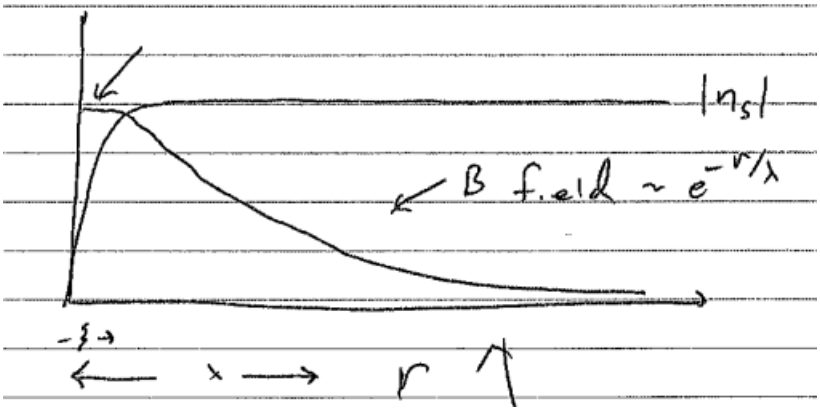


Figure 6.5: The order parameter heals over a short length scale ξ whereas the magnetic field is screened over a longer scale λ.

To understand where this term comes from, we roughly say that at radius less than λ we can neglect the screening due to the electromagnetism and the order parameter around the vortex core will be similar to what it is for a neutral superfluid. In this case, the order parameter is $\psi \sim e^{i\theta}$ so there is a velocity $v \sim \nabla\theta \sim 1/r$ in the $\hat{\theta}$ direction. The ginzburg-Landau kinetic energy density will give us something of the form

$$KE = \frac{mv^2}{2} \sim \frac{1}{r^2}$$

we then have a total energy

$$E \sim \int d^2r \frac{1}{r^2} \sim \int_{\xi}^{\lambda} dr \frac{1}{r} \sim \log(\lambda/\xi)$$

where we have cut off the integral at ξ because below this, the order parameter drops and we also cut off at λ because above this radius the screening makes the current drop exponentially.

Chapter 7

Interacting Fermions

7.1 Why study fermions

Having spent the entire course so far discussing bosons, we now turn our attention to fermions, and interacting fermions in particular.

Why should we study interacting fermions? There are several **good reasons** for this

Electrons (which are fermions) are the world[1] They physics of every metal, every semiconductor, every insulator, is completely controlled by the behavior of its electrons. In fact essentially all of chemistry is nothing more than the study of the behavior of electrons in different environments.

Usually when a condensed matter physicist says they are studying fermions, they mean they are studying electrons. There is one notable exception to this: the fermion ^{3}He. This fermionic isotope[2] of Helium is a favorite of condensed matter. As with the bosonic version, the light mass of Helium prevents it from forming a solid at low temperatures, and instead we get a quantum fluid — or fermi liquid. However, as compared to electrons, it has short range interactions rather than long range Coulomb interactions, and this makes its physics somewhat simpler in many ways[3]. An enormous amount has been learned from

[1] You can imagine all the electrons getting together and holding hands and singing "We are the world...!". At this point, anyone reading this footnote probably thinks I have gone crazy, but I've been typing these notes for a lot of hours in a row, and yes, maybe I'm going a bit batty.

[2] Helium-3 (^{3}He) was discovered experimentally in 1934 by Mark Oliphant at Cambridge. A mere few milligrams of the material became available for experiments as an offshoot of the post-war nuclear program. Now it is much more plentiful due to the fact that it is a waste product of nuclear missiles (Tritium, a fuel of hydrogen bombs, has a half-life of 12 years, and decays into ^{3}He). The price of Helium 3 fluctuates between 100 and 10000 dollars per litre, depending on the global supply at the time.

[3] One interesting feature we will not discuss in depth is that at extremely low temperaturures (meaning sub milli Kelvin) ^{3}He actually becomes a susprfluid. The experimental discovery of this in 1972 earned Lee, Osheroff and Richardson a Nobel prize in 1996. Theoretical work on the subject earned a Nobel prize for Tony Leggett[4]here in 2003. Similar to electons pairing at low temperature to superconduct, Helium 3

the study of this fermion. We will return to discussion of this below in section ***.

We need to understand strongly interacting fermions. In all of our introductory courses on solid state physics, we learn about metals, semiconductors, and insulators completely ignoring the interactions between electrons. But in fact in typical materials, the interaction energy is on the order of the kinetic energy, or even larger. It seems crazy to have ignored it! So why on earth is it OK for us to ignore interactions altogether in these simple pictures. At some level the interactions must have some effect — what are these effects?

Eventually we want to study superconductivity!. We have so far treated superconductivity crudely as simply thinking about bosonswith charge $e* = 2e$, but this is completely wrong for a number of reason

- Electrons repel each other *very* strongly. It seems crazy to think of them forming pairs[5].
- Even if you coudl manufacture some weak attraction between fermions, to make a true boson that you coudl condense, you would need a binding radius smaller than the inter-electron distance. This would require a binding energy on the order of the Fermi energy, which is huge!

7.2 Some Mathematical Preliminaries Regarding Fermions

Although it is possible to do almost every calculation we will discuss in first quantized notation, it becomes rapidly extremely messy to do so. It is really better to just bite the proverbial bullett and introduce second quantization and then talk in that language. The preliminaries introduced here are the fermionic analogs of the preliminaries introduced in section 4.1 for bosons.

7.2.1 Second Quantization

Orthonormal Single Particle Basis

Suppose we have a set of orthonormal orbitals which we will label $i, j, k, \ldots$. What we mean by this is wavefunctions $\varphi_i(\mathbf{r}, \sigma), \varphi_j(\mathbf{r}, \sigma), \varphi_k(\mathbf{r}, \sigma), \ldots$. Here note that the wavefunction is

forms pairs at low tempertaure in order to form a superfluid.

[4]See also comment about Leggett's opinion of number non-conserving order parameters in section 4.4. Tony Leggett was an undergraduate at Oxford, *in Classics!*. (More properly the degree was called "greats" or something like that at the time). After his undergrad degree he manage to convince a tutor to let him study physics, which he says he struggled with at first. In his Nobel biography he tells an entertaining story about rowing in his first year at Oxford (since everyone was doing it) and feeling like he was actually doing well, until they swapped him for the coxswain.

[5]Landau famously said "You cannot repeal Coulomb's law!"

a function of both position and particle spin. The orthonormality condition is[6]

$$\langle i|j\rangle = \sum_{\sigma} \int d\mathbf{r}\ \varphi_i^*(\mathbf{r},\sigma)\varphi_j(\mathbf{r},\sigma)$$

we will frequently abbreviate this kind of integral as

$$\langle i|j\rangle = \int d(1)\ \varphi_i^*(1)\varphi_j(1)$$

where here (1) is meant to indicate positions and spins (if we have particles with spin).

Many-Fermion Slater Determinant

A many body fermionic wavefunction must be fully antisymmetric. We can write down a convenient basis of fully antisymmetric states using so-called *Slater* determinants[7]. We write

$$\Psi(\tilde{1},\tilde{2},\ldots,\tilde{M}) = \frac{1}{\sqrt{M!}} \begin{vmatrix} \varphi_1(\tilde{1}) & \varphi_1(\tilde{2}) & \ldots & \varphi_1(\tilde{M}) \\ \varphi_2(\tilde{1}) & \varphi_2(\tilde{2}) & \ldots & \varphi_2(\tilde{M}) \\ \vdots & \vdots & & \vdots \\ \varphi_M(\tilde{1}) & \varphi_M(\tilde{2}) & \ldots & \varphi_M(\tilde{M}) \end{vmatrix}$$

Here for clarity, the numbers with tildes over them $\tilde{1},\tilde{2},\ldots$ are the position and spin variables, whereas the subscripts $_{1,2,\ldots}$ are orbital indices. If the consituent orbitals are orthonormal then the slater determinants are properly normalized

$$\langle\Psi|\Psi\rangle = \int d(\tilde{1})d(\tilde{2})\ldots d(\tilde{M})\Psi^*(\tilde{1},\tilde{2},\ldots,\tilde{M})\ \Psi(\tilde{1},\tilde{2},\ldots,\tilde{M}) = 1 \tag{7.1}$$

where again the integrals $d(\tilde{1})$ means both to integrate over space and sum over spin. Further, two slater determinants made from different sets of orthonormal orbitals will be orthogonal.

Fermionic Creation Operators

We define a set of Fermionic creation operators $c_i^\dagger$ corresponding to the orbitals φ_i. These operators are defined by the following statement: Applying creation operators to the

[6]The observant reader will realize this is nothing more than a completeness relationship

$$\langle i|j\rangle = \sum_x \langle i|x\rangle\langle x|j\rangle$$

where x is the positionn and spin basis.

[7]Slater was a professor at MIT for many years.

vacuum gives a slater determinant of the corresponding orbitals. In particular

$$c_1^\dagger c_2^\dagger \dots c_M^\dagger |0\rangle = \frac{1}{\sqrt{M!}} \begin{vmatrix} \varphi_1(\tilde{1}) & \varphi_1(\tilde{2}) & \dots & \varphi_1(\tilde{M}) \\ \varphi_2(\tilde{1}) & \varphi_2(\tilde{2}) & \dots & \varphi_2(\tilde{M}) \\ \vdots & \vdots & & \vdots \\ \varphi_M(\tilde{1}) & \varphi_M(\tilde{2}) & \dots & \varphi_M(\tilde{M}) \end{vmatrix}$$

Let us look at the normalization condition Eq. 7.1. In terms of these operators we have

$$1 = \langle \Psi | \Psi \rangle = \langle 0 | c_M \dots c_1 \;\; c_1^\dagger \dots c_M^\dagger | 0 \rangle \tag{7.2}$$

We should thus think of $c_i^\dagger$ as an operator that adds a fermion to orbital i, and correspondingly c_i is an operator that removes a fermion from orbital i. So in Eq. 7.2 we start on the far right with the vacuum, we add a fermion in orbital M and then in $M-1$ and so forth until we add a fermion in orbital 1, then continuing towards the left we remove the fermions in the opposite order until we are back to the vacuum. Alternately we can think of the c_i operators as just being creation operators that have been hermitian conjugated so that they act on the dual space to the left. I.e., $\langle 0|c_i$ is the dual (hermitian conjugate) to the wavefunction $c_i^\dagger|0\rangle$, and both represent one particle created in an orbital.

Anticommutations

Note that the fermionic creation operators must anticommute

$$c_i^\dagger c_j^\dagger = -c_j^\dagger c_i^\dagger$$

This is because if we switch the order of creation of two orbitals, this corresponds to switching two rows of the slater determinant — which incurs a minus sign. Similarly, we can conclude

$$c_i c_j = -c_j c_i$$

Further, we have

$$c_i^\dagger c_i^\dagger = 0$$

since you cannot put two fermions in the same orbital (or equivalently, if two rows of a slater determinant are the same, the determinant vanishes). Similarly we have the dual statement

$$c_i c_i = 0$$

meaning that you can only annihilate a particle, at most, once.

Finally we note that

$$c_i^\dagger c_i + c_i c_i^\dagger = 1 \tag{7.3}$$

To see this is true we apply this expression to an arbitrary $|\text{state}\rangle$. We can decompose the $|\text{state}\rangle$, into two parts, one in which orbital i is filled and one in which orbital i is empty (there are no other possibilities for fermions). If the orbital is filled then

$$c_i^\dagger c_i |\text{state}\rangle = |\text{state}\rangle$$

since the fermion in orbital i is removed and then put back. On the other hand

$$c_i c_i^\dagger |\text{state}\rangle = 0$$

since it is trying to create another fermion in orbital i which is already filled.

On the other hand, if orbital i is empty we have

$$c_i c_i^\dagger |\text{state}\rangle = |\text{state}\rangle$$

since we can add a particle to orbital i then remove it again. And also we have

$$c_i^\dagger c_i |\text{state}\rangle = 0$$

since we are trying to annihilate a particle from an orbital that is already empty. Putting these statements together we find that Eq. 7.3 is satisfied independent of whether it acts on a filled or empty orbital.

We can summarize many of these results by defining anticommutator brackets. For any operators let us define

$$\{A, B\} = AB + BA$$

All of the previous results in this subsection are summarized with the following statements[8]:

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \tag{7.4}$$

$$\{c_i, c_j^\dagger\} = \delta_{ij} \tag{7.5}$$

7.2.2 Change of Basis

As in the bosonic case we can consider changing the basis for our orbitals. Let us suppose we have two sets of orthonormal basis orbitals. One set we call $\{|\alpha\rangle\}$ and the other set we call $\{|i\rangle\}$. We can derive creation operators in a new basis in terms of the creation operators in the old basis (this is entirely analogous to Eq. 4.4 for bosons)

$$c_\alpha^\dagger = \sum_i \langle i|\alpha\rangle c_i^\dagger$$

A useful example of such a basis change is from tight binding orbitals to plane waves on a lattice (where we leave the spin unchanged in this particular case).

$$c_{\mathbf{r};\sigma}^\dagger = \sum_{\mathbf{k}} \langle \mathbf{k}, \sigma | \mathbf{r}, \sigma \rangle c_{\mathbf{k};\sigma}^\dagger$$

[8]The observant reader will notice that in fact we have not yet shown Eq. 7.5 for $i \neq j$. This is required by consistency. To see this let us try writing (with $i \neq j$)

$$c_j^\dagger |0\rangle = c_j^\dagger c_i c_i^\dagger |0\rangle$$

But also

$$c_j^\dagger |0\rangle = c_i c_i^\dagger c_j^\dagger |0\rangle = -c_i c_j^\dagger c_i^\dagger |0\rangle$$

Since these two lines must equal each other, we must have $c_j^\dagger c_i = -c_i c_j^\dagger$

Often we would like to use continuum fields $\mathbf{r}$ rather than lattice points, in which case we write $\hat{\psi}^\dagger_\sigma(\mathbf{r})$ instead of $c^\dagger_\sigma(\mathbf{r})$. In this case the fields $\hat{\psi}$ and $\hat{\psi}^\dagger$ obey the anticommutations

$$\{\hat{\psi}^\dagger_\sigma(\mathbf{r}), \hat{\psi}_{\sigma'}(\mathbf{r}')\} = \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma,\sigma'}$$

If we have an orbital basis $\varphi_i(\mathbf{r},\sigma)$ we can write the creation operators in this basis in terms of the $\hat{\psi}$ operators as

$$\begin{aligned} c^\dagger_i &= \sum_\sigma \int d\mathbf{r}\varphi_i(\mathbf{r},\sigma)\hat{\psi}_\sigma(\mathbf{r}) \\ &= \int d(1)\varphi_i(1)\hat{\psi}^\dagger(1) \end{aligned}$$

Important Example: Fermi Sea As an example, let us consider a sytem of $\mathbf{k}$ states filling a fermi sea. We can write

$$|\text{Fermi Sea}\rangle = \prod_{|\mathbf{k}|<k_f}\prod_{\sigma=\uparrow,\downarrow} c^\dagger_{\mathbf{k},\sigma}|0\rangle \tag{7.6}$$

We note that there is some presumed fiducial ordering of operators in these products. Without an ordering we cannot establish the sign of the wavefunction. Fortunately, we may never need to actually specify the ordering, but we should be very careful to keep track of any changes to the ordering, since any exchange incurs a minus sign.

7.2.3 Writing our Hamiltonian in Second Quantized Form

We will typically be concerned with a Hamiltonian of the form

$$H = H_0 + H_{int}$$

where[9]

$$H_0 = \sum_i \left[\frac{\mathbf{p}_i^2}{2m} + U(\mathbf{r}_i)\right] = \sum_i \hat{h}_i$$

is the single particle Hamiltonia of particles in a trapping potential $U(\mathbf{r})$ and

$$H_{int} = \frac{1}{2}\sum_{i\neq j} V(\mathbf{r}_i - \mathbf{r}_j)$$

is the interaction between particles. This might be, for example, a coulomb interaction if we are considering electrons.

We now want to rewrite these in second quantized form.

[9] I apologize that here I've used U for single particle potential and V for interaction, whereas in prior sections it was the other way around. I hope this does not create too much confusion!

To do this we can write the particle density,

$$\rho(\mathbf{r}) = \sum_\sigma \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})$$

so that we can write the interaction as

$$\begin{aligned} H_{int} &= \frac{1}{2}\int d(1)\int d(2) : \rho(1)\, V(1-2)\, \rho(2) : \\ &= \frac{1}{2}\int d(1)\int d(2) : \hat{\psi}^\dagger(1)\hat{\psi}(1)\; V(1-2)\; \hat{\psi}^\dagger(2)\hat{\psi}(2) : \end{aligned}$$

As in section 4.3 we have added colons : to indicate that the expression should be normal ordered which implies we should move all the creation operators to the left (and remember to add a minus sign for each exchange). To justify this we consider a system with a single fermion — without the normal ordering colons, this single fermion would have a nonzero self-interaction.

We can thus rewrite the interaction term as

$$H_{int} = \frac{1}{2}\int d(1)\int d(2) : \hat{\psi}^\dagger(1)\hat{\psi}^\dagger(2)\; V(1-2)\; \hat{\psi}(2)\hat{\psi}(1) :$$

The single particle term, we can write as

$$H_0 = \int d(1)\; \hat{\psi}^\dagger(1)\left[\frac{-\hbar^2\nabla^2}{2m} + U(\mathbf{r})\right]\hat{\psi}(1) \tag{7.7}$$

To see that this is correct, we rewrite $\psi^\dagger$ in terms of some single particle basis $|\alpha\rangle$.

$$\hat{\psi}^\dagger(1) = \sum_\alpha \varphi^*_\alpha(1) c^\dagger_\alpha$$

so that we have

$$H_0 = \sum_{\alpha,\beta} h_{\alpha\beta} c^\dagger_\alpha c_\beta \tag{7.8}$$

where

$$h_{\alpha,\beta} = \langle\alpha|\hat{h}|\beta\rangle = \int d(1)\; \varphi^*_\alpha(1)\left[\frac{-\hbar^2\nabla^2}{2m} + U(\mathbf{r})\right]\varphi_\beta(1)$$

It is most convenient at this point (although certainly not necessary) to choose a basis $|a\rangle$ that are eigenvectors of the operator $\hat{h}$ with eigenvalues ϵ^0_a, so we have

$$\hat{h}|a\rangle = \epsilon^0_a|a\rangle$$

Thus we can write

$$H_0 = \sum_a \epsilon^0_a\; c^\dagger_a c_a \tag{7.9}$$

The meaning of this expression is quite clear. The operators $\hat{n}_a = c_a^\dagger c_a$ counts the number of fermions (0 or 1) in orbital a, and if there is a fermion in the orbital, it is assigned an energy ϵ_a^0.

It is then useful to write the interaction part of the Hamiltonian Eq. 7.7 in an orbital basis to obtain

$$H_{int} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} v_{\alpha\beta\gamma\delta}\ c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \tag{7.10}$$

where the matrix element $v_{\alpha\beta\gamma\delta}$ is given by

$$v_{\alpha,\beta,\gamma,\delta} = \langle \alpha\beta | V | \gamma\delta \rangle = \int d(1) \int d(2)\ \varphi_\alpha^*(1)\varphi_\beta^*(2)\, V(1-2)\, \varphi_\gamma(1)\varphi_\delta(2) \tag{7.11}$$

Note carefully the ordering of the indices in Eq. 7.10 (the last two indices in the two sets of subscript are switched). To see where this comes from compare Eq. 7.7 to Eq. 7.11. We will continue to use this convention, although other conventions are possible as well.

Obviously the matrix element $\langle \alpha\beta | V | \gamma\delta \rangle$ in Eq. 7.11 uses a two-particle basis

$$|\gamma\delta\rangle \to \varphi_\gamma(1)\varphi_\delta(2)$$

which is not properly symmetrized for fermions. The symmetrization is automatic though once we put these matrix elements into Eq. 7.10 using the fermionic creation operators.

Note also that the matrix element has a number of obvious symmetries including

$$v_{\alpha\beta\gamma\delta} = v_{\beta\alpha\delta\gamma} \tag{7.12}$$

The Hamiltonian $H = H_0 + H_{int}$ with H_{int} written in the form of Eq. 7.10 and H_0 written in the form of Eq. 7.8 or Eq. 7.13 will be our object of study for the rest of this chapter. This form is extremely general and can be used for study of any interacting fermi system, such as electrons in a metal, electrons in an atom, or even Helium 3.

We will use several different "first pass" approximations (First order perturbation theory, Hartree approximation, Hartree Fock, etc). Sometimes these approximations will give the same results, but sometimes they will not.

7.3 First Order Perturbation Theory

Let us work in a basis such that the single particle Hamiltonian H_0 is diagonal. We thus have

$$H_0 = \sum_a \epsilon_a^0\ c_a^\dagger c_a \tag{7.13}$$

Ignoring the interaction ("zeroth" order in interaction) the groun state is just to fill up all orbitals below the chemical potential μ.

$$|\text{Noninteracting Ground State}\rangle = |\text{GS}^0\rangle = \left[\prod_{a\ \text{occupied}} c_a^\dagger \right] |0\rangle \tag{7.14}$$

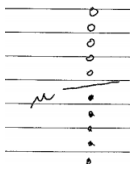


Figure 7.1: (Ignore the lined paper!). This depicts filling all orbitals up to the chemical potential.

where here an orbital a is occupied if

$$\epsilon_a^0 < \mu$$

as depicted schematically in Fig.7.1. As in Eq. 7.6, there is some presumed ordering of orbitals in Eq. 7.14 which we will not specify.

Next we want to include the interaction term. We write this term as above in the form (Same as Eq. 7.10)

$$H_{int} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} v_{\alpha\beta\gamma\delta}\ c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \tag{7.15}$$

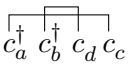
At first order in perturbation theory the correction to the energy is

$$\delta E = \langle \mathrm{GS}^0 | H_{int} | \mathrm{GS}^0 \rangle$$

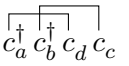
We now have to evaluate this expectation. We could do this by commuting a bunch of operators around, but there is a simple "shortcut" way of thinking:

$$\delta E = \underbrace{\langle 0| \prod_{e \text{ occupied}} c_e \,|}_{\text{same filled state}} \ \tfrac{1}{2} \sum_{abcd} v_{abcd} \ \underbrace{c_a^\dagger c_b^\dagger}_{\text{return same two}} \ \underbrace{c_d c_c}_{\text{remove two}} \ \underbrace{| \prod_{f \text{ occupied}} c_f^\dagger |0\rangle}$$

Here we note that the initial ket and final bra are exactly the same state. This means whichever particles are removed by $c_d c_c$ have to be returned by $c_a^\dagger c_b^\dagger$. There are exactly two ways in which this can happen: Either a matches c and b matches d,



or a matches d and b matches c



We thus obtain

$$\delta E = \langle H_{int} \rangle = \frac{1}{2} \sum_{a,b \text{ occupied}} (v_{abab} - v_{abba}) \tag{7.16}$$

It is clear that the two terms should have opposite signs since one commutation will make them look the same. To be more precise about the signs, note that in the first case (were a matches c) we can write the contribution as

$$\langle 0| \prod_{e \text{ occupied}} c_e \,|\ \tfrac{1}{2} c_a^\dagger c_b^\dagger \quad c_b c_a \ | \prod_{f \text{ occupied}} c_f^\dagger |0\rangle = \langle \text{state} | \text{state} \rangle$$

so we end up with a postive sign. On the other hand, to get the second case into this form we need to anticommute two of the operators and thus pick up an minus sign.

This approach, can at least in principle, be extended systematically to higher order perturbation theory.

7.3.1 Hartree and Fock Terms

The two terms in Eq. 7.16 have different meanings. Let us study them one at a time.

Hartree, or Direct, Term

Using Eq. 7.11 the first term in Eq. 7.16 is given by

$$v_{abab} = \int d(1) \int d(2) |\varphi_a(1)|^2 |\varphi_b(2)|^2 V(1-2) \tag{7.17}$$

This is known as the Hartree[10] or Direct interaction term. This is simply the interaction of the density in orbital a with the density in orbital b. If we keep only this term in Eq. 7.16 we have what is known as the Hartree approximation, which is somewhat simpler than the full first order perturbation calculation.

Self-Consistent Hartree We can also consider doing a self-consistent version of this calculation. This is a common approach known as Self-Consistent Hatree. It amounts to solving the Schroenger equation in a potention which includes the interaction from all the other electrons in the system. In other words we write

$$\begin{aligned} U^{eff}(\mathbf{r}) &= U(\mathbf{r}) + \int d\mathbf{r}' \sum_{n \text{ occupied}} |\varphi_n(\mathbf{r}')|^2 V(\mathbf{r}-\mathbf{r}') \\ &= U(\mathbf{r}) + \int d\mathbf{r}' \ \langle \rho(\mathbf{r}') \rangle \ V(\mathbf{r}-\mathbf{r}') \end{aligned}$$

The procedure for implementing self-consistent Hartree is as follows:

1. Solve the schroedinger equation in the presence of the potential $U^{eff}(\mathbf{r})$
2. Fill the lowest N orbitals, and calculate $\langle \rho(\mathbf{r}) \rangle$
3. Recalculate U^{eff}
4. Go back to step 1, and repeat until converged.

[10] Douglas Hartree was a British Numerical expert. He has a unit, the Hartree, named after him (which is $e^2/(4\pi\epsilon_0 a_0) = 2\text{Ry} \approx 27.2\text{eV}$).

Fock, or Exchange, Term

Using Eq. 7.11 the second term in Eq. 7.16 is given by

$$v_{abba} = \int d(1) \int d(2)\ \varphi_a^*(1)\varphi_b^*(2)\, V(1-2)\, \varphi_b(1)\varphi_a(2) \tag{7.18}$$

Note in particular that this term is zero unless the orbitals a and b overlap[11]. Note in particular that this means that orbital a and b need to overlap both in space *and* in spin space[12]. Eq. 7.18 is known as the Fock[13] or exchange term. This term cannot be described as simply some sort of effective potential that an electron moves in, as the Hartree term was. Note also that if the potential $V(r)$ is repulsive, the Fock term (which enters in Eq. 7.16 with a minus sign) is attractive.

Further Comments on First Order Perturbation Theory

It should be noted that, despite the fact that we have a Hartree term and a Fock term, what we have calculated so far (Eq. 7.16) is NOT the Hartree-Fock approximation (admittedly the nominclature is confusing).

We should also note that first order perturbation theory can also be used to (approximately) calculate the energy shift, due to interactions, of excited states. Again, if we begin with the noninteracting system, we can write an excited state as

$$|\text{Excited}\rangle = c_j^\dagger c_i |\text{GS}^0\rangle$$

where i is one of the orbitals which is filled in the noninteracting ground state, and j is one of the orbitals which is empty in the noninteracting ground state. Without interactions the energy of this excited state is

$$E^0_{excited} = \epsilon^0_j - \epsilon^0_i + E^0_{groundstate}$$

Again we can calculate the energy shift due to interactions as

$$\delta E = \langle H_{int} \rangle = \frac{1}{2} \sum_{a,b \text{ occupied}} (v_{abab} - v_{abba})$$

[11] If the *support* of φ_a and φ_b (meaning the region where they are nonzero) is disjoint then there is no value of the variable 1 for which the integrand is nonzero

[12] For example, since

$$\int d(1)\varphi_a^*(1)\varphi_b(1) = \int d\mathbf{r} \sum_\sigma \varphi_a^*(\mathbf{r},\sigma)\varphi_b(\mathbf{r},\sigma)$$

If we work with orbitals having a definite spin, the two orbitals woudld have to have the same spin for this to be nonzero.

[13] Vladimir Fock was the creator of the idea of second quantization in 1932 (although some of the ideas were presented by Dirac as early as 1927). Fock is immortalized through the idea of "Fock space". Much of Fock's later career was devoted to philosophy of science. He became a defender of relativity in a hostile Marxist world. Unfortunately, some of the Marxist philosophers thought that modern physics was "Bourgeois" and therefore dangerous to the state. Fock was forced to become a philosopher, speak their language, and clarify what is physics and what is philosophy. It is unclear how well soviet physics would have survived were it not for Fock.

with the expectation given in the excited state, meaning that the sum over occupied states includes orbital j but not orbital i.

7.4 Hartree-Fock Approximation

The so-called Hartree-Fock approximation is a self-consistent mean-field theory approach. It is often the first approach a theorists tries, and it is used extensively in condensed matter physics, but also in nuclear physics, atomic physics, molecular chemistry[14], and so forth.

Let us briefly recall the (Weiss) mean field method for understanding ferromagnets. Here we have a Hamiltonian like the Heisenberg Hamiltonian

$$H = \frac{J}{2} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

where, for example, the sum is over neighboring spins i, j. To handle this interacting we average one of the spins and leave the other one un-averaged,. So we have instead a Hamiltonian for a single spin given by

$$h_j = J \sum_{j \text{ neighbors } i} \mathbf{S}_i \cdot \langle \mathbf{S}_j \rangle$$

with $\langle \mathbf{S}_j \rangle = \langle \mathbf{S} \rangle$ is the average of the spin on any site. We can then solve the single site problem, and we need to "self-consist" meaning that the solution of the single-site problem should give us $\langle \mathbf{S} \rangle$.

We hope to use the same mean-field idea to handle the interaction term of our Hamiltonian. We thus take

$$H_{int} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} v_{\alpha\beta\gamma\delta} \; c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma \tag{7.19}$$

and we replace it with

$$H^{eff}_{int} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} v_{\alpha\beta\gamma\delta} \left[\langle c^\dagger_\alpha c_\gamma \rangle c^\dagger_\beta c_\delta + \langle c^\dagger_\beta c_\delta \rangle c^\dagger_\alpha c_\gamma - \langle c^\dagger_\alpha c_\delta \rangle c^\dagger_\beta c_\gamma - \langle c^\dagger_\beta c_\gamma \rangle c^\dagger_\alpha c_\delta \right] \tag{7.20}$$

Here we have taken all possible (nonzero) averages of two operators and left two other operators unaveraged[15] Note also that due to the symmetry Eq. 7.12 the first two terms in

[14] A Nobel Prize in chemistry was awarded to John Pople in 1998 for developing numerical Hartree Fock methods for simulating molecules.

[15] When we get to superconductivity, we will also consider the possibility of needing terms like $\langle c^\dagger c^\dagger \rangle$ and $\langle cc \rangle$. However if we insist on a system with a definite number of particles, such expectations are strictly zero.

the square brackets are identitical to each other and the last two terms are also identical to each other.

We can thus write a more abbreviated form

$$H_{int}^{eff} = \sum_{\alpha,\delta} f_{\alpha\delta}\ c_\alpha^\dagger c_\delta \tag{7.21}$$

where

$$f_{\alpha\delta} = \sum_{\beta gamma} \langle c_\beta^\dagger c_\gamma \rangle \left[v_{\alpha\beta\delta\gamma} - v_{\alpha\beta\gamma\delta} \right] \tag{7.22}$$

Including the single-body terms $h_{\alpha\beta}$ (See Eq. 7.8) we have

$$H^{eff} = \sum_{\alpha\delta} \left[h_{\alpha\delta} + f_{\alpha\delta} \right]\ c_\alpha^\dagger c_\delta \tag{7.23}$$

The two equations Eq. 7.22 and 7.23 consitute the Hartree-Fock approximation. Our procudure for solving these two equations at the same time is iterative (similar to the above described, self-consistent Hartree approach). While in principle one can produce a solution in any basis, it is convenient to successively change basis as we iterate to convergence. We thus follow the following procedure

1. Let ϵ_μ be the eigenvalues of $h_{\alpha\delta} + f_{\alpha\delta}$ with corresponding eigenvectors $|\mu\rangle$.

2. Change to this eigenbasis by defining

$$\tilde{c}_\mu^\dagger = \sum_\alpha \langle \alpha | \mu \rangle c_\alpha^\dagger$$

   In this basis, the Hamiltonian is of the form

$$H^{eff} = \sum_\mu \epsilon_\mu \tilde{c}_\mu^\dagger \tilde{c}_\mu$$

3. Fill the lowest N states with our fermions (Assuming we have an N fermion system)

$$|\Psi\rangle \prod_{\text{lowest } N} \tilde{c}_\mu^\dagger |0\rangle$$

4. Recalculate $f_{\alpha\delta}$ in this new ground state using Eq. 7.22. Note that this recalculation is why we wanted to work in the diagonal basis. In this basis we have

$$\langle c_\mu^\dagger c_\nu \rangle = \delta_{\mu\nu} \times \begin{cases} 1 & \text{if } \mu \text{ is filled} \\ 0 & \text{if } \mu \text{ is empty} \end{cases}$$

   We thus have

$$f_{\alpha\delta} = \sum_{\mu \text{ occupied}} \left[v_{\alpha\mu\delta\mu} - v_{\alpha\mu\mu\delta} \right] \tag{7.24}$$

5. Go back to step 1 and repeat until convergence. When it converges, the old basis and the new basis match. This means, that in this basis, $h + f$ is already diagonal. Thus we have
$$\epsilon_\mu = h_{\mu\mu} + f_{\mu\mu} = h_{\mu\mu} + \sum_{\nu \text{ occupied}} [v_{\mu\nu\mu\nu} - v_{\mu\nu\nu\mu}]$$
The first term the square brackets being from the Hartree term and teh second term being from the Fock term.

Note that if we were to follow exactly the same procedure, but using only the first (Hartree) of the two v terms, we would have the self-consistent Hartree approximation, as described above.

The energies ϵ_μ can be thought of as the Hartree fock ionization energies. I.e., this is the energy (in Hartree fock approximation) required to remove the electron in the μ orbital. This results is known as Koopmans' theorem[16]. The total energy of the Hartree fock system is given by
$$E_{total} = \sum_{\mu \text{ filled}} \left[h_{\mu\mu} + \frac{1}{2} f_{\mu\mu} \right]$$
The factor of 1/2 here is similar to what occurs in Weiss mean field theory. In writing down the total energy of the system, one does not want to overcount the energy of spin i interaction with spin j and also spin j interacting with spin i. It is quite similar here. Simple addition of all of the ϵ_μ hartree fock ionization energies would count interaction of each particle μ with all the other particles ν but then would again count the interaction of each ν with μ. Thus we need to introduce the factor of 1/2 in the interaction.

7.4.1 Hartree Fock as Optimal Slater Determinant

We claim that the solution of the Hartree Fock equations provides the best (lowest energy) variational wavefunction in the form of a single slater determinant. This optimal wavefunction is
$$|\text{HF}\rangle = \prod_{\mu \text{ occupied}} c_\mu^\dagger |0\rangle$$
for the Hartree fock orbitals μ. This brings us to an equivalent definition of the Hartree fock approximation:

Hartree Fock is an approximation by which one finds the optimal ground state wavefunction in the form of a single slater determinant.

[16] Tjalling Koopmans is a Nobel laureate in the field of economics (never mind that economics was not one of the original subjects that Nobel had established prizes for — so it is strictly speaking a Nobel memorial medal, not a Nobel prize). He did his work on Hartree Fock in 1934 when he was a 24 year old grad student, but shortly thereafter switched fields to economics. His prize in 1975 was awared for the theory of optimal allocation of resources. Apparently his own resource was more optimally allocated in the field of economics.

Proof that this statement is equivalent to the Hartree fock equations derived as a mean field theory above (Eq. 7.22 and 7.23) is nontrivial. We will present it here.

Proof:

Consider a basis of orbitals μ and a single slater determinante (or "filled fermi sea") made of these orbitals.

$$|\text{GS}\rangle = \prod_{\text{lowest } N \text{ states}} c_\mu^\dagger |0\rangle$$

We would like to find a condition such that $|\text{GS}\rangle$ is a variational minimum. To find this condition we want to try varyin h the basis μ and seeing if the energy decreases. So let us imagine switching to a new basis

$$\tilde{c}_\alpha^\dagger = \sum_\mu \langle \mu|\alpha\rangle c_\mu^\dagger = \sum_\mu U_{\alpha\mu} c_\mu^\dagger \tag{7.25}$$

where U is a unitary matrix. Note that we are only concerned with a change of basis which mixes filled and empty orbitals. If we change basis in a way that that mixes two filled orbitals with each other, or in a way that mixes two empty orbitals with each other, the resulting slater determinant remains unchanged[17]. At the same time we want the variation to be very small, so we can write

$$U = e^{i\epsilon M}$$

with $M = M^\dagger$ is a Hermitian matrix[18]. With ϵ small, we have

$$U = \mathbf{1} + i\epsilon M + \ldots$$

which we plug into Eq. 7.25 to give

$$\tilde{c}_\mu^\dagger = c_\mu^\dagger + i\epsilon \sum_\nu M_{\mu\nu} c_\nu^\dagger + \ldots$$

Here, as mentioned above, to have any change in the resulting slater determinant we are only interested in M that mixes filled and empty orbitals. Thus we can assume that $M_{\mu\nu}$

[17] Let us see an example of this. Suppose we make the basis transform

$$\begin{aligned} \tilde{c}_a^\dagger &= (c_1^\dagger + c_2^\dagger)/\sqrt{2} \\ \tilde{c}_b^\dagger &= (c_1^\dagger - c_2^\dagger)/\sqrt{2} \end{aligned}$$

It is easy to check that if both orbitals are filled, the basis change does not change the resulting slater determinant:

$$\tilde{c}_a^\dagger \tilde{c}_b^\dagger |0\rangle = c_1^\dagger c_2^\dagger |0\rangle$$

However if we only fill one of these two orbitals

$$\tilde{c}_a^\dagger |0\rangle \neq c_1^\dagger |0\rangle \neq c_2^\dagger |0\rangle$$

Thus to change the slater determinant, we need to mix a filled state with an empty state.

[18] Let us check that exponentiating a hermitian matrix gives a unitary matrix. For a matrix to be unitary we must have $UU^\dagger = \mathbf{1}$. So let us check $(e^{i\epsilon M})(e^{i\epsilon M})^\dagger = (e^{i\epsilon M})(e^{-i\epsilon M}) = \mathbf{1}$.

is nonzero only if either μ is fileld and ν is empty or ν is filled and μ is empty. (...and in particular $\mu \neq \nu$).

Thus we consider trial states of the form

$$\begin{aligned} |\Psi\rangle_\epsilon &= \prod_{\mu \text{ in lowest } N} \tilde{c}^\dagger_\mu |0\rangle \\ &= \prod_{\mu \text{ in lowest } N} \left(c^\dagger_\mu + i\epsilon \sum_{\nu \text{ not in lowest } N} M_{\mu\nu} c^\dagger_\nu \right) |0\rangle \end{aligned} \tag{7.26}$$

where the sum over ν must be only over unoccupied states, such that we have μ occupied and ν unoccupied (or equivalently M is simply zero for all other cases). We now want to expand this product order by order in ϵ. We get

$$|\Psi\rangle_\epsilon = \left[\prod_{\mu \text{ in lowest } N} c^\dagger_\mu |0\rangle \right] + i\epsilon \sum_{\nu \text{ empty; } \mu \text{ filled}} M_{\mu\nu} c^\dagger_\nu c_\mu \left[\prod_{\lambda \text{ in lowest } N} c^\dagger_\lambda |0\rangle \right] + \dots$$

Let us walk through this result. The first term in brackets, the product of the $c^\dagger_\mu$ is the product of all of the first terms in Eq. 7.26. This just gives the unperturbed ground state $|\text{GS}\rangle$ (ie., the $\epsilon = 0$ wavefunction). The order ϵ^1 term is more complicated. To get this term from the product of Eq. 7.26 one chooses only a single μ win the product where instead of taking the first term $c^\dagger_\mu$ one instead chooses the M term. We write this term in a creative way, by starting with $|\text{GS}\rangle$ (the term in square brackets on the far right) and removing the orbital μ with c_μ and then putting in the sum over M instead. As a shorthand we can write

$$|\Psi\rangle_\epsilon = |\text{GS}\rangle + \epsilon |\delta\Psi\rangle + \dots$$

where

$$|\delta\Psi\rangle = i\epsilon \sum_{\nu \text{ empty; } \mu \text{ filled}} M_{\mu\nu} c^\dagger_\nu c_\mu \, |\text{GS}\rangle \tag{7.27}$$

At this linear order in ϵ it is easy to see that

$$\langle \delta\Psi | \text{G}S \rangle = 0$$

since $\delta\Psi$ always has some orbitals ν filled which are not filled in the ground state, GS. This then implies that

$${}_\epsilon\langle \Psi | \Psi \rangle_\epsilon = 1 + \mathcal{O}(\epsilon^2)$$

Finally we turn to the variational condition. We would like our wavefunction to be at an extremum of the energy. Thus we want

$$\left. \frac{\partial E}{\partial \epsilon} \right|_{\epsilon=0} = 0$$

which we write as

$$\left. \frac{\partial}{\partial \epsilon} \right|_{\epsilon=0} \frac{{}_\epsilon\langle \Psi | H | \Psi \rangle_\epsilon}{{}_\epsilon\langle \Psi | \Psi \rangle_\epsilon} = 0$$

where this condition should now be true for *any* hermitian matrix M that mixes filled and unfilled orbitals. Note that the denominator of this fraction we just found to be 1 up to corrections of order ϵ^2 so we can thow this out. Expanding our condition and taking the ϵ derivative gives us the condition

$$0 = \langle \delta\Psi | H | \mathrm{GS} \rangle + \langle \mathrm{GS} | H | \delta\Psi \rangle = \mathrm{Re} \langle \mathrm{GS} | H | \delta\Psi \rangle$$

And indeed since this needs to be true for any matrix M in Eq. 7.27, we can equivalently state the condition

$$\mathrm{Re} \langle \mathrm{GS} | H c_\nu^\dagger c_\mu | \mathrm{GS} \rangle = 0$$

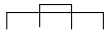
where μ is filled in the ground state GS and ν is empty in the ground state GS. Writing H out explicitly we get

$$\mathrm{Re} \langle \mathrm{GS} | \left[\sum_{\alpha\beta} h_{\alpha\beta} c_\alpha^\dagger c_\beta + \sum_{\alpha\beta\gamma\delta} \frac{1}{2} v_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \right] c_\nu^\dagger c_\mu \, | \mathrm{GS} \rangle = 0 \tag{7.28}$$

Let us attack this term by term. In the first term, we have

$$\langle \mathrm{GS} | c_\alpha^\dagger c_\beta c_\nu^\dagger c_\mu \, | \mathrm{GS} \rangle$$

Since μ is occupied and ν is unoccupied in GS, this expression can only be nonzero if $\mu = \alpha$ and $\nu = \beta$.



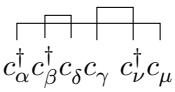
$$\langle \mathrm{GS} | c_\alpha^\dagger \, c_\beta \, c_\nu^\dagger \, c_\mu \, | \mathrm{GS} \rangle = \delta_{\nu\beta} \delta_{\alpha\mu}$$

Thus the first term in the correlator Eq.7.28 is simply $h_{\mu\nu}$.

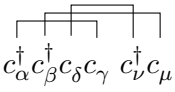
We next examine the second, more complicated, term in Eq. 7.28. This has the form

$$\langle \mathrm{GS} | \, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \, c_\nu^\dagger c_\mu \, | \mathrm{GS} \rangle$$

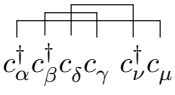
Now there are four different ways in which this can be nonzero, which we now list here. For all of these we must have μ initially filled and ν initially empty.



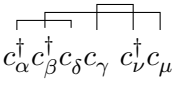
$$\langle \mathrm{GS} | \, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \, c_\nu^\dagger c_\mu \, | \mathrm{GS} \rangle \quad \rightarrow \quad +\delta_{\alpha\mu} \delta_{\beta\delta} \delta_{\gamma\nu} \qquad \delta \text{ initially filled}$$



$$\langle \mathrm{GS} | \, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \, c_\nu^\dagger c_\mu \, | \mathrm{GS} \rangle \quad \rightarrow \quad +\delta_{\alpha\gamma} \delta_{\beta\mu} \delta_{\delta\nu} \qquad \gamma \text{ initially filled}$$



$$\langle \mathrm{GS} | \, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \, c_\nu^\dagger c_\mu \, | \mathrm{GS} \rangle \quad \rightarrow \quad -\delta_{\alpha\mu} \delta_{\beta\gamma} \delta_{\delta\nu} \qquad \gamma \text{ initially filled}$$



$$\langle \mathrm{GS} | \, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \, c_\nu^\dagger c_\mu \, | \mathrm{GS} \rangle \quad \rightarrow \quad -\delta_{\alpha\delta} \delta_{\beta\mu} \delta_{\gamma\nu} \qquad \delta \text{ initially filled}$$

Putting these results together we obtain the condition

$$h_{\mu\nu} + \frac{1}{2} \sum_{x \text{ occupied}} \left[v_{\mu x \nu x} + v_{x \mu x \nu} - v_{\mu x x \nu} - v_{x \mu x \nu} \right] = 0$$

Now using the symmetry of v given in Eq. 7.12 we find that the first two v terms are the same and the last two v terms are the same thus giving us

$$h_{\mu\nu} + \sum_{x \text{ occupied}} [v_{\mu x \nu x} - v_{\mu x x \nu}] = 0$$

for all mu filled and ν emtpy. We recognize the sum over x as being precisely $f_{\mu\nu}$ as given in Eq. 7.24. So our condition is

$$h_{\mu\nu} + f_{\mu\nu} = 0$$

for μ initially filled and ν initially unfilled. Thus if we started with a Hartree fock basis, where $h+f$ is diagonal, this condition in necessarily satisfied (since it will only be nonzero for $\mu = \nu$). Thus we conclude that the solution to the Hartree fock equations indeed produces the lowest possible energy single slater determinant! QED. $\square$. Yay. etc.

7.5 Application of Hartree-Fock to Translationally Invariant Fermions

We now would like to apply Hartree-Fock theory to a very simple, but also very important case. : The translationally invariant interacting fermi gas.

This situation is supposed to model electrons in metals, but we have thrown away the crystal lattice for simplicity and just kept the electrons. (So, for example, we will have a perfectly spherical fermi sea, as compared to what we get in real metals). Note that if we completely throw away the positive ions in the crystal lattice, the coulomb energy of all the electrons interacting with each other becomes infinite. To avoid this problem, one usually smears out a neutralizing positive charge which we keep along with the electrons, so that the entire system is charge neutral (but still completely translationally invariant). This model is known as the "jellium" model[19] (with the idea that the positive charge is like a smeared out jelly that has been spread evenly around the system).

Another way to handle the problem coming from the infinite coulomb interaction is to just consider fermions with shorter range interaction $V(\mathbf{r})$. While this does not apply to real electrons, it does apply to fermi systems such as ^{3}He.

Whether we use a jellium background or not, our Hamiltonian will always be of the form

$$H = H_0 + H_{int}$$

with

$$H_0 = \sum_{\mathbf{k},\sigma} \frac{\hbar^2 \mathbf{k}^2}{2m} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

[19]The Jellium model (including the name) was constructed by Conyers Herring. Herring was an extremely important condensed matter physicist in the mid 1900s — and his influence was often in the background of other great works. Herring was the first head of the famous Bell Labs theory department. Many years later, when Bell Labs was closing down its fundamental research effort, I was the last head of the Bell Labs theory department – a rather dubious distinction I'm afraid.

is the kinetic (single particle, noninteracting part) of the Hamiltonian, and

$$H_{int} = \frac{1}{2} \sum_{(\mathbf{k}_1\sigma_1)(\mathbf{k}_2\sigma_2)(\mathbf{k}_3\sigma_3)(\mathbf{k}_4\sigma_4)} v_{(\mathbf{k}_1\sigma_1)(\mathbf{k}_2\sigma_2)(\mathbf{k}_3\sigma_3)(\mathbf{k}_4\sigma_4)} \quad c^\dagger_{\mathbf{k_1}\sigma_1} c^\dagger_{\mathbf{k_2}\sigma_2} c_{\mathbf{k_4}\sigma_4} c_{\mathbf{k_3}\sigma_3}$$

Note when comparing to the form written in Eq. 7.10 the indices we used as a, b, c, d are now replaced by the combined indices $(\mathbf{k}_1\sigma_1), (\mathbf{k}_2\sigma_2), (\mathbf{k}_3\sigma_3), (\mathbf{k}_4\sigma_4)$. The matrix element is given by

$$v_{(\mathbf{k}_1\sigma_1)(\mathbf{k}_2\sigma_2)(\mathbf{k}_3\sigma_3)(\mathbf{k}_4\sigma_4)} = \langle \mathbf{k}_1\sigma_1; \mathbf{k}_2\sigma_2 | V(\mathbf{r} - \mathbf{r}') | \mathbf{k}_3\sigma_3; \mathbf{k}_4\sigma_4 \rangle$$

Here the kets are normalized (but unsymmetrized) plane wave state of two particles

$$\langle \mathbf{r}\sigma_3; \mathbf{r}'\sigma_4 | \mathbf{k}_3\sigma_3; \mathbf{k}_4\sigma_4 \rangle = \frac{1}{\mathcal{V}} \, e^{i\mathbf{k}_3\cdot\mathbf{r} + i\mathbf{k}_4\cdot\mathbf{r}'}$$

with $\mathcal{V}$ the volume of the system. Thus we have

$$\begin{aligned} v_{(\mathbf{k}_1\sigma_1)(\mathbf{k}_2\sigma_2)(\mathbf{k}_3\sigma_3)(\mathbf{k}_4\sigma_4)} &= \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} \int d\mathbf{r} \int d\mathbf{r}' \frac{1}{\mathcal{V}^2} e^{-i\mathbf{k}_1\cdot\mathbf{r} - i\mathbf{k}_2\cdot\mathbf{r}'} e^{i\mathbf{k}_3\cdot\mathbf{r} + i\mathbf{k}_4\cdot\mathbf{r}'} V(\mathbf{r} - \mathbf{r}') \\ &= \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4} \frac{1}{\mathcal{V}} \delta_{\mathbf{k}_1+\mathbf{k}_2, \mathbf{k}_3+\mathbf{k}_4} \tilde{V}(\mathbf{k}_4 - \mathbf{k}_2) \end{aligned}$$

where

$$\tilde{V}(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} V(\mathbf{r})$$

We can thus rewrite

$$H_{int} = \frac{1}{2\mathcal{V}} \sum_{(\mathbf{k}_1,\sigma_1),(\mathbf{k}_4,\sigma_4),\mathbf{q}} c^\dagger_{\mathbf{k_1}\sigma_1} c^\dagger_{(\mathbf{k_4}-\mathbf{q})\sigma_4} c_{\mathbf{k_4}\sigma_4} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1} \tilde{V}(\mathbf{q}) \tag{7.29}$$

Note that there is another, potentially more physical way to write this expression

$$H_{int} = \sum_{\mathbf{q}} : \rho(\mathbf{q}) \tilde{V}(\mathbf{q}) \rho(-\mathbf{q}) :$$

where ρ is the density written in Fourier space

$$\rho(\mathbf{q}) = \sum_{\mathbf{k},\sigma} c^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} c_{\mathbf{k}\sigma} = \text{FourierTransform}_{\mathbf{q}}[\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})] \tag{7.30}$$

Although we don't intend to generally write our perturbation theory in termms of Feynman diagrams, it is occassionally useful to write them anyway — not the least reason being that one will often see these diagrams in the literature, and it is useful to be able to convert the diagram into physical expressions. The interaction 7.29 can be written diagrammatically as shown in the left of Fig. 7.2. When we make Hartree-Fock approximation, we want to average one creation and one annihilation operator to give $\langle c^\dagger_a c_b \rangle$, and this can be done in two ways, corresponding to the direct and exchange (Hartree and Fock) terms.

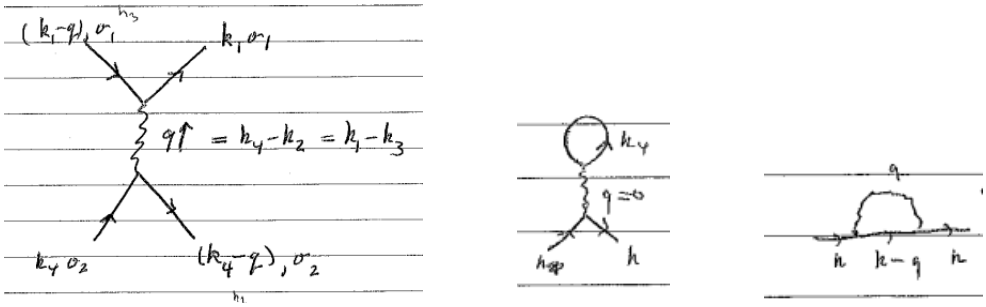


Figure 7.2: Left: The interaction in Eq. 7.29 drawn as a diagram. Middle: connecting up the legs of the diagram to make the Hartree contribution. Right: Connecting the legs up to make the Fock contribution.

The first possibility is the direct or Hartree term

$$\overbrace{c^\dagger_{\mathbf{k_1}\sigma_1} c^\dagger_{(\mathbf{k_4}-\mathbf{q})\sigma_4} c_{\mathbf{k_4}\sigma_4} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}}$$

and the second is the exchange or Fock term

$$c^\dagger_{\mathbf{k_1}\sigma_1} \overbrace{c^\dagger_{(\mathbf{k_4}-\mathbf{q})\sigma_4} c_{\mathbf{k_4}\sigma_4} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}}$$

We will examine these one at a time.

Note that we are going to assume that the ground state is in the form of a Fermi sea

$$|\mathrm{FS}\rangle = \prod_{\sigma,\mathbf{k}<k_F} c^\dagger_{\mathbf{k}\sigma}|0\rangle$$

and we will justify this assumption post-facto.

Direct (Hartree) Term

We have

$$H_{Hartree} = \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} \left[\sum_{\mathbf{k_1},\sigma_1} \langle c^\dagger_{\mathbf{k_1}\sigma_1} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1} \rangle \right] \sum_{\mathbf{k}_4,\sigma_4} c^\dagger_{(\mathbf{k_4}-\mathbf{q})\sigma_4} c_{\mathbf{k_4}\sigma_4} \tilde{V}(\mathbf{q})$$

Here we examine the expectation. If we are taking the expection in a Fermi sea state, we have

$$\langle c^\dagger_{\mathbf{k_1}\sigma_1} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1} \rangle = \delta_{\mathbf{q},0} \times n_F(\mathbf{k})$$

where

$$n_F(\mathbf{k}) = \begin{cases} 1 & |\mathbf{k}| < k_F \\ 0 & \text{otherwise} \end{cases} \tag{7.31}$$

is the fermi occupation factor at zero temperature for the fermi sea where k_F is the fermi wavevector. Thus the expression in the square brackets is

$$\left[\sum_{\mathbf{k_1},\sigma_1} \langle c^\dagger_{\mathbf{k_1}\sigma_1} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}\rangle\right] = N\delta_{\mathbf{q},0}$$

with N the total particle number. We then get

$$H_{Hartree} = \frac{N}{\mathcal{V}}\tilde{V}(0)\sum_{\mathbf{k}_4,\sigma_4} c^\dagger_{\mathbf{k_4}\sigma_4} c_{\mathbf{k_4}\sigma_4}$$

This is nothing more than a shift of the chemical potential and is therefore trivial. Indeed, if one considers a jellium model where the positive charge is neutralized by a uniform background charge, $\tilde{V}(0) = 0$, and this term vanishes exactly. Diagramatically, this is expressed by the diagram in the middle of Fig. 7.2.

Exchange (Fock) Term

Here we have

$$H_{Fock} = \frac{-1}{\mathcal{V}}\sum_{\mathbf{k_1},\sigma_1}\left[\sum_{\mathbf{k}_4,\sigma_4,\mathbf{q}} \langle c^\dagger_{((\mathbf{k_4}-\mathbf{q})\sigma_4} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}\rangle \tilde{V}(\mathbf{q})\right] c^\dagger_{\mathbf{k_1}\sigma_1} c_{\mathbf{k_4}\sigma_4}$$

We again examine the expectation in the Fermi sea ground state giving us

$$\langle c^\dagger_{((\mathbf{k_4}-\mathbf{q})\sigma_4} c_{(\mathbf{k_1}-\mathbf{q})\sigma_1}\rangle = \delta_{\sigma_1,\sigma_4}\delta_{k_1,k_4}\; n_F(\mathbf{k}_4-\mathbf{q})$$

so the fermi occupation factor here is unity only if $|\mathbf{k}_4 - \mathbf{q}| < k_F$ and is otherwise zero. We can then write the Fock term as

$$H_{Fock} = \sum_{\mathbf{k},\sigma} \Sigma_{Fock}(\mathbf{k})\; c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

where Σ_{Fock} is knonw as the *self-energy* and is given by

$$\Sigma_{Fock}(\mathbf{k}) = -\frac{1}{\mathcal{V}}\sum_{\mathbf{q}} \tilde{V}(\mathbf{q}) n_F(|\mathbf{k}-\mathbf{q}|)$$

Diagrammatically this result is shown in the far right of Fig. 7.2.

Putting the Hartree-Fock pieces together

Adding together the Hatree and Fock contributions we get the effective Hartree-Fock Hamiltonian

$$H_{HF} = \sum_{\mathbf{k},\sigma} \epsilon_{HF}(\mathbf{k})\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}\sigma} \tag{7.32}$$

where

$$\epsilon_{HF}(\mathbf{k}) = \frac{\hbar^2\mathbf{k}^2}{2m} + \frac{N}{\mathcal{V}}\tilde{V}(0) + \Sigma_{Fock}(\mathbf{k}) \tag{7.33}$$

What is crucial to note here is that Eq. 7.32 is "diagonal" in the variables $\mathbf{k}$ and σ. This means we have the correct Hartree-Fock eigenstates. Recall that we were supposed to iterate Hartree-Fock until we converge to diagonal. Here we simply guessed the right starting wavefunction, and we found it was diagonal immediately. This may seem surprising, but actually it is not. Before we turned on the interaction, we had a translationally invariant system with a ground state which was a simple fermi sea. When the interaction was turned on, we did not ruin translational invariance, and this greatly constrains what kind of wavefunctions we can write down. As a result, the Hartree fock best single slater determinant is simply the filled non-interacting fermi sea. And there, Hartree fock just gives a modification to $\epsilon(\mathbf{k})$. This results is the same as what we would get for first order perturbation theory in this case, although that is not always true for Hartree-Fock.

It is worth looking at the three terms in Eq. 7.33. The first term is simply the noninteracting kinetic energy. When we sum this up over the entire fermi sea in Eq. 7.32 we obtain (this is an easy exercise to show!)

$$E_0 = \frac{3}{5}NE_F^0 \tag{7.34}$$

where E_F^0 is the noninteracting Fermi energy. The total Hartree energy summed over all of the particles is

$$E_{Hartree} = \frac{1}{2}\frac{N^2}{\mathcal{V}}\tilde{V}(0) \tag{7.35}$$

with $\mathcal{V}$ the volume of the system as usual; and the total Fock energy summed over all the particles is

$$E_{Fock} = \frac{-1}{2\mathcal{V}}\sum_{\mathbf{q},\mathbf{q}'} n_F(\mathbf{q})n_F(\mathbf{q}')\tilde{V}(\mathbf{q}-\mathbf{q}') \tag{7.36}$$

Note that this rather intuitive expresion gives only interaction between aligned spins, as is required for the Fock term. The factors of $1/2$ in Eq.7.35 and 7.36 are included to avoid overcounting as described in the discussion of Koopmans' theorem above.

7.5.1 Hartree Fock Effective Mass

The interesting physics of a metal is often the low energy physics compared to E_F, since E_F for a metal is often huge. We are thus interested in the low energy excitations near the fermi surface.

For a noninteracting fermi gas we can expand around the Fermi surface and write

$$\begin{aligned}\epsilon^0(\mathbf{k}) &= E_F + \frac{\hbar k_F}{m}\hbar(|\mathbf{k}| - k_F) \\ &= E_F + v_F\,\hbar(|\mathbf{k}| - k_F)\end{aligned}$$

where we have defined the fermi velocity to be

$$v_F = \hbar k_F/m$$

Note that we are dropping terms which are $(|\mathbf{k}| - k_F)^2$ and higher powers being that we are assuming we are close to the fermi surface.

For an interacting fermi system we can write instead

$$\epsilon(\mathbf{k}) = E_F^* + \frac{\hbar k_F}{m^*}\hbar(|\mathbf{k}| - k_F)$$

where we have defined an effective mass m^* by

$$\frac{\hbar^2}{m^*} = \frac{\partial^2}{\partial k^2}\epsilon_{HF}(k)\Big|_{k=k_F}$$

For example, for ^{3}He, the effective mass ranges from 3-5 times the bare mass of the Helium atom, depending on the pressure applied to the system.

Effective Mass for Coulomb Interaction

We now return to the Coulomb interaction, which is slightly troublesome due to its long range nature. We start with

$$V(\mathbf{r}) = \frac{e^2}{4\pi\epsilon_0|\mathbf{r}|}$$

which we Fourier transform to get[20]

$$\tilde{V}(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}}\frac{e^2}{4\pi\epsilon_0|\mathbf{r}|} = \frac{e^2}{\epsilon_0|\mathbf{k}|^2} \tag{7.37}$$

Here we note that $\tilde{V}(0)$ (which we need for the Hartree energy) is divergent for the Coulomb interaction. This is a result of having not included the neutralizing positive (jellium) background. If we put this in, it will fully cancel $\tilde{V}(0)$ and we don't have to worry about this divergence.

[20] On dimensional grounds, and by rotational invariance we know that it has to be proportional to $\frac{1}{|\mathbf{k}|^2}$, so let us call the result $\frac{\alpha}{|\mathbf{k}|^2}$. To get the prefactor right it is useful to look at the inverse Fourier transform

$$V(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}}\frac{\alpha}{|\mathbf{k}|^2}$$

Then take the laplacian

$$\nabla^2 V(\mathbf{r}) = \alpha\int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} = \alpha\delta(\mathbf{r})$$

and by Gauss' law we can then fix the prefactor $\alpha = e^2/\epsilon_0$.

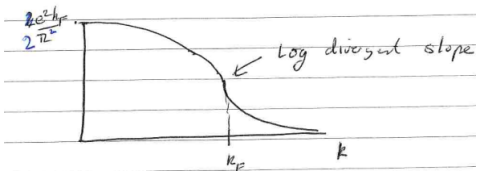


Figure 7.3: A plot of the self-energy in the case of the coulomb interaction

Let us now calculate the Fock self-energy

$$\begin{aligned}\Sigma_{Fock}(\mathbf{k}) &= -\frac{1}{\mathcal{V}}\sum_{\mathbf{q}}\tilde{V}(\mathbf{q})n_F(|\mathbf{k}-\mathbf{q}|) \\ &= \frac{e^2}{\epsilon_0}\frac{1}{\mathcal{V}}\sum_{|\mathbf{k}'|<\mathbf{k_F}}\frac{1}{|\mathbf{k}-\mathbf{k}'|^2} = \frac{e^2}{\epsilon_0}\int_0^{|\mathbf{k}'|=\mathbf{k_F}}\frac{d\mathbf{k}'}{(2\pi)^3}\frac{1}{|\mathbf{k}-\mathbf{k}'|^2} \qquad (7.38)\end{aligned}$$

which is sketched in Fig. 7.3. For $\mathbf{k}=0$ it is easy to calculate that $\Sigma = e^2k_f/(\epsilon_0 2\pi^2)$. And it is also easy to see that Σ must decay for very large $\mathbf{k}$. However, what is not as obvious is that the self energy has a log-divergent slope at k_F. The calculation that shows this is given just below.

Given the log divergent slope, m^* then goes to zero at the Fermi surface. The reason for the log divergence is the long-ranged coulomb interaction. Over long distances, other electrons rearrange themselves to cancel the coulomb potential, and this is not properly accounted for in simple Hartee fock. This rearrangement of charges to remove the long range coulomb interaction is known as *screening* and will be treated in some detail in the next chapter.

7.6 Appendix: Showing the Log Divergence at The Fermi Surface

We want to calculate the self energy Eq. 7.38 as $\mathbf{k}$ approaches the fermi surface. Let us consider $\mathbf{k}$ (without loss of generality) in the x direction and approaching the fermi surface k_F, as shown in Fig. 7.4. We divide the integral over $\mathbf{k}'$ into an integral in the x direction and an inegral in the directions perpendicular to x, which we call $\mathbf{k}'_\perp$.

$$\begin{aligned}\Sigma_{HF}(\mathbf{k}) &= \int d\mathbf{k}'_\perp \int dk'_x \frac{1}{|\mathbf{k}-\mathbf{k}'|^2} \\ &= \int_{-k_F}^{k_F} dk'_x 2\pi \int_0^{\sqrt{k_F^2-(k'_x)^2}} dk'_\perp k'_\perp \frac{1}{|k-k'_x|^2+k_\perp^2} \\ &\approx 2\pi\int_{-k_F}^{k_F} dk'_x \log(|k-k'_x|^2/\text{cutoff}) \\ &\sim (k-k_F)\log(|k-k_F|)\end{aligned}$$

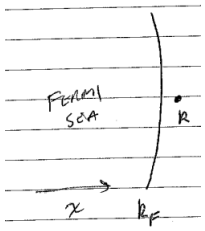


Figure 7.4: A plot of the self-energy in the case of the coulomb interaction

Thus we have

$$\frac{\partial \epsilon_{HF}}{\partial k} \sim \log(|k - k_F|)$$

and

$$\frac{1}{m*} \sim \frac{\partial^2 \epsilon_{HF}}{\partial k^2} \sim \frac{1}{|k - k_F|}$$

Chapter 8

Screening and Linear Response

In the previous chapter we had some problems with the long-rangedness of the Coulomb interaction. While we will not completely solve this problem here, we understand that the solution to this problem comes from allowing other particles to respond to the potential created, thus *screening* the long range interaction. Indeed, we know that if we try to put a postive charge in a metal at one point and a negative charge at another point (so as to keep the total charge neutral) the other charges in the metal should rearrange so as to make the metal look overall neural everywhere — at least when looked at from far away.

More generally we are interested in how a system responds to any arbitrary perturbation. We will study this at various levels of sophisitication.

8.1 Thomas-Fermi Screening

Let us consider a uniform electron gas and we imagine there is some potential $U(\mathbf{r})$ that the electrons feel. We thus have a Hamiltonian which is

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + U(\mathbf{r}_i)$$

Let us further assume taht $U(\mathbf{r})$ varies slowly in space and $\langle U \rangle = 0$ for simplicity. For example, we might assume that $U(\mathbf{r}) = U_0 \cos(\mathbf{q} \cdot \mathbf{r})$ with small $|\mathbf{q}|$.

To determine what happens in this situation we start by thinking locally: Locally we have fermi sea which is filled up to the chemical potential μ. If the potential U increases, this pushes some of the electrons above the chemical potential and the density drops by

$$\delta n(\mathbf{r}) = -D(E_F)U(\mathbf{r}) \tag{8.1}$$

where $D(E_F)$ is the density of states per unit volume. This is shown in Fig. 8.1.

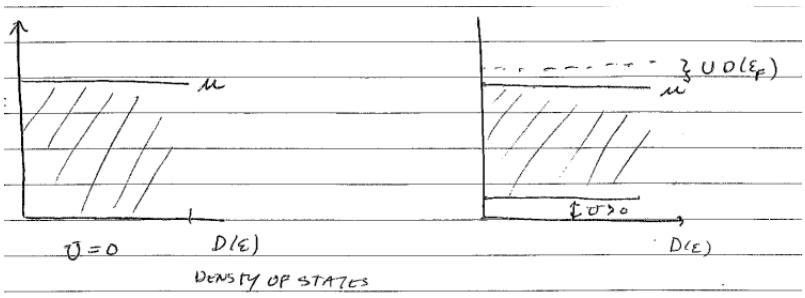


Figure 8.1: Left: States are filled up to the chemical potential μ. Right: If an additional potential U is added to the system, some states are pushed above the chemical potential, and the local denstity drops by $D(E_F)U$ where D is the density of states per unit volume.

In this situation, we sometimes call the quantity $-D(E_F)$ in Eq. 8.1 a *response function*[1]

At this point, we are still ignoring interactions between the electrons, we are only keeping the interaction between the electrons and the potential U. With more careful thought, we realize that the interaction beween electrons should matter. When the electrons move around in response to the potential U, they then create a new electrostatic potential that the other electrons then should respond to. Thus we need to consider some sort of self-consistent approach. First, however, we should convert our response equation into an equation that explains how charge moves around, rather than how density moves around.[2]

$$\delta\rho(\mathbf{r}) = -e\,\delta n(\mathbf{r})$$

The potential felt by an electron moving in an *electrostatic* potential $\phi(\mathbf{r})$ is

$$U(\mathbf{r}) = -e\phi(\mathbf{r})$$

Thus, our above response equation Eq. 8.1 can be rewritten as a charge response to an electrostatic potential

$$\delta\rho(\mathbf{r}) = -e^2 D(E_F)\phi(\mathbf{r}) \tag{8.2}$$

Now if there is a change in density, there is a resulting change in the electrostatic potential. The resulting electrostatic potential is given by Gauss' law

$$\begin{aligned} \nabla^2\phi &= \frac{-\delta\rho}{\epsilon_0} \\ &= \frac{e^2}{\epsilon_0} D(E_F)\phi \end{aligned} \tag{8.3}$$

[1]Later we will call a quantity essentially equivalent to this (up to some factors of e, the response function χ^0. The superscript 0 indicating that it does not yet include interaction between electrons, but only interaction of electrons with the potential U.

[2]This is going to be one of those times when we really wish we could go back in time and tell Benjamin Franklin to switch the definition of positive charge so that the electron is positive! The minus signs here are a common source of error!

where we have used Eq. 8.2 in going to the second line. This resulting equation for ϕ is precisely the self-consistent Hartree equation: Electrons respond to a density which is created by all the other electrons.

It is useful now to define the so-called Thomas-Fermi[3] wavevector[4]

$$k_{TF}^2 = \frac{e^2}{\epsilon_0} D(E_F) \tag{8.4}$$

So that our self consistent screening equation 8.3 is just

$$\nabla^2 \phi = k_{TF}^2 \phi$$

Such an equation has a characteristic decay of the form

$$\phi \sim e^{-k_{TF}|\mathbf{r}|}$$

The potential decays exponentially because it is *screened* by other electrons. To be more precise, let us consider the field near a point of charge Q inserted into our system of electrons. The resulting electrostatic potential is given by the Yukawa[5] form

$$\phi = \frac{Q}{4\pi\epsilon_0 |\mathbf{r}|} e^{-k_{TF}|\mathbf{r}|} \tag{8.5}$$

This potential solves the equation

$$\nabla^2 \phi = k_{TF}^2 \phi + \frac{Q}{\epsilon_0} \delta(\mathbf{r})$$

where the second term on the right represents the source charge that is inserted.

Let us now estimate the Thomas-Fermi wavevector. The density of states in a noninteracting fermi liquid is given by[6]

$$D(E_F) = \frac{3}{2} \frac{n}{E_F} = \frac{m k_F}{\hbar^2 \pi^2}$$

We thus have

$$k_F = \sqrt{\frac{D(E_F) e^2}{\epsilon_0}} = \sqrt{\frac{m k_F e^2}{\hbar^2 \pi^2 \epsilon_0}} = \sqrt{\frac{4}{\pi}} \sqrt{\frac{k_F}{a_0}}$$

[3]Llewelyn Thomas invented this in 1927 : Frighteningly soon after Fermi-Dirac statistics was invented (1925).

[4]It is worth checking that k_{TF} does indeed have the dimensions of a wavevector. First, note that $D(E_F)$ is is a density of states per unit volume, so it has dimension $1/(\text{Energy} - \text{Volume})$. Next note that $e^2/(\epsilon_0 \times \text{length})$ is an energy. The rest is easy.

[5]Yukawa won a Nobel prize in 1949 for his work on nuclear forces.

[6]To derive this $E \sim k_F^2 \sim n^{2/3}$, so $dE/dn = (2/3)E/n$, and $dn/dE = (2/3)E/n$. We also need $E_F = \hbar^2 k_F^2/(2m)$ and an expression for the density in terms of k_F which is given by $n = 2/(2\pi)^3 (4\pi k_F^3)/3$ where the prefactor of 2 is for two spin states.

where a_0 is the Bohr radius. Now in a typical metal we have a screening length $1/k_F \approx a_0 \approx 1\mathring{A}$ which is very short. However, in a semiconductor, this screening length can be 10-100 $\mathring{A}$ or more due to a small k_F and a large a_0 (the small k_F coming from a low density of electrons, and the large a_0 coming from a low mass and a large effective dielectric constant).

The Thomas-Fermi approximtion is a good first approach for understanding screening. In particular it removes the long range singularity of the Coulomb interactions. However, there are some things that are obviously wrong with the Thomas-Fermi appraoch. The main problem is that it is an "instantaneous" approximation, whereas if we add a charge to a system it actually takes some time for the electrons to rearrange so as to screen the charge. This time delay can turn out to be very important. This brings us to the topic of dynamical screening and dynamical response.

8.2 Response More Generally

We will now consider response functions more generally – including time dependent response. Let us generally write our Hamiltonian

$$H = \hat{H}_0 + \delta\hat{H}(t)$$

where $\delta\hat{H}(t)$ is the small perturbation applied to the system (and $\hat{H}_0$ is the Hamiltoninan in the absence of the perturbation). Although we will here be interested in the response of an interacting fermi liquid to a perturbation, the same principles we use here are far more general and can be applied to many other systems. It is always conventient to assume that the perturbation goes to zero at time $t = -\infty$ and turns on slowly.

An important example of such a perturbation (for our electron system) would be a weak time dependent externally applied electrostatic potential, in which case we have

$$\delta\hat{H}(t) = \int d\mathbf{r}\,(-e\phi_{ext}(\mathbf{r},t)\hat{n}(\mathbf{r})) \tag{8.6}$$

However, we could perturb the system with many other things, such as a magnetic field, or pressure, etc, and much of the calculation of response will be similar.

We now want to ask how the system responds to this perturbation. To probe this response we measure some observable operator $\hat{B}$. So we are interested in

$$\langle\hat{B}\rangle_t = \langle\psi(t)|\hat{B}|\psi(t)\rangle$$

where $|\psi(t)\rangle$ is the time dependent many particle wavefunction.

An example here is that we might be interested in the density operator

$$\hat{B} = \delta n(\mathbf{r})$$

so, if we perturb (in Eq. 8.6) with the potential $\phi(\mathbf{r}, t)$ what is the resulting change in density at some later time.

One key priniciple to keep in mind is that of causality: If a perturbation occurs at time t we should only have a response at times $t' \geqslant t$.

Time Dependent Perturbation Theory

So how are we going to find the general response $\langle \hat{B} \rangle_t$. The strategy here is to assume the perturbation $\delta\hat{H}(t)$ is small and use time dependent perturbation theory.

Let us start with the time dependent Schroedinger equation.

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_S = \left[H_0 + \delta\hat{H}(t) \right] |\psi(t)\rangle_S$$

The subscript S her indicates that the kets are in the Schroedinger representation. Also note that inside the square brackets is the full Hamiltonian — which is a combination of the bare part H_0 and the small perturbation.

We now switch to so-called "interaction" representation.

$$|\psi(t)\rangle_I = e^{iH_0 t/\hbar} |\psi(t)\rangle_S$$

In this representation, operators are time dependent

$$\begin{aligned} \hat{B} \quad &\to \hat{B}_I(t) \quad = e^{iH_0 t/\hbar}\ \hat{B}_S\ e^{-iH_0 t/\hbar} \\ \delta\hat{H} \quad &\to \delta\hat{H}_I(t) \quad = e^{iH_0 t/\hbar}\ \delta\hat{H}_S\ e^{-iH_0 t/\hbar} \end{aligned}$$

In this representation, the Schroedinger equation becomes

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I = \delta\hat{H}(t)\ |\psi(t)\rangle_I \tag{8.7}$$

Note that in this representation, if $\delta H = 0$ then $|\psi\rangle_I$ is actually time independent.

We can now write out a formal solution of the Schroedinger Equation in the form

$$|\psi(t)\rangle_I = |\psi\rangle_{I0} - \frac{i}{\hbar} \int_{-\infty}^{t} dt' \delta\hat{H}_I(t') |\psi\rangle_{I0} + \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' \delta\hat{H}_I(t') \delta\hat{H}_I(t'') |\psi\rangle_{I0} + \ldots \tag{8.8}$$

where $|\psi\rangle_{I0}$ is the wavefunction in the absence of the perturbation, in the interaction rep (and it is therefore a time independent ket). We can confirm that Eq. 8.8 solves the Schroedinger equation Eq. 8.7 by plugging the expansion into both sides of the Schroedinger equation.

We will now make use of the fact that $\delta\hat{H}$ is small and we will truncate the expansion at first order, throwing away terms of order $(\delta\hat{H})^2$ and higher. We can now use the time

dependent wavefunction in Eq. 8.8 to calculate the time dependence of some operator to be observed

$$\begin{aligned}
&\langle\hat{B}\rangle_t = \langle\psi_I(t)|\hat{B}_I(t)|\psi_I(t)\rangle \\
= &\left[{}_{I0}\langle\psi| + \frac{i}{\hbar}\int_{-\infty}^{t} dt' \; {}_{I0}\langle\psi|\delta\hat{H}_I(t')\right]\hat{B}_I(t)\left[|\psi\rangle_{I0} - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\delta\hat{H}_I(t')|\psi\rangle_{I0}\right] \\
= &\; {}_{I0}\langle\psi_I|\hat{B}_I(t)|\psi_I\rangle_{I0} - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \;\; {}_{I0}\langle\psi|\left[\hat{B}_I(t), \delta\hat{H}_I(t')\right]|\psi\rangle_{I0}
\end{aligned}$$

The first term in the last line is just the value of $\langle B\rangle_t$ in the absence of the perturbation. Thus we have a change in the value of B given by

$$\langle\delta\hat{B}\rangle_t = -\frac{i}{\hbar}\int_{-\infty}^{t} dt' \;\; \langle[\hat{B}_I(t), \delta\hat{H}_I(t')]\rangle$$

where the expectation is taken in the unperturbed state $|\psi\rangle_{I0}$ as above. This formula is a general linear respsonse equation, otherwise known as the Kubo formula[7]. The importance of this type of formula can hardly be overstated, as it is used universally to calculate the response of a system to a perturbation.

Example of Externally Applied Potential

Let us go back to the main example we want to study: the density response to an externally applied potential. The perturbation is generally of the form

$$\delta\hat{H}_S(t') = \int d\mathbf{r}\left(-e\phi_{ext}(\mathbf{r}, t')\hat{n}_S(\mathbf{r})\right)$$

with the operators being expressed here in the Schroedinger representation. The operator we would like to measure is again the density operator

$$\hat{B} = \hat{n}_S(\mathbf{r})$$

It is often easier to work in Fourier space. By using Parseval's theorem[8]

$$\delta\hat{H}_S(t) = \frac{-e}{\mathcal{V}}\sum_{\mathbf{k}} \phi_{ext}(\mathbf{k}, t')\,\hat{n}_S(-\mathbf{k}) \tag{8.9}$$

wiht $\mathcal{V}$ the volume as usual. Since we are considering *linear* response, we can imagine applying a single wavevector perturbation $\mathbf{k}$ at a time — and if we have an initial perturubation which is a sum of different wavevectors we can just add up the responses to each wavevector at the end of the calculation.

[7] Named for the Japanese physicist Ryogo Kubo who constructed this general formula in 1957.

[8] Named for Marc-Antoine Parseval des Chênes who published it in 1799 without proof, stating that it was self-evident.

We also write the quantity we want to measure (the density) in **k**-space

$$\delta B = \delta \hat{n}_S(\mathbf{k})$$

again in the Schroedinger representation.

We can then write our Kubo formula as

$$\begin{aligned} \langle \delta n(\mathbf{k}) \rangle_t &= \int_{-\infty}^{t} dt' \ \langle [\hat{n}_I(\mathbf{k},t), \hat{n}_I(-\mathbf{k},t')] \rangle \phi_{ext}(\mathbf{k},t') \qquad (8.10) \\ &= \int_{-\infty}^{\infty} dt' \ \tilde{\chi}(\mathbf{k}, t-t') \qquad (8.11) \end{aligned}$$

where

$$\tilde{\chi}(\mathbf{k}, t-t') = \theta(t-t') \frac{ie}{\hbar \mathcal{V}} \langle [\hat{n}_I(\mathbf{k},t), \hat{n}_I(-\mathbf{k},t')] \rangle$$

and

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

is the usual step function. The insertion of the step function in Eq.8.11 implements the correct boundary conditions given explitily in Eq. 8.10. The function $\tilde{\chi}$ is known as the linear response function (or susceptibility) and note that it is translationally invariant in time. I.e., if we perturb a system at time 0 and measure at time a, this is the same as perturbing at time b and measuring at time $a+b$.

Note that here on the left hand side of Eq. 8.10, we have indicated the response at wavevector **k** which was the same wavevector which we perturbed with on the right. In other words we are assuming that the response is diagonal in wavevector. It turns out that this is necessarily true in any tranlationally invariant system — a system that is perturbed at some wavevector **k**, in linear response theory, will only only respond at the same wavector. We will prove this statement below.

Our next step is to realize that the integral in Eq. 8.11 is a convolution in the t variables. As is usual with a convolution, it is then conventient to fourier transform. Further, we remember that since we are thinking about *linear* response, we can always decompose the perturbation into a sum of pieces and think about the response to each piece separately. Thus let us just think about a perturbation at a fixed frequency

$$\phi_{ext}(\mathbf{k}, t) = e^{-i\omega t} \phi_{ext}(\mathbf{k}, \omega)$$

If we have a more complicated time dependence we can always sum signals over many frequencies.

Note that we had previously decided that to make sure things are well-behaved, we want to make sure the perturbation is turned off at time $t = -\infty$. Thus we write instead

$$e^{-i(\omega + i\varepsilon)t} \qquad (8.12)$$

where ε is an infinitesimle positive number. This will then properly vanish at $t = -\infty$. We will often not write the $+i\varepsilon$ but we should remember that it is there.

The integral Eq. 8.11 in Fourier space instead reads

$$\delta n(\mathbf{k},\omega) = \chi(\mathbf{k},\omega)\phi_{ext}(\mathbf{k},\omega)$$

where the response χ is given by

$$\begin{aligned}\chi(\mathbf{k},\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\,\tilde{\chi}(\mathbf{k},t) \\ &= \frac{ie}{\hbar V}\int_0^{\infty} dt\, e^{i\omega t}\,\langle[\hat{n}(\mathbf{k},t),\hat{n}(-\mathbf{k},0)]\rangle \end{aligned} \tag{8.13}$$

Note that the $+i\varepsilon$ we added to ω in Eq. 8.12 regularizes this integral at $t = +\infty$.

Eq. 8.13 has two terms in the commutator. We will consider these one of these terms explicitly (and we assume the reader can fill in the rest of the calculation for the second term!). We will assume we are at temperature $T = 0$ and that the system is initially in the ground state, which we write as $|\mathrm{GS}\rangle$. The first term in the commutator is

$$\begin{aligned}\langle \mathrm{GS}|\hat{n}(\mathbf{k},t)\hat{n}(-\mathbf{k},0)\mathrm{GS}\rangle &= \langle \mathrm{GS}|e^{iH_0t/\hbar}\hat{n}(\mathbf{k})e^{-iH_0t/\hbar}\hat{n}(-\mathbf{k})|\mathrm{GS}\rangle \\ &= \sum_m \langle \mathrm{GS}|e^{iH_0t/\hbar}\hat{n}(\mathbf{k})e^{-iH_0t/\hbar}|m\rangle\ \langle m|\hat{n}(-\mathbf{k})|\mathrm{GS}\rangle\end{aligned}$$

where we have inserted a complete set of eigenstates $|m\rangle$ in the last line (their corresponding energies will be taken to be E_n with E_0 being the ground state energy). We now make use of the fact that $\hat{n}(-\mathbf{k}) = \hat{n}^\dagger(\mathbf{k})$ to write

$$\langle \mathrm{GS}|\hat{n}(\mathbf{k},t)\hat{n}(-\mathbf{k},0)\mathrm{GS}\rangle = \sum_m\ e^{i(E_{\mathrm{GS}}-E_m)t}\ \langle \mathrm{GS}|\hat{n}(\mathbf{k})|m\rangle\ \langle m|\hat{n}^\dagger(\mathbf{k})|\mathrm{GS}\rangle$$

At this point we think back to the claim made after Eq. 8.11: That a perturbation at wavevetor $\mathbf{k}$ will only ilicit a response at the same wavevector $\mathbf{k}$. We can now see why this is the case. Reading this equation from right to left: We start with the grounds state $|\mathrm{GS}\rangle$ which has wavevector zero. The operator $\hat{n}^\dagger(\mathbf{k})$ adds wavevector $\mathbf{k}$ to the ground state and generates an excited state $|m\rangle$ with wavevector $\mathbf{k}$. Then the operator $\hat{n}(\mathbf{k})$ removes this wavevector and returns us to the ground state. If we had measured a response at a different wavevector $\mathbf{k}' \neq \mathbf{k}$, the operator $\hat{n}(\mathbf{k}')$ would not be able to return us to the ground state and we would end up getting zero, as claimed.

We thus have the result

$$\chi(\mathbf{k},\omega) = \frac{ie}{\hbar\mathcal{V}}\int_0^{\infty} e^{i\omega t}\sum_m \left\{e^{i(E_{\mathrm{GS}}-E_m)t/\hbar}|\langle \mathrm{GS}|\hat{n}(\mathbf{k})|m\rangle|^2 - e^{-i(E_{\mathrm{GS}}-E_m)t/\hbar}|\langle \mathrm{GS}|\hat{n}(-\mathbf{k})|m\rangle|^2\right\}$$

where the second term in the brackets is from the other term of the commutator. Taking the integral now gives

$$\chi(\mathbf{k},\omega) = \frac{-e}{\hbar\mathcal{V}}\sum_m \left\{\frac{|\langle \mathrm{GS}|\hat{n}(\mathbf{k})|m\rangle|^2}{\omega + i\varepsilon - (E_m - E_{\mathrm{GS}})/\hbar} - \frac{|\langle \mathrm{GS}|\hat{n}(-\mathbf{k})|m\rangle|^2}{\omega + i\varepsilon - (E_{\mathrm{GS}} - E_m)/\hbar}\right\} \tag{8.14}$$

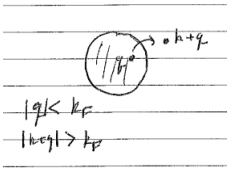


Figure 8.2: The relevant excitations for this calculation are excitations of a single electron out of the fermi sea.

We now are left with the problem of calculating the matrix elements such as $\langle \mathrm{GS}|\hat{n}(\mathbf{k})|m\rangle$. This depends entriely on what particular Hamiltonian we are working with. So far, what we have written is entirely general, and it is still exact at linear response level.

8.3 Lindhard Response Function (Response of Noninteracting Electrons)

So, let us consider a very simple case to start with, that of free electrons. We take

$$H_0 = \sum_i \frac{\mathbf{p}_i^2}{2m}$$

only. (In principle, one might want to include interactions in the Hamiltonian — which we will do later at least in some approximation. However, writing down a complete set of eigenstates is extremely hard when we have interactions, whereas it is fairly easy for the noninteracting case). In this noninteracting case, the ground state $|\mathrm{GS}\rangle$ is simply the filled fermi sea. We can write the density operator again as (See Eq. 7.30, with apologies that we changed notation for ρ to $\hat{n}$)

$$\hat{n}(\mathbf{k}) = \sum_{\mathbf{q},\sigma} c^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} c_{\mathbf{q}\sigma} = \mathrm{FourierTransform}_{\mathbf{k}}[\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})] \tag{8.15}$$

We thus see that $\hat{n}(\mathbf{k})$ can excite a single electron out of the fermi sea. Thus, the intermediate states $|m\rangle$ are all of the form

$$|m\rangle = c^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} c_{\mathbf{q}\sigma}|\mathrm{GS}\rangle$$

with $|\mathbf{q}| < k_F$ and $\mathbf{k}+\mathbf{q} > k_F$ as shown in Fig. 8.2. The corresponding energy difference is given by

$$E_m - E_{\mathrm{GS}} = \frac{\hbar^2|\mathbf{k}+\mathbf{q}|^2}{2m} - \frac{\hbar^2|\mathbf{q}|^2}{2m} = \epsilon^0_{\mathbf{k}+\mathbf{q}} - \epsilon^0_{\mathbf{q}}$$

where $\epsilon^0_{\mathbf{q}} = \hbar^2|\mathbf{q}|^2/(2m)$ as usual, the superscript 0 indicating that this is the energy of noninteracting electrons. Plugging these results into Eq. 8.14, and using $\chi(\mathbf{k}) = \chi(-\mathbf{k})$ we obtain

$$\chi^0(\mathbf{k},\omega) = \frac{-e}{\mathcal{V}} \sum_{\mathbf{q},\sigma} \frac{n_F(\mathbf{q}) - n_F(\mathbf{q}+\mathbf{k})}{\hbar(\omega + i\varepsilon) - (\epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}})} \tag{8.16}$$

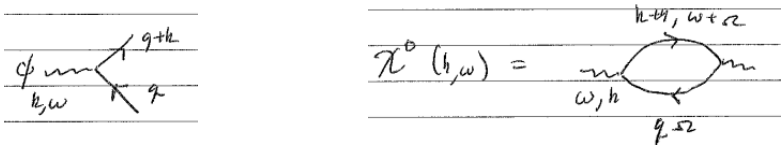


Figure 8.3: Left: Vertex representing a density operator.

with n_F the fermi function, which is simply a step function at the fermi surface at zero temperature (See Eq. 7.31). The superscript 0 here on χ^0 indicates that we are thinking about noninteracting electrons. This rather important result is known as the Lindhard response function[9].

Aside: Green's function language

For those who like to think in Feynman diagrams and Green's functions it is sometimes useful to rephrase this result in this language. For those who are not familiar with this technique, it is OK to mostly ignore it (it is not examinable in this course) and skip down to section 8.3.1. It is simply useful to be able to talk different languages sometimes.

First, the "source" for the response function is the density $\hat{n}(\mathbf{k})$, which we think of in the form of Eq. 8.15 which therefore includes terms of the form $c^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} c_{\mathbf{q}\sigma}$. We write this diagrammatically as the vertex shown in the left of Fig.8.3 We then also write the Greens' function for the electron as

$$G(\mathbf{k},\Omega) = \frac{1}{\Omega - (\epsilon^0_{\mathbf{k}} - \mu) + i\varepsilon \mathrm{sgn}(\epsilon^0_{\mathbf{k}} - \mu)}$$

which we write as a line with an arrow. The response function χ^0 is then given by the diagram in the right of Fig. 8.3. This diagram corresponds to the integral over the Green's functions

$$\chi^0(\mathbf{k},\omega) = \sum_{\mathbf{q}} \int d\Omega \; G(\mathbf{q},\Omega) G(\mathbf{k}+\mathbf{q}, \omega+\Omega)$$

Carrying out the integrals here will generate precisely the same result as Eq 8.16 (up to a prefactor which I may have dropped).

For complicated diagrams, meaning high order perturbation theory calculations, these Green's functions and diagrammatics are a very useful bookkeeping tool. However, at this level it is easier to just do the calculation directly without bothering with diagrams. Nonetheless, it is useful to draw the diagram, because one often sees it in the literature, and it is good to know what it means!

[9]Named for Jens Lindhard who wrote it down for the first time in 1954 — rather late for such an important result to be first discovered, although perhaps this is not surprising being that the Kubo formula had not yet been discovered at this time.

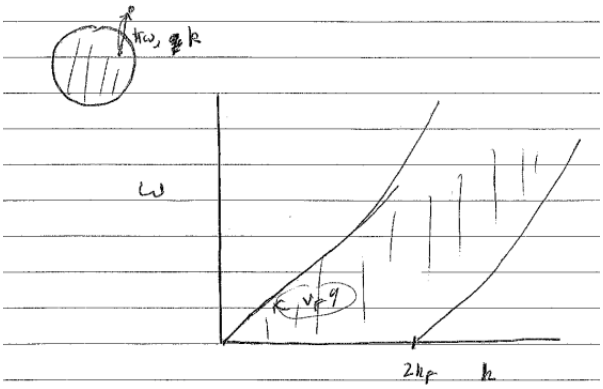


Figure 8.4: The region of q,ω space where there is an imaginary part of χ. This is precisely the region where Eq. 8.17 can be satisfied.

8.3.1 Interpretations

We now would like to interpret the result we have derived Eq. 8.16. We will look at some properties of χ^0, partially to understand it, and partially as a sanity check that we have gotten a reasonable answer!

Imaginary Dissipative Part

First, let us examine the imaginary part of χ. What does it mean that our response function has an imaginary part rather than all real? This simply means that the response is dissipative – energy is absorbed by they system (this is precisely analogous to a conductivity being real rather than imaginary – we will see the connection to conductivity below in section ***).

To find out when χ^0 has an imaginary part recall that

$$\lim_{\varepsilon \to 0^+} \frac{1}{x + i\varepsilon} = i\pi\delta(x)$$

In Eq. 8.16, it is implied that we are taking a limit of $\varepsilon \to 0^+$. Thus the response has an imaginary part when

$$\hbar\omega = \epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}} \quad \text{where} \quad \begin{cases} |\mathbf{q}+\mathbf{k}| > k_F & \text{and} \quad |\mathbf{q}| < k_F \\ & \text{OR} \\ |\mathbf{q}+\mathbf{k}| < k_F & \text{and} \quad |\mathbf{q}| > k_F \end{cases} \tag{8.17}$$

In Fig. 8.4 we sketch the region of q, ω space where this condition is satisfied. This is the region of space where we can add a wavevector $\mathbf{k}$ to the system and get an excitation of energy ω.

Let us make a few quick calculations to determine the rough shape of this region. First we notice that that the longest vector across the Fermi surface is the diameter which

is $k = 2k_F$. It is impossible to make any zero energy excitations (ie., from the fermi surface to the fermi surface) for wavevectors larger than this. This is why the shaded region in Fig. 8.4 has a boundary at $\omega = 0$ and $k = 2k_F$. Secondly it is useful to look at what happens for small k. Here we can have the condition

$$\hbar\omega = \epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}} = \frac{\hbar^2|\mathbf{k}+\mathbf{q}|^2}{2m} - \frac{\hbar^2|\mathbf{q}|^2}{2m}$$

but for small k we need to have $q \approx k_F$ to satosfy te conditions in Eq. 8.17. Thus we can write

$$\hbar\omega \approx \frac{\hbar k_F}{m} k\cos\theta$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{q}$. The largest ω is then given by $\cos\theta = 1$ or

$$\omega = v_F k$$

with $v_F = \hbar k_F/m$ the fermi velocity, which is shown in Fig. 8.4.

Low Frequency, Small k

Let us look at the limite $\omega \to 0$ with small k. We tehn have

$$\chi^0(k,\omega) = \frac{e}{\mathcal{V}} \sum_{\mathbf{q},\sigma} \frac{n_F(\epsilon^0_{\mathbf{q}}) - n_F(\epsilon^0_{\mathbf{q}+\mathbf{k}})}{(\epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}})}$$

where n_F is now a step function in energy at the chemical potential μ. If k is small, then the difference in the denominator is small, as is the difference of the arguments of n_F in the numerato4, and we can view the fraction on the right as being a derivative. Since the derivative of a step function is a delta function, we then have

$$\begin{aligned}\chi^0(k,\omega) &= \frac{e}{\mathcal{V}} \sum_{\mathbf{q},\sigma} \delta(\epsilon_{\mathbf{q}} - \mu) \\ &= e\int d\epsilon D(\epsilon)\delta(\epsilon-\mu) = eD(\mu)\end{aligned}$$

where in going to the second line, we have replaced a sum over $\mathbf{q}$ as an integral over energy dimens a density of states $D(\epsilon)$. The final result here is just the density of states, which is the static compressibility we derived previously (See Eq. 8.2).

8.3.2 High Frequency $\omega \gg E_F$ and small k

Another limit we can consider is that of high frequency.

Explicit Limit

Here we expand the denominator of Eq. 8.16 for large ω obtaining

$$\chi^0(\mathbf{k},\omega) = \frac{-e}{\mathcal{V}} \sum_{\mathbf{q},\sigma} \frac{n_F(\mathbf{q}) - n_F(\mathbf{q}+\mathbf{k})}{\hbar\omega} \left[\frac{1}{1 - \frac{(\epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}})}{\hbar\omega}} \right] \tag{8.18}$$

The leadingg term in this expansion replaces the square brackets with unity, bu then the sum over $\mathbf{q}$ vanihses. For the next term it is useful to write for small $\mathbf{k}$,

$$(\epsilon^0_{\mathbf{q}+\mathbf{k}} - \epsilon^0_{\mathbf{q}}) \approx \mathbf{k} \cdot \nabla_{\mathbf{q}} \epsilon^0_{\mathbf{q}}$$

and similarly

$$n_F(\mathbf{q}+\mathbf{k}) - n_F(\mathbf{q}) \approx \mathbf{k} \cdot \nabla_{\mathbf{q}} n_F(\mathbf{q})$$

We thus have

$$\chi^0(\mathbf{k},\omega) = \frac{e}{\mathcal{V}(\hbar\omega)^2} \sum_{\mathbf{q},\sigma} (\mathbf{k} \cdot \nabla_{\mathbf{q}} n_F(\mathbf{q}))(\mathbf{k} \cdot \nabla_{\mathbf{q}} \epsilon^0_{\mathbf{q}}) \tag{8.19}$$

$$= \frac{-e}{\mathcal{V}(\hbar\omega)^2} \left[\sum_{\mathbf{q},\sigma} n_F(\mathbf{q}) \right] \left[(\mathbf{k} \cdot \nabla_{\mathbf{q}})^2 \epsilon^0_{\mathbf{q}}) \right] \tag{8.20}$$

In obtaining the second line, we have integrated by parts (convert to integral, integrate by parts and convert back to a sum). The quantity in the second square bracket is $\hbar^2 k^2/(m)$ and is $\mathbf{q}$ independent. The quantity in the first square bracket can thus be summed alone to just give N. We thus have in this limit of large ω

$$\chi^0(\mathbf{k},\omega) = \frac{-k^2 n}{m\omega^2} \tag{8.21}$$

where n is the electron density. In fact this result is extremely general — independent of many details of the system, as we will see next.

More general f-sum rule approach

The limit can be obtained by invoking the so-called f-sum rule. We return to the primitive integral form of our response function (See Eq. 8.13)

$$\chi(\mathbf{k},\omega) = \frac{ie}{\hbar\mathcal{V}} \int_0^\infty dt\ e^{i(\omega+i\varepsilon)t} \langle [\hat{n}(\mathbf{k},t), \hat{n}(-\mathbf{k},0)] \rangle$$

Where

$$\hat{n}(\mathbf{k},t) = e^{iHt/\hbar} \hat{n}(\mathbf{k}) e^{-iHt/\hbar}$$

and here we would like to be completely general, so we consider *any* Hamiltonian H at this point (which may include electron-electron interactions, for example).

Since we are interested in high frequency, we equivalently want to look at small times t. Thus we expand for small t to write

$$\hat{n}(\mathbf{k},t) \approx \hat{n}(\mathbf{k}) + \frac{it}{\hbar}[H,\hat{n}(\mathbf{k})] + \dots$$

so that we have

$$\chi(\mathbf{k},\omega) = \frac{ie}{\hbar\mathcal{V}}\int_0^\infty dt\ e^{i(\omega+i\varepsilon)t}\ \frac{it}{\hbar}\langle[[H,\hat{n}(\mathbf{k},t)],\hat{n}(-\mathbf{k},0)]\rangle$$

This double commutator is familiar from our discussion of the Feynman theory of superfluids. In Eq. 5.11 we discovered that this double commutator is *independent of interactions between particles* and yields the constant $\hbar^2\mathbf{k}^2N/m$. Thus we can perform the integral to obtain the same result

$$\chi = \frac{-k^2n}{m\omega^2} \tag{8.22}$$

Drude Theory Approach

In fact one can get the same result out of simple Drude theory for a translationally invariant system. Translational invariance here means there should be no scatterers. Let us start with the current conservation equation (with the overdot being time derivative)

$$\dot{\delta n}(\mathbf{r},\mathbf{t}) + \nabla\cdot\mathbf{j}(\mathbf{r},t) = 0$$

where here δn is the local change in particle density and $\mathbf{j}$ is the local particle current. Let us rewrite this in terms of its frequency and wavevector fourier modes

$$-i\omega\,\delta n(\mathbf{k},\omega) + i\,\mathbf{k}\cdot\mathbf{j}(\mathbf{k},\omega) = 0$$

which we can write as

$$j_\parallel = \frac{\omega(\delta n)}{k} \tag{8.23}$$

We can then use the equations of motion when an electric field is applied

$$m\dot{\mathbf{v}} = -e\mathbf{E}$$

where the velocity is related to the current density by

$$\mathbf{j} = \bar{n}\mathbf{v}$$

with $\bar{n}$ the average density[10]. We thus have

$$m\dot{\mathbf{j}} = -e\bar{n}\mathbf{E} = e\bar{n}\nabla\phi$$

again moving to Fourier space we have

$$-i\omega m j_\parallel(k,\omega) = ie\bar{n}k\ \phi(k,\omega)$$

Plugging in Eq. 8.23 we obtain

$$\delta n(\mathbf{k},\omega) = \frac{-k^2\bar{n}e}{m\omega^2}\ \phi(\mathbf{k},\omega)$$

[10]We would also have a term $\delta n\mathbf{v}$ but this is order $(small)^2$, since both δn and $\mathbf{v}$ are assumed small.

8.4 Response of Interacting Electrons: RPA

In the last section we have been considering non-interacting electrons. We have the charge density response to an applied potential

$$\delta n(\mathbf{q},\omega) = \chi^0(\mathbf{q},\omega)\phi_{ext}(\mathbf{q},\omega)$$

where the superscript 0 indicates noninteracting. We would like to put the interactions back into the system in the simplest way possible. What do the interactions do? Well, if a nonuniform density δn occurs, this will induce a Coulomb interaction

$$\phi_{induced}(\mathbf{r},t) = \int d\mathbf{r}' V(\mathbf{r}-\mathbf{r}')\delta n(\mathbf{r}',t) \tag{8.24}$$

where we will assume here that the interaction V is of coulomb form

$$V(r) = \frac{-e}{4\pi\epsilon_0 r}$$

although our approach will work for any form of V.

Equation 8.24 is a convolution so we can write it more simply in fourier space

$$\phi_{induced}(\mathbf{q},\omega) = \tilde{V}(\mathbf{q})\delta n(\mathbf{q},\omega) \tag{8.25}$$

where $\tilde{V}$ is the fourier transform of $V(\mathbf{r})$.

Now the system must respond to both the externally applied ϕ_{ext} and the induced $\phi_{induced}$. A simple approximation is to assume the system responds like a noninteracting system — and let the entire effect of the interaction be included in the fact that we let the system respond to both the external and the induced potnentials. Thus we write

$$\begin{aligned}\delta n(\mathbf{q},\omega) &= \chi^0(\mathbf{q},\omega)\left[\phi_{ext}(\mathbf{q},\omega) + \phi_{induced}(\mathbf{q},\omega))\right] \\ &= \chi^0(\mathbf{q},\omega)\left[\phi_{ext}(\mathbf{q},\omega) + \tilde{V}(\mathbf{q})\delta n(\mathbf{q},\omega))\right]\end{aligned}$$

We can then solve this to obtain

$$\delta n(\mathbf{q},\omega) = \frac{\chi^0(\mathbf{q},\omega)}{1-\chi^0(\mathbf{q},\omega)\tilde{V}(\mathbf{q})}\ \phi_{ext}(\mathbf{q},\omega)$$

or equivalently

$$\delta n(\mathbf{q},\omega) = \chi^{RPA}(\mathbf{q},\omega)\phi_{ext}(\mathbf{q},\omega)$$

where

$$\chi^{RPA}(\mathbf{q},\omega) = \frac{\chi^0(\mathbf{q},\omega)}{1-\chi^0(\mathbf{q},\omega)\tilde{V}(\mathbf{q})} \tag{8.26}$$

This approximation of the response function of an interacting system is known as the RPA approximation[11] or time-dependent self-consistent Hartree approximation, since we

[11] RPA stands for "Random Phase Approximation". However these words mean almost nothing now. The approximation was first used by Bohm and Pines in 1952, and it was derived in a very roundabout way which is no longer used. In that language it was related to random phases, but this is only of historical interest.

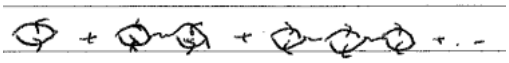


Figure 8.5: The RPA diagrams or bubble sum

are simply treating the effect of the interaction as being an effective potential (Eq. 8.24) that the electrons respond to, analogous to the Hartree approximation we used previously in section 7.3.1.

One way of understanding the RPA approximation is expand the denominator and write

$$\chi^{RPA} = \chi^0 + \chi^0 \tilde{V} \chi^0 + \chi^0 \tilde{V} \chi^0 \tilde{V} \chi^0 + \dots$$

which is shown in diagrammatic language in Fig. 8.5

8.4.1 Relation to Dielectric Constant

The response function χ is closely related to the relative dielectric constant. Recall that

$$\mathbf{E} = \frac{\mathbf{1}}{\epsilon_{\mathbf{r}}} \mathbf{D}$$

meaning that[12]

$$\phi_{total} = \frac{1}{\epsilon_r} \phi_{ext}$$

But we have

$$\begin{aligned} \phi_{total} &= \phi_{ext} + \phi_{induced} \\ &= \left[1 + \tilde{V}\chi\right] \phi^{ext} \end{aligned}$$

This equation is exact, so long as one uses the exact response function χ in the equation. So we have the exact result

$$\epsilon_r = \frac{1}{1 + \tilde{V}\chi}$$

Note that ϵ_r in principle depends on frequency and wavevector.

Using the RPA approximation for χ we substitute in to obtain

$$\epsilon_r = \frac{1}{1 + \tilde{V} \frac{\chi^0}{1 - V\chi^0}} = 1 - V\chi^0 \tag{8.27}$$

[12]Recall that $\mathbf{D}$ is the field applied normal exteranlly to a material, whereas $\mathbf{E}$ is the physical field.

Static Limit

It is useful to look a the static $\omega = 0$ limit. Recall that in this limit (Eq. 8.2)

$$\chi^0 = eD(E_F)$$

and we have the coulomb interaction in fourier space (Eq. 7.37)

$$\tilde{V}(k) = \frac{-e}{\epsilon_0 k^2}$$

We thus plug into Eq. 8.27 to get

$$\epsilon_r(\mathbf{k}) = 1 + \frac{e^2}{\epsilon_0 k^2} D(E_F) = 1 + \frac{k_{TF}^2}{k^2}$$

where k_{TF} is the Thomas-Fermi wavevector, Eq. 8.4.

We can then try to find out what happens if we insert a test charge of charge Q into our system. We then have

$$\phi_{ext}(\mathbf{k}) = \frac{Q}{\epsilon_0 k^2}$$

which gives us

$$\phi_{total}(\mathbf{k}) = \frac{1}{\epsilon_r}\phi_{ext} = \frac{Q/\epsilon_0}{k_{TF}^2 + k^2}$$

Fourier transforming this immediately gives

$$\phi_{total}(\mathbf{r}) = \frac{Q}{4\pi\epsilon_0 |\mathbf{r}|} e^{-k_{TF}|\mathbf{r}|}$$

matching the yukawa form we derived in Eq. 8.5.

8.4.2 High Frequency, Low k response: Plasmons

Let us consider interactions in the small k high frequency limit. As we derived above (in several ways!) we have the noninteracting response (Eq. 8.21) given by

$$\chi^0 = \frac{-e\bar{n}k^2}{m\omega^2}$$

If we plug this into the RPA equation (Eq. 8.26) we discover that the denominator $1 - \tilde{V}\chi^0$ diverges when

$$1 = \tilde{V}\chi^0 = \frac{e}{\epsilon_0} e\bar{n}k^2 m\omega^2$$

or

$$\omega = \sqrt{\frac{e^2 n}{\epsilon_0 m}}$$

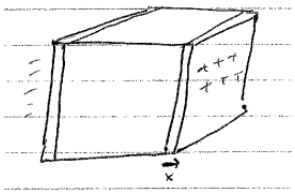


Figure 8.6: Displacing all of the mobile charges by a distance x builds up a surface charge $\rho_{surface} = \bar{n}xe$
.

The divergence in χ indicates an excitation mode of the system – in other words, the system responds with infinitessimly small amplitude perturbation if you perturb it in resonance with the excitation energy. This particular excitation mode is known as *plasma oscillation* or *plasmon* (when we think of it as a quantized object like a phonon or photon).

There is actually a very simple physical explanation for the plasmon. We consider a big cube of our material — with mobile negative chargees and a stationary positive background. Now let us imagine moving all of our negative charge a distance x in the x direction. This builds up a charge on the two x faces of our cube as shown in Fig. 8.6. The surface charge density that is built up is $\bar{n}xe$. We thus have a capacitor formed by the two charged faces. We may recall that from Gauss' law $\nabla \cdot \mathbf{E} = \rho/\epsilon_0$ we can obtain the electric field from a capacitor

$$\mathbf{E} = \rho/\epsilon_0 = \bar{n}xe/\epsilon_0$$

The electric field then applies a force

$$\mathbf{F} = -e\rho/\epsilon$$

to all of the electrons. Newtons law then gives us

$$m\ddot{x} = -e\rho/\epsilon_0 = \frac{-\bar{n}e^2}{\epsilon_0}x$$

thus resulting in harmonic motion with frequency

$$\omega = \sqrt{\frac{e^2 n}{\epsilon_0 m}}$$

It is important to note that this result holds with the mass m not being renormalized by any interactions (We discussed mass renormalization in the previous chapter, but that does not matter here). The reason the mass remains unrenormalized is because the plasma frequency describes the motion of the center of mass of all of the electrons in the system, and this is completely independent from the details of interaction between electrons. This is quite related to the argument leading up to Eq. 8.22, that the high frequency response is unchanged by interactions between particles.

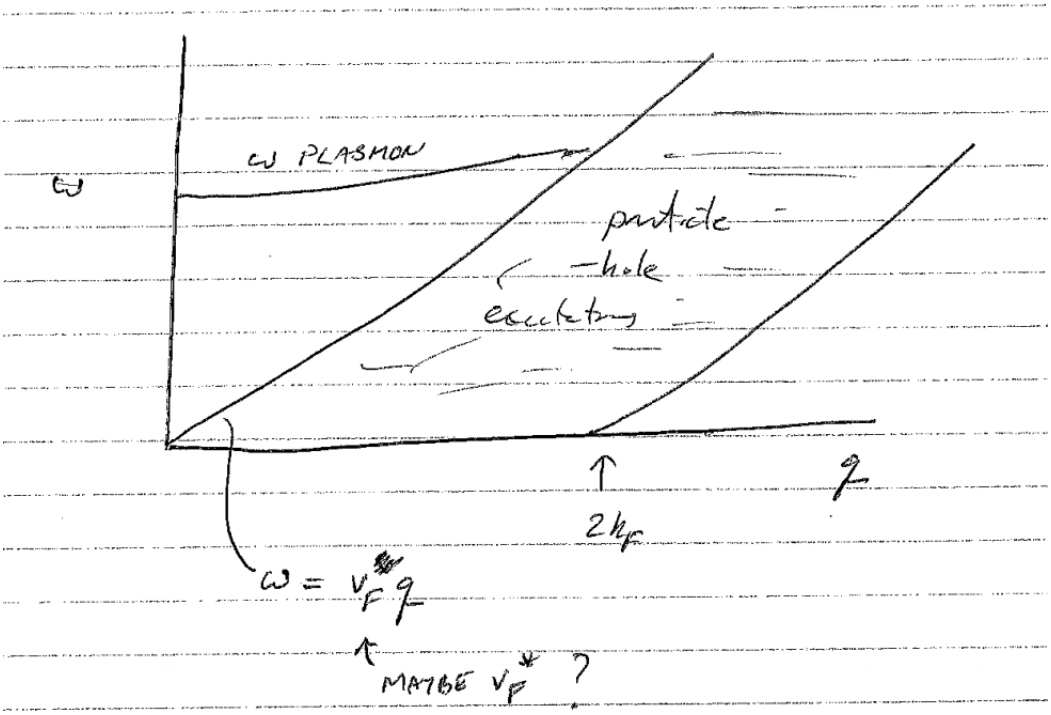


Figure 8.7: The excitation spectrum of an electron gas in three dimensions, with coulomb interaction between particles. This is qualitiatively similar to Fig. 8.4 except that the coulomb interaction gives an isoltated plasma mode at small k and high frequency. In RPA calculation, the upper edge of the particle-hole excitation band is at $\omega = v_F q$ with v_F the unrenormalized fermi velocity. However, in more detailed calculations this will be modified to $\omega = v_F^* q$ with a renormalized effective mass. However, the frequency of the plasma mode remains unrenormalized.

In Fig. 8.7 we sketch the excitation spectrum of a three dimensional electron gas with coulomb interactions. The spectrum is qualitatively similar to the noninteracting fermion spectrum shown in Fig. 8.4 except for the addition of the plasma mode at $\omega_{plasmon}$ at small wavevector 1. In RPA calculation, the upper edge of the particle-hole excitation band is at $\omega = v_F q$ with v_F the unrenormalized fermi velocity. However, in more detailed calculations this will be modified to $\omega = v_F^* q$ with a renormalized effective mass. However, the frequency of the plasma mode remains unrenormalized.

Chapter 9

Landau Fermi Liquid Theory

9.1 Background

What we have done so far (first order perturbation theory, Hartree-Fock, RPA) is fairly accurate for weakly interacting Fermi systems. However, real physical fermion systems usually have strong interactions[1]. Whether we are talking about metals, ^{3}He, neutron stars, or seminconductors[2], we typically have the interaction larger than the fermi energy

$$E_{interaction} > E_F$$

As a result the calculations we have done so far cannot be used quantitatively[3], although they can be used for qualitative inspiration. Despite this strong warning, we almost always get away with completely ingnoring interactions completely. Indeed, almost all of seminconductor physics (including the whole semiconductor industry) is built on the idea of mostly non-interacting electrons. Why does this make any sense at all? I'm glad you asked!

Understanding of strongly interacting fermions really began with experiments on ^{3}He. This system is much simpler than systems of electrons because of the absence of long ranged Coulomb interactions. In 1953-1954, William Fairbank[4] manged to cool ^{3}He to below about 1K which is less than the Fermi energy $E_F \approx 5$K. At low temeperature he

[1] In recent years people have been able to make cold atomic fermi gases where one can tune the interaction strength, and almost turn it off if desired. A huge amount of the pioneering research on cold fermionic atomic systems was done by Debbie Jin, who very sadly died of cancer at the young age of 47 in 2016.

[2] One might think that the low density of semiconductors might help. However, this turns out not to be true. The interaction is on the scale of $e^2/(\epsilon a)$ where a is the distance between fermions, whereas the kinetic energy is on the scale $\hbar^2/(2ma^2)$, so as we make the density lower, in fact the ratio of interaction to fermi energy actually increases!

[3] There is an exception: At small enough q and high enough ω, RPA becomes exact even for strongly interacting systems.

[4] Fairbanks was at Duke university at the time (where he recruited Fritz London in 1952). A few milligrams of ^{3}He was supplied by Oak Ridge National Lab, where much of the research for the american nuclear project was being done. This small amount was plenty for conducting the key experiments.

was able to see evidence of the Fermi-dirac distribution. In particular, he measured

$$\begin{aligned} C_v &\sim T \\ \chi &\sim \text{indep of } T \end{aligned}$$

where here χ means the pauli paramagnetic susceptibility. Both of these relations are indicative of fermions. However, in both cases, the proportionality constants did not match the predictions of the noninteracting fermion model. Now in our discussion of Hartree-Fock approximation above, we already have seen that the particle mass can be renormalized by interactions. However, this alone does not fix the problem in a consistent manner.

9.2 Basics Idea of Fermi Liquid Theory

In 1956, Landau, in one of his classic papers[5], explained how we should understand interactions of fermions. This work, based on brilliant intuition, set the language for our understanding of ferimons, and was fully justified many years later using both perturbation thoery and renormalization group methods.

9.2.1 Landau's Conjecture

Landau conjectured that interacting fermions should be just like noninteracting fermions, but "dressed" by interactions. What he meant by this is that

- The ground state shold be a "dressed" fermi sea
- Low energy excitations, can be described in terms of *quasiparticle* excitations of the ground state. These are "dressed" versions of the noninteracting excitations of the fermi sea.

The key question here is what we mean by "dressed". Here we mean that it needs to include a cloud of interactions with its surroundings. This very vague statement we will make more definite by the following argument:

Landau Adiabaticity Argument

Let us imagine starting with the noninteracting case and we imagine adiabatically turning on the interactions. Since this is a procedure that can be implimented using a Hamiltonian that we modify in time, it must be representable using a unitary (time evolution) operator. The result of this procedure gives the dressed fermi sea. This is depicted as a cartoon in the

[5]Titled, "The Theory of Fermi Liquids". This is a rather remarkable paper. It is only 6 pages long and has only a single citation (to the experiment by Fairbank).

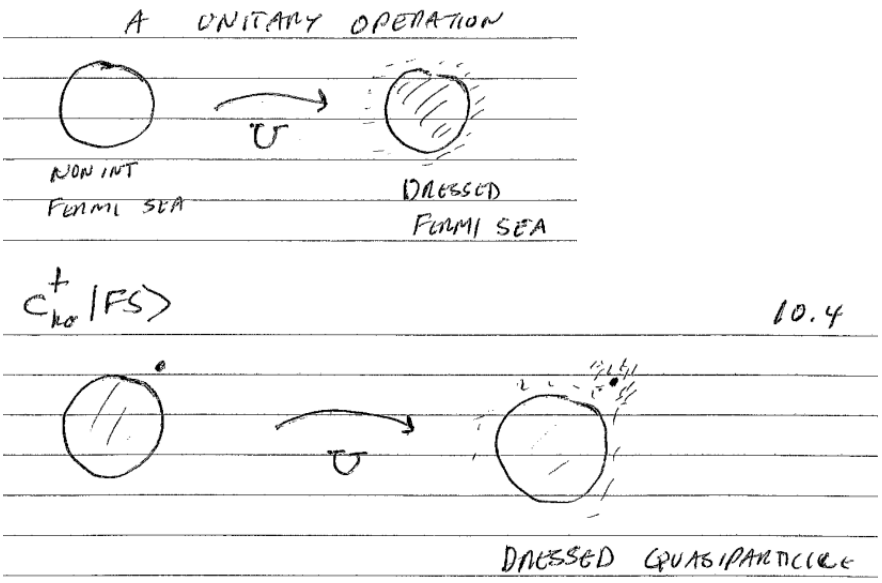


Figure 9.1: Top: turning on interaction adiabatically turns a noninteracting fermi sea into the interacting "dressed" ground state. Bottom: If we start with a fermi sea plus a single particle outside the fermi sea, when we turn on the interaction, we obtain a *quasiparticle*.

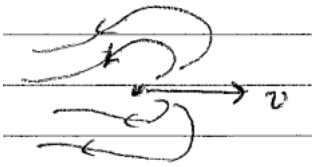


Figure 9.2: Fluid backflow around a moving object.

top of Fig. 9.1. Similarly, we can start with a single fermion added to the noninteracting fermi sea and adiabatically turn on the interaction. Here we get a dressed fermi sea with a dressed additional particle outside of the fermi sea as shown in the bottom of Fig. 9.1. We call this dressed additional particle a *quasiparticle*.

Here it is key to realize that in turning on the interaction, the quantum numbers of the system do not change — in particular, the momentum and spin are unchanged. Thus the dressed quasiparticles are in one-to-one correspondence with the noninteracting particles. However, in contrast to the noninteracting particles, the quasiparticles carry with the a cloud of interactions with their environment. This is very much like the idea of backflow around a moving object in a fluid as shown in Fig. 9.2.

Why does this picture of dressed quasiparticles make sense? To answer this we should ask the opposite question: how could this picture fail? (Of course one could always have a first order transition when the interaction turns on and the new ground state could be something completely different, like a crystal, but let us assume that such a first order

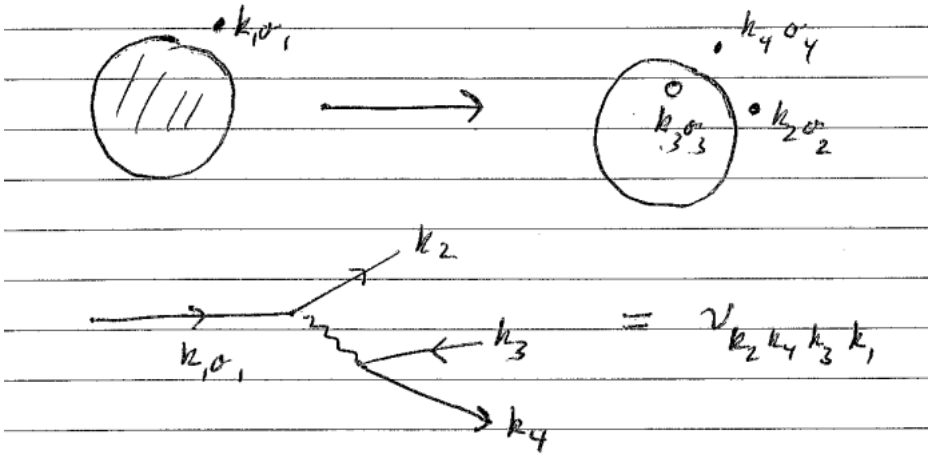


Figure 9.3: Two different depictions of quasiparticle decay of a single particle added above a fermi surface.

transition does not occur.) The only way our picture of dressed particles can fail is if the introduction of interactions lets the quasiparticle decay into multiple other quasiparticles — then the idea that we have a "single-particle" excitation will fail.

Let us think about what would have to be the case if such a decay were to happen. Of course we need to conserve both energy and momentum. If we have an initial momentum of our additional particle is $\mathbf{k}_1$ above the fermi surface ($|\mathbf{k}_1| > k_F$), we can imagine that it decays into two quasipartcles with momenta $\mathbf{k}_2, \mathbf{k}_4$ above the fermi surface and a quasihole with momentum $\mathbf{k}_3$ below the fermi surface. Such a process is shown in Fig. 9.3.

The key claim here is that due to phase space restrictions associated with energy conservation, the scattering lifetime for such a process is

$$\tau \sim |k_1 - k_F|^{-2} \tag{9.1}$$

so if we are considering quasielectrons or quasiholes very close to the fermi surface, they are very long lived, i.e., they do not fall apart. If a particle is "close enough" to the fermi surface it lives essentially forever, meaning it is in an eigenstate.

Here is a quasiproof of the statement Eq. 9.1. In the process shown in Fig. 9.3, all of the particles have energy $v_F|k - k_F|$, whether they are quasiparticles or quasiholes (a quasihole below the fermi surface costs positive energy). Enforce that the intitial energy must be the same as the final energy, so in calculating the scattering rate using Fermi's golden rule, we will have integrals of the form

$$\frac{1}{\tau} \sim \int_0^\infty d\epsilon_2 \int_0^\infty d\epsilon_3 \int_0^\infty d\epsilon_4 \;\; \delta(\epsilon_1 - (\epsilon_2 + \epsilon_3 + \epsilon_4))$$

where ϵ_1 is the initial energy and $\epsilon_{2,3,4}$ are the three final energies of the three final particles. As shown in Fig. 9.4 the value of this integral is equal to the area of a triangular region in $\epsilon_{2,3,4}$ space which intersects each axis at a value ϵ_1. Thus we obtain

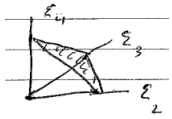


Figure 9.4: The region that conserves energy is the area of triangular piece of a plane a distance ϵ_1 out along each axis.

$$\text{Area} \sim \epsilon_1^2 \sim |k_1 - k_F|^2$$

Thus the scattering rate decreases as we approach the fermi surface and we have well defined quasiparticles[6]

9.3 Properties of the Dressed Fermi Liquid

Let us then ask what the dressing of the fermi liquid looks like in more detail. As written figuratively in Fig. 9.1, the dressing is given by some unitary transformation U. So that the interacting ground state can be written in terms of the noninteracting ground state

$$|\text{GS}\rangle = U|\text{GS}^0\rangle$$

Similarly we can write creation operators for the dressed quasiparticles $\tilde{c}^\dagger_{\mathbf{k},\sigma}$ by dressing the noninteracting quasiparticles $c^\dagger_{\mathbf{k},\sigma}$

$$\tilde{c}^\dagger_{\mathbf{k},\sigma} = U c^\dagger_{\mathbf{k},\sigma} U^\dagger$$

Now notice that the occupation of these dressed quasiparticles in the ground state is simply a step function, since

$$\begin{aligned} n^{qp}(\mathbf{k},\sigma) &= \langle \hat{n}_{qp}(\mathbf{k},\sigma)\rangle = \langle \text{GS}|\tilde{c}^\dagger_{\mathbf{k},\sigma}\tilde{c}_{\mathbf{k},\sigma}|\text{GS}\rangle \\ &= \langle \text{GS}^0|U^\dagger U\tilde{c}^\dagger_{\mathbf{k},\sigma}U^\dagger U\tilde{c}_{\mathbf{k},\sigma}U^\dagger U|\text{GS}^0\rangle \\ &= \langle \text{GS}^0|c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}|\text{GS}^0\rangle = n_F(k) \end{aligned}$$

It is much more complicated to find the occupancy of the *noninteracting* plane wave orbitals in the *interacting* ground state. Generally, this will be a hard task. However, at least if the interaction is weak, we can apply perturbation theory to write the interacting

[6]There has recently been a lot of study of so-called non-fermi liquid cases where the quasiparticle is not well defined because $1/\tau < \epsilon$. Certain models of high temperature superconductors have this property, for example.

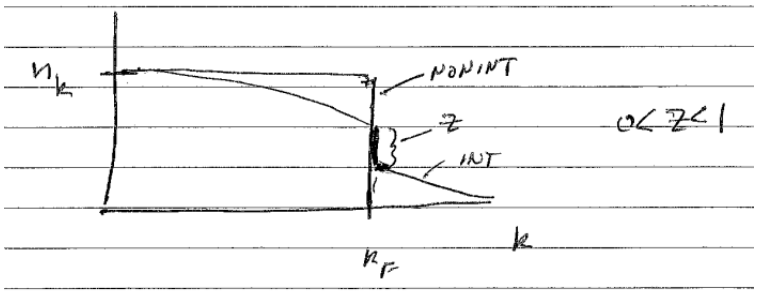


Figure 9.5: An interacting fermi liquid still has a step in the occupation at k_F, although the step is not as big as for a noninteracting fermi system.

ground state in tersm of the noninteracting one.

$$
\begin{aligned}
|\mathrm{GS}\rangle &= \eta \left[|\mathrm{GS}^0\rangle + \sum_{n \neq GS} \frac{|n\rangle\langle n|V|\mathrm{GS}^0\rangle}{E_n - E_{GS}} + \ldots \right] \qquad (9.2) \\
&= \eta \left[|\mathrm{GS}^0\rangle + \sum_{\mathbf{q}_1,\mathbf{q}_2>k_F;\mathbf{q}_3,\mathbf{q}_4<k_F} c^\dagger_{\mathbf{q_1}} c^\dagger_{\mathbf{q_2}} c_{\mathbf{q_3}} c_{\mathbf{q_4}} |\mathrm{GS}^0\rangle \frac{v_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_4,}}{E_{\mathbf{q}_1} + E_{\mathbf{q}_2} - E_{\mathbf{q}_3} + E_{\mathbf{q}_4}} + \ldots \right]
\end{aligned}
$$

where η is a factor included to keep the wavefunction properly normalized (and we have dropped spin indices for simplicity).

Now when we calculate the occupation of the original orbitals we have

$$
\begin{aligned}
n(\mathbf{k},\sigma) &= \langle \hat{n}(\mathbf{k},\sigma)\rangle = \langle \mathrm{GS}|c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}|\mathrm{GS}\rangle \\
&= \langle \mathrm{GS}^0|U^\dagger c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} U|\mathrm{GS}^0\rangle
\end{aligned}
$$

and the unitary transform is precisely the series shown in Eq. 9.2. The key thing to note here is that, at least perturbatively, there must remain a step in the occupation $n(k)$ coming from the first term in the series. It is a less pronounced step than for a purely interacting series, but it is a step nonehtheless as shown in Fig. 9.5.

This brings us to an important fact about interacting fermi systems. (We can even generalize our consideration now to arbitrary band structures in crystals, not just simple spherically symmetric systems).

Let us define a fermi surface to be the locus of points in k-space where there is a discontinuity in $\hat{n}(\mathbf{k})$.

Luttinger's Theorem:[7] The volume of the fermi sea in k-space is unchanged by interactions.

In a rotationally invariant system, this means k_F is unchanged by interactions.

[7] Joaquin (Quin) Mazdak Luttinger discovered this (partially with John Ward) in 1960. Those who know field theory know Ward from the famous Ward identities, which are key to the derivation of this theorm.

9.4 Landau Free Energy Functional

Given this quasiparticle concept, how are we going to deccribe the physics of a fermi liquid. The general idea is to always describe a system by the occupation of the quasiparticle states $n_{\mathbf{p},\sigma}$. (Above we called this $n^{qp}(\mathbf{k},\sigma)$ to distinguish it from the noninteracting particle occupation. Here we will drop the qp and also write this as a function of $\mathbf{p}$ rather than $\mathbf{k}$ as is more conventional in the field.) Remember that we are describing the quasiparticle occupancy here!

As mentioned, above at $T = 0$ we expect to have the ususal step function occupancy

$$T = 0 \qquad n^0_{\mathbf{p},\sigma} = \begin{cases} 1 & |\mathbf{p}| < p_F \\ 0 & |\mathbf{p}| > p_F \end{cases}$$

The superscript 0 means this is the occupancy in equilibrium (i.e., unperturbed). At finite temperature we would have a fermi function instead of a step function.

Let us now consider small perturbations to this distribution such that any excited quasiparticle or quasihole stays near the fermi surface. We can then Taylor expand

$$\delta n_{\mathbf{p},\sigma} = n_{\mathbf{p},\sigma} - n^0_{\mathbf{p},\sigma}$$

We the expect the change of free energy to be given by

$$\mathcal{F} - \mathcal{F}_0 \approx \sum_{\mathbf{p},\sigma} (\epsilon_p - \mu)\delta n_{\mathbf{p},\sigma} + \dots$$

Since we are near the fermi surface we have

$$\epsilon_{\mathbf{p}} - \mu = v^*_F(|\mathbf{p}| - p_F)$$

where we have linearized around the fermi surface. Note in particular that we are using the effective mass here

$$v^*_F = p_F/m^*$$

which tells us the energy of a single quasiparticle above (or below) the fermi surface.

A key realization by Landau is that the energy difference $F - F_0$ is second order in small quantities: Both $|\mathbf{p}| - p_F$ is small and δn is also small. As a result, to be consistent, we must consider other terms of roughly the same size — i.e., the next terms in the Taylor expansion giving

$$\mathcal{F} - \mathcal{F}_0 = \sum_{\mathbf{p},\sigma} (\epsilon_p - \mu)\delta n_{\mathbf{p},\sigma} + \frac{1}{2} \sum_{\mathbf{p},\mathbf{p}',\sigma,\sigma'} f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}')\delta n_{\mathbf{p},\sigma}\delta n_{\mathbf{p}',\sigma'} + \dots \tag{9.3}$$

The quantity $f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}')$ is some arbitrary interaction between a quasiparticle with momentum $\mathbf{p}$ with spin σ and another quasiparticle with momentum $\mathbf{p}'$ with spin σ'. What is crucial here is that this allows for a shift in energy, but it does not allow for scattering

— i.e, changing momentum! (The reason for this being the idea that the quasiparticle is very close to being an eigenstate when it is near the fermi surface).

Aside: We've been thinking in terms of spins σ which can be $\uparrow$ or $\downarrow$. However, more generally we would have to consider cases when the spin is polarized in the x-direction. As such we would write a density matrix $\delta n_{\alpha,\beta}(\mathbf{p})$ rather than just a density. So for example, the spin of the quasiparticle would be

$$\langle \overrightarrow{s} \rangle = \mathrm{Tr}[\overrightarrow{\sigma}_{\beta,\alpha} \delta n_{\alpha,\beta}]$$

and the interaction function would be a more complicated $f_{\alpha,\beta;\gamma,\delta}(\mathbf{p},\mathbf{p}')$. Fortunately, we will never need to deal with this more complicated situation. **end of aside**

Differentiating Eq. 9.3 we can obtain the energy of a quasiparticle $\tilde{\epsilon}$ when it is in the presence of other quasiparticles

$$\tilde{\epsilon}_{\mathbf{q},\sigma} - \mu = \epsilon_{\mathbf{p}} - \mu + \sum_{\mathbf{p}',\sigma'} f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}') \delta n_{\mathbf{p}',\sigma'}$$

The term including f here gives the energy shift of the quasiparticle due to the presence of other quasiparticles!

We now implement a number of simplifications.

1. We assume **p** and **p'** are both near the fermi surface, so that

   $$f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}') = f_{\sigma,\sigma'}(\hat{\mathbf{p}},\hat{\mathbf{p}}')$$

   with $\hat{\mathbf{p}}$ being the direction of **p**.

2. Further assuming rotational invariance we have

   $$f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}') = f_{\sigma,\sigma'}(\theta_{\hat{\mathbf{p}},\hat{\mathbf{p}}'})$$

   with θ being the angle between $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$.

   We can then further decomposte f into harmonics

   $$\begin{aligned} f_{\sigma,\sigma'}(\theta) &= \sum_{l \geqslant 0} f^{l,\sigma,\sigma'} P_l(\cos\theta) \\ f_{l,\sigma,\sigma'} &= \frac{2l+1}{2} \int_{-1}^{1} P_l(\cos\theta) f_{\sigma,\sigma'}(\theta) \end{aligned}$$

   where P_l is the Legendre polynomial.

   In particular, this implies

   $$f_{0,\sigma,\sigma'} = \frac{1}{4\pi} \int_{sphere} d\hat{\Omega}\, f_{\sigma,\sigma'}(\theta_{\hat{\Omega}})$$

3. We further assume our system is spin rotationally invariant this means that

$$\begin{aligned} f_{l,\uparrow\uparrow} &= f_{l,\downarrow\downarrow} \\ f_{l,\uparrow\downarrow} &= f_{l,\downarrow\uparrow} \end{aligned}$$

So that it is convenient to define the symmetric and antisymmetric combinations

$$\begin{aligned} f_l^s &= \frac{1}{2}\left(f_{l,\uparrow\uparrow} + f_{l,\uparrow\downarrow}\right) \\ f_l^a &= \frac{1}{2}\left(f_{l,\uparrow\uparrow} - f_{l,\uparrow\downarrow}\right) \end{aligned}$$

Finally we note that f has dimensions of energy (everything else in the least term of Eq. 9.3 is dimensionless). It is then convenient to define a dimensionless quantity. Let us define the density of states

$$D^*(\epsilon_F) = \frac{\mathcal{V} m^* p_F}{\hbar^3 \pi^2}$$

Note that this quantity has dimensionsl of 1/energy, and represents the density of states for quasiparticles (having a factor of m^* in it rather than m). We can then define the dimensionless quantities

$$F_l^{s,a} = D^*(\epsilon_F) f_l^{s,a}$$

known as fermi liquid coefficients. These parameters along with m^* and k_F completely describe our fermi liquid. Note that not all these parameters are completely independent: in particular we will see that m^* is related to F_1^s.

These F_l parameters describe the energy renormalizations associated with making a deformation of the fermi surface in the shape of the l^{th} spherical harmonic The s superscript means both spin fermi surfaces are deformed in the same way whereas the a supescript means the two fermi surfaces are deformed in opposite ways.

Aside: Although the following may look complicated, i think it clarifies a number of issues (Ref: See book by Baym and Pethick). If we write the shape of the deformed surface as

$$\delta p_F(\hat{\mathbf{p}}, \sigma) = p_\sigma P_l(\cos\theta)$$

with θ measured from some given point on the sphere, we get an energy of deformation given by

$$\mathcal{F} - \mathcal{F}_0 \sim p_s^2 \left(1 + \frac{F_l^s}{2l+1}\right) + p_a^2 \left(1 + \frac{F_l^a}{2l+1}\right)$$

where $p_s = p_\uparrow + p_\downarrow$ and $p_a = p_\uparrow - p_\downarrow$. Note the stability condition that $F_l > -(2l+1)$. If this condiditon is violated then the fermi sea deforms spontaneously in the ground state. **end aside**

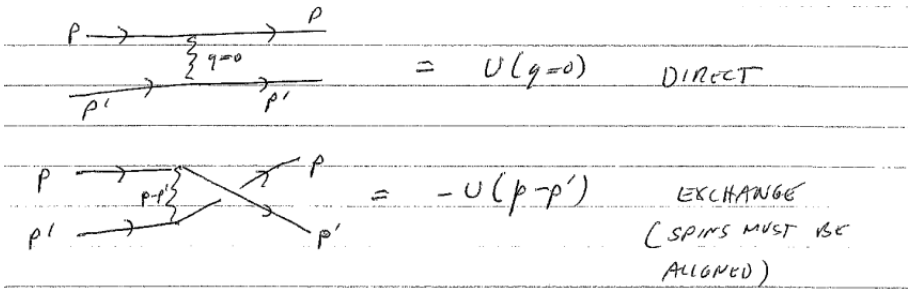


Figure 9.6: The two processes contributing to the interaction energy between $\mathbf{p}$ and $\mathbf{p}'$ included at first order in interaction strength.

Example: f at first order

It is useful to try calculating the interaction f at first order in the interactions. Recall that $f(\mathbf{p}, \mathbf{p}')$ is the interaction between quasiparticles at $\mathbf{p}$ and $\mathbf{p}'$ but does not allow scattering to another momentum $\mathbf{p}''$. (Again this is the well-defined quasiparticle assumption).

There are two processes in this interaction which we can label direct and exchange, analogous to the interactions we discussed in prior chapters. These two processes are shown in Fig. 9.6. The direct process (as in prior chapters) is the direct term, and it simply contributes $\tilde{V}(\mathbf{q} = 0)$ (the interaction bewtween two uniform densities). This is independent of the spin state of the two quasiparticles. The more interesting contribution is the exchange term which gives $-\tilde{V}(\mathbf{p} - \mathbf{p}')$, and this contribution requires both spin states to be aligned. Thus we have

$$\begin{aligned} f_{\uparrow,\downarrow}(\mathbf{p}, \mathbf{p}') &= \tilde{V}(0) \\ f_{\uparrow,\uparrow}(\mathbf{p}, \mathbf{p}') &= \tilde{V}(0) - \tilde{V}(\mathbf{p} - \mathbf{p}') = \tilde{V}(0) - \tilde{V}(2p_F \cos\theta_{\mathbf{p},\mathbf{p}'}) \end{aligned}$$

Example: ^{3}He

Examples of the Fermi liquid parameters for ^{3}He are given in the following table (Book Helium 3 by L. Pitaevskii and W. Halprin)

	m^*/m	F_0^s	F_0^a	F_1^s	F_1^a	F_2^s	F_2^a
1 atm	2.03	11.5	-0.71	5.8	-0.61	-0.18	-0.8
33.5 atm	5.81	87.1	-0.75	14.4	-1.01	0.83	0.0

Note that the F_0^a parameters is close to the stability boundary -1 where it deforms spontaneously in the ground state (in this case meaning that it becomes ferromagnetic, see section 9.5.2 below).

Figure 9.7: To find compressibility we imagine an expansion of the fermi surface by dp_F

9.5 Results from Fermi Liquid Theory

We are now in a position to use Landau's Fermi liquid theory to calculate some physical responses to small external perturbations.

9.5.1 Compressibility

Let us try to find the compressibility $\partial N/\partial\mu$. changing the number density involves an expansion or compression of the fermi surface as shown in Fig. 9.7 Let us imagine expanding the fermi surface by dp_F. We then want to calculate the new chemical potential

$$\begin{aligned}\mu^{new} &= \text{Energy of qp on the new fermi surface} \\ &= \tilde{\epsilon}_{p_F+dp_F} \\ &= \epsilon_{p_F+dp_F} + \sum_{\mathbf{p}',\sigma} f_{\sigma,\sigma'}(\mathbf{p},\mathbf{p}')\delta n_{\mathbf{p}',\sigma'}\end{aligned}$$

Here we have

$$\epsilon_{p_F+dp_F} = \mu^{old} + v_F^* dp_F$$

with $v_F^* = p_F/m^*$, and in the interaction term we should use

$$\delta n_{\mathbf{p},\sigma} = \begin{cases} 1 & p_F < |\mathbf{p}| < p_F + dp_F \\ 0 & \text{otherwise} \end{cases}$$

representing the change in the fermi surface. We thus have

$$\mu^{new} = \mu^{old} + v_F^* dp_F + \sum_{p_F<|\mathbf{p}'|<p_F+dp_F,\sigma'} f_{\sigma\sigma'}(\mathbf{p},\mathbf{p}')$$

I.e., the renormalization of the energy at the fermi surface contains the usual dispersion of energy ($v_F^* dp_F$) plus the change in the interaction term. We can rewrite this as

$$\mu^{new} = \mu^{old} + v_F^* dp_F + \begin{pmatrix} \text{number of } p \text{ states} \\ \text{between } p_F \text{ and } p_F + dp_F \end{pmatrix} \left[\frac{1}{4\pi} \int d\hat{\Omega} \sum_{sigma'} f_{\sigma,\sigma'}(\hat{\Omega}) \right]$$

The quantity in the square brackets we recognize as $2f_0^s$ and the quantity in the round brackets we recognize as

$$\begin{pmatrix} \text{number of } p \text{ states} \\ \text{between } p_F \text{ and } p_F + dp_F \end{pmatrix} = \frac{1}{2} D(E_F) v_F dp_F = \frac{1}{2} D^*(E_F) v_F^* dp_F$$

Putting these together and recalling the definition of F_0^s we obtain

$$\frac{\partial \mu}{\partial p_F} = v_F^*(1 + F_0^s)$$

Noninteracting Case: For noninteracting fermions we have

$$\frac{\partial \mu}{\partial p_F} = v_F$$

So the compressibility is

$$\frac{\partial N}{\partial \mu} = \frac{\partial N}{\partial p_F}\frac{\partial p_F}{\partial \mu}$$

and here it is easy to show $\partial N/\partial p_F = D(E_F)v_F$, so we have

$$\frac{\partial N}{\partial \mu} = [D(E_F)v_F]\frac{1}{v_F} = D(E_F)$$

which is what we usually expect.

Interacting case: Here we use instead

$$\frac{\partial \mu}{\partial p_F} = v_F^*(1 + F_0^s)$$

So that

$$\begin{aligned} \frac{\partial N}{\partial \mu} &= \frac{\partial N}{\partial p_F}\frac{\partial p_F}{\partial \mu} \\ &= [D(E_F)v_F]\frac{1}{v_F^*(1 + F_0^s)} \end{aligned}$$

But using the fact that

$$D(E_F)v_F = D^*(E_F)v_F^*$$

we get the final result

$$\frac{\partial N}{\partial \mu} = \frac{D^*(E_F)}{1 + F_0^s}$$

which shows that the compressibility is renormalized both by the expected mass renormalization (resulting in the * on $D^*(E_F)$) but also by the fermi liquid coefficient F_0^s.

9.5.2 Spin Susceptibility

Here we want to consider a similar expansion/compression of the fermi surface. However, in this case we let the up spins expand and the down spins compress, corresponding to a net change in magentization, as shown in Fig. 9.8. This is an *spin-antisymmetric* deformation of the fermi surface, and hence will couple to F_0^a as compared to the spin-symmetric deformation we considered in calculating the compressibility. For noninteracting fermions,

Figure 9.8: To determine spin susceptibility, we increase the size of the fermi surface for spin up and reduce the size of the fermi surface for spin down

this gives the usual Pauli spin susceptibility calculation. Yielding the result

$$\chi_{Pauli} = (\frac{1}{2}g\mu_B)^2\mu_0 D(E_F)$$

with μ_B being the Bohr magneton and g the g-factor. However, with a very similar calculation as we did for compressibility above, we determine the susceptibility for interacting fermions is

$$\chi = (\frac{1}{2}g\mu_B)^2\mu_0 \frac{D^*(E_F)}{1+F_0^a}$$

so that the spin susceptibility is again renormalized both by the mass renormalization and the fermi liquid parameter, F_0^a in this case.

Note that if $F_0^a < -1$ we have $\chi < 0$. This means that it is energetically favorable[8] for the ground state to deform by making a spin-antisymmetric deformation of the fermi surface — i.e., the fermi surface spontaneously magnetizes and we have a ferromagnet!

9.5.3 Mass Renormalization

Since this is a homework assignment, I'm not going to solve it here, but I'll give hints. The renormalization of mass is related to the F_1^s fermi liquid parameter via

$$\frac{m^*}{m} = 1 + \frac{F_1^s}{3} \tag{9.4}$$

Why is this related to F_1^s?. The $l = 1$ fourier spherical mode of the Fermi surface, shown in Fig. 9.9 corresponds to a simple displacement of the fermi surface — which is the same as a Galilean boost. One could calculate the energy of this Galilean boost either by starting with the Fermi liquid expression Eq. 9.3, or by realizing that a boost must have energy $N\frac{1}{2}mv^2$, with m the bare mass of the particles! Equating these two gives Eq. 9.4.

[8]Recall that for any magnetic system we can write the energy as a function of the magnetization as

$$E(M) = \frac{M^2\mu_0}{2\chi} - MB + \ldots$$

Figure 9.9: To determine spin susceptibility, we increase the size of the fermi surface for spin up and reduce the size of the fermi surface for spin down

9.5.4 More?

It may seem at this point that we have simply introduced a new fudge factor F for each experiment we want to do. However, once we fix these fermi liquid parameters, it turns out that many different experiments can be explained.

9.6 Further extensions of Fermi Liquid Theory

9.6.1 Local Dynamical Properties and Boltzmann Transport

Similar to the idea of going from Landau theory of phase transition to Landau-Ginzburg theory of phase transitions, our next bold step will be to promote the occupations from global to local quantities

$$n_{\mathbf{p},\sigma} \to n_{\mathbf{p},\sigma}(\mathbf{r})$$

Admittedly this appears to violate the uncertainty relation, since we can't specify $\mathbf{p}$ and $\mathbf{r}$ at the same time. However, we can indulge in some amount of semiclassical thinking. As long as we don't try to specify precise values of either, it will still be acceptable. As such, n will become some sort of momentum and position phase space density. We can then construct a Boltzmann equation or dynamical theory. We will not derive the Boltzmann equation here, but ...

.. it has solutions that are oscillations of the *shape* of the fermi surface, without oscillations in the local density. This phenomenon is known as *zero sound*. It was predicted by Landau and then observed in the 1960s in ^{3}He. Note that as the temperature goes to zero, regular ound vanishes. The reason for this is the lack of quasiparticle scattering when the quasiparticles are at low energy. Regular sound is derived by assuming local thermodynamic quantities, such as pressure, which is calculated from a local equation of state (pressure as a function of density). However, if the quasiparticles are not scattering, one never gets thermodynamic equilibrium and resular sound then no longer makes sense.

In contrast, zero sound persists down to zero temeprature, since it is derived without assuming any scattering of quasiparticles (the assumption of fermi liquid theory!).

9.6.2 Landau-Silin Theory: Long Range Coulomb Interactions

Finally we return to fermi liquids in metals. These are omnipresent in our world and so are of great interest. The long range coulomb interaction presents some problems for Fermi liquid theory. However, Landau and Silin (1956) developed a good method to address this, which can be thought of as a combination of Landau theory of fermi liquids and the RPA or self-consistent Hartree approximation which we apply in two steps:

(1) First, we imagine a fermi system with short range interaction only. Since the Fock interaction is short range (it requires wavefunction overlap), we can treat this part of the interaction between particles, but we throw out the long range hartree part. With this modified short range interaction, we have something we can treat properly with conventional Fermi liquid theory. We then calculate the properties of this fictitious interaction-truncated fermi system. For example, we might have

$$\tilde{\chi}^0 = \frac{\partial n}{\partial \mu} = \frac{D^*(E_F)}{1 + F_0^s}$$

(2) Once we have calculated all of these responses, we then add back in the long range Hartree part of the interaction at RPA level. For example,

$$\chi = \frac{\tilde{\chi}^0}{1 - \tilde{V}\tilde{\chi}^0} \tag{9.5}$$

So this approach is just like RPA, except instead of using the noninteracting response χ^0 in Eq. 9.5, we use a response $\tilde{\chi}^0$ which includes fermi liquid corrections due to the short range part of the interaction. We can check, for example, that in this approach, the Thomas-Fermi wavevector becomes modified to get

$$k_{TF}^2 = \frac{e^2}{\epsilon_0} \frac{D^*(E_F)}{1 + F_0^s}$$

So we see that the compressibility is modified by the mass renormalization and the F_0^s fermi liquid correction.

Chapter 10

BCS Theory

OK, this part is nonexaminable so I'm not going to write notes. Sorry!