

Lecture I

The goal of this course, broadly speaking, is to understand how the seemingly simple laws of quantum mechanics and electromagnetism give rise to a rich variety of highly organized phases of matter. Some of these phases, such as superconductors and superfluids, are so different in their properties from our everyday experience that to their original discoverers they must have seemed nearly magical. This first lecture gives a nontechnical overview of the main topics to be covered and the “big picture” ideas, and has a short discussion/review of second quantization and coherent states.

Useful textbooks are listed on the course information sheet. The two texts closest to the presentation in class are Schrieffer and Auerbach, but there will be some topics discussed, such as the Kondo effect, that are not mentioned in either book. The prerequisites for the course are a solid understanding of quantum mechanics and one semester each of statistical mechanics and solid-state physics.

Some examples of correlated states that we may discuss are superconductors and superfluids, the “Fermi liquid” description of metals, quantum ferromagnetism and antiferromagnetism, the integer and fractional quantum Hall effect, the “Luttinger liquid” theory of one-dimensional systems like carbon nanotubes, and the Kondo effect. A large part of the course will be devoted to understanding both the various instabilities of the Fermi liquid (to attractive interactions, to magnetic order, in one dimension, etc.) and its exceptional stability to repulsive interactions in two and three dimensions. All of these emerge from what is sometimes known as the “theory of almost everything”: nonrelativistic kinetic terms for electrons and ions, plus the instantaneous Coulomb interaction.

The main theoretical techniques used will be second quantization as a way to write new types of many-body states, such as the BCS wavefunction, and many-body perturbation theory (Feynman diagrams) for Green’s functions. Second quantization, which we will begin at the end of this lecture, is a compact way to write states with strong correlations or variable particle number; many-body perturbation theory is a clever way to compute corrections to physical quantities without having to deal with the entire wavefunction of 10^{26} particles.

Adiabatic continuity and discontinuity

Example I of continuity: In describing most metals and insulators, one starts from a picture of noninteracting electrons in e.g. calculating the band structure and other properties. However, the Coulomb interaction energy is actually very large, and one might wonder why it is appropriate to assume that noninteracting electrons (a free Fermi gas) make a sensible starting point.

The underlying idea, first phrased in these terms by Landau, is that electrons in a real metal form a “Fermi liquid”, which bears the same relation to the “Fermi gas” of free electrons that a normal liquid bears to a normal gas: the interactions are much stronger, but there is no change in symmetry or in the fundamental nature of the state. In particular, the “elementary excitations” of the ground state (those that are found to carry current, heat, and other properties) bear the same quantum numbers as ordinary electrons. We can imagine looking at the full energy spectrum of a many-particle system and trying to identify mobile low-energy excitations: Landau’s theory, which we will justify later in this course, explains how these excitations can wind up as electrons “dressed” by particle-hole pairs, which renormalize the mass (by up to a factor 10^3 in so-called heavy fermion compounds) and some other properties but not the charge e and fermionic statistics.

It turns out that electrons in a typical metal are stable to strong *repulsive* interactions, but can be unstable to even weak *attractive* interactions. The resulting superconducting state is an example of how adiabatic continuity can be violated: the lowest-energy charged excitations in a traditional superconductor are “Cooper pairs” of charge $2e$.

Example I of discontinuity: The natural energy scale of noninteracting electrons in a solid is the Fermi energy, which can be tens of thousands of kelvins. The natural Coulomb interaction energy scale $e^2n^{-1/3}$ is comparable to the Fermi energy. Both these energies are very large in comparison to the superconducting transition temperature T_c , which for an old-fashioned BCS superconductor is of order 10 K. It turns out that this new small energy scale is a signal of adiabatic discontinuity or “nonperturbative” behavior.

The superconducting gap in BCS theory scales as

$$T_c \sim De^{-1/\lambda N(0)}, \quad (1)$$

where D is a bandwidth or Fermi energy, λ is the energy of the attractive electron-electron interaction, and $N(0)$ is the electron DOS at the Fermi level. Looking at this formula, suppose we try to expand it as a power series in λ around $\lambda = 0$, when the system should be a noninteracting Fermi gas. You will find that all the derivatives at $\lambda = 0$ are 0, so the Taylor series looks like

$$T_c \sim 0 + \lambda 0 + \frac{\lambda^2}{2!} 0 + \dots \quad (2)$$

This is often stated as “ T_c is zero to all orders in perturbation theory”. Its practical meaning is that we need to find a new starting point for the description of the superconductor, rather than just starting from the free Fermi gas and trying to incorporate interactions perturbatively. A large part of this course will be devoted to the new starting points or organizational principles that emerge from the simple rules of nonrelativistic QM and the Coulomb interaction.

Example II of continuity: A superfluid is “like” a pure (noninteracting) BEC, even though the strong interactions in the superfluid make its quantitative properties very different. For instance, in a noninteracting bosonic gas, at temperature $T = 0$ all of the particles are in the lowest eigenstate; for an atomic BEC, about 99 percent or more are in the lowest eigenstate, as the interactions are weak; for superfluid helium-4, only about 10 percent are in the lowest eigenstate. However, helium-4 still shows amazing properties such as an absence of viscosity for low-velocity flows, because in some sense the interactions do not change the basic nature of the state.

Second quantization and states with variable particle number

You are all familiar, I’m sure, with Slater determinants for states of multiple identical fermions. A convenient way to write the overall wavefunction of three electrons in states ψ_1, ψ_2, ψ_3 is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \begin{vmatrix} \psi_1(\mathbf{r}_1) & \psi_1(\mathbf{r}_2) & \psi_1(\mathbf{r}_3) \\ \psi_2(\mathbf{r}_1) & \psi_2(\mathbf{r}_2) & \psi_2(\mathbf{r}_3) \\ \psi_3(\mathbf{r}_1) & \psi_3(\mathbf{r}_2) & \psi_3(\mathbf{r}_3) \end{vmatrix}. \quad (3)$$

This satisfies the requirement of asymmetry; note that the wavefunction vanishes if any two of the \mathbf{r}_i or ψ_i are equal.

An example of when we might want to use Slater determinants is when we study a many-body system in the **Hartree** approximation. Suppose we want to approximate the many-body state of N electrons moving in some constant background potential V_b (for example, from the ions of a

solid). We seek N lowest-energy eigenstates of the time-independent Schrödinger equation in the form

$$H\psi = \left(-\frac{\hbar^2 \nabla^2}{2m} + V(r) + V_b(r) \right) \psi_i = E_i \psi_i, \quad (4)$$

where the self-consistent potential $V(r)$ is determined through

$$V(r) = \int d\mathbf{r}_2 \frac{e^2 n(\mathbf{r}_2)}{|\mathbf{r}_2 - \mathbf{r}|} = \int d\mathbf{r}_2 \sum_i \frac{e^2 |\psi_i(\mathbf{r}_2)|^2}{|\mathbf{r}_2 - \mathbf{r}|}. \quad (5)$$

Here $n(\mathbf{r})$ is the electron number density.

Now the Hartree approximation is to find a self-consistent solution of these equations. However, the natural resulting many-body wavefunction that gives the potential above is the symmetric combination of the ψ_i , which does not satisfy the requirement of asymmetry under particle exchange. To be more precise, the Hartree equations can be justified as minimizing the total energy over all wavefunctions of the form

$$\Psi = \psi_1(\mathbf{r}_1) \psi_2(\mathbf{r}_2) \dots \quad (6)$$

which is not properly asymmetric.

The main error in the Hartree description, as you probably know, is that it ignores the “exchange” interaction between identical particles. We can make a better approximation by taking the Slater determinant of some orbitals ψ_i as the many-body ground state. Note that the many-body state still can be thought of as N independent “orbitals”, which is not true for a general state of N electrons, as we shall see. Minimizing over Slater determinants of independent orbitals gives the famous Hartree-Fock equation,

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_i(\mathbf{r}) + (V(\mathbf{r}) + V_b(\mathbf{r})) \psi_i(\mathbf{r}) - \sum_j \int d\mathbf{r}_2 \frac{e^2}{|\mathbf{r} - \mathbf{r}_2|} \psi_j^*(\mathbf{r}_2) \psi_i(\mathbf{r}_2) \psi_j(r) \delta_{s_j s_i} = E_i \psi_i. \quad (7)$$

Note that the exchange term (the last term on the left side) is now an integral operator, rather than just acting on $\psi_i(\mathbf{r})$. Here we have put back a spin delta-function as a reminder that the exchange term only occurs for equal spin (so that the particles are identical). It is important to remember that the Hartree-Fock description, which can be improved in various ways that are discussed in the 240 series, is qualitatively quite good for the majority of materials.

This course will concentrate, however, on the minority of materials for which the true quantum-mechanical many-body state is completely different from the simple Hartree picture. Let us first introduce a compact notation for Slater determinants. First, focus on problems with translational invariance, so that the single-particle states have well-defined momentum and can be labeled by their momentum \mathbf{k} . We assume for now that the particles are spinless, to simplify the notation. You may have seen a similar notation before for raising and lowering operators of harmonic oscillators, which we connect below to creation and annihilation operators of **bosons**. For now we stick to **fermions**, which will be created by c^\dagger and annihilated by c .

Write $|0\rangle$ for the state of zero particles (sometimes this notation will also be used for the ground state of a many-particle system, so be careful). Then the state of one particle of momentum \mathbf{k} is written

$$c_k^\dagger |0\rangle. \quad (8)$$

The adjoint of c_k^\dagger we write as c_k . The zero-particle state is annihilated by all the c_k :

$$c_k |0\rangle = 0. \quad (9)$$

Another requirement is that trying to put two fermions into the same single-particle state should also give 0, as should trying to get rid of two fermions:

$$c_k^\dagger c_k^\dagger = c_k c_k = 0, \quad (10)$$

where this notation means that the operators give 0 applied to any many-body state.

The most important condition on the c_k is the anticommutation relation:

$$\{c_k^\dagger, c_k\} = c_k^\dagger c_k + c_k c_k^\dagger = 1. \quad (11)$$

This essentially says that the probability of single-particle state k being empty in many-body state $|\Psi\rangle$, which is $\langle\Psi|c_k^\dagger c_k|\Psi\rangle$, plus the probability of its being occupied, which is $\langle\Psi|c_k^\dagger c_k|\Psi\rangle$, should sum to 1. Recall that this anticommutation relation holds only for **fermions**; clearly something different will be required for **bosons**.

Now we need to add the spin of the fermions and ask how the operators of different states k alter each other. For instance, is the state $c_{k_1}^\dagger c_{k_2}^\dagger |0\rangle$ the same as $c_{k_1}^\dagger c_{k_2}^\dagger |0\rangle$? There is an element of choice here, but the simplest way to think about it is to consider the operator $c_{k_1}^\dagger$ as “adding on” a new row to the Slater determinant (3). Then, since interchanging two rows of a determinant changes the sign of a determinant, we should have

$$c_{k_1}^\dagger c_{k_2}^\dagger |0\rangle = -c_{k_2}^\dagger c_{k_1}^\dagger |0\rangle, \quad (12)$$

which we summarize as

$$\{c_{\sigma_1 k_1}^\dagger, c_{\sigma_2 k_2}^\dagger\} = \{c_{\sigma_1 k_1}, c_{\sigma_2 k_2}\} = 0. \quad (13)$$

so that the two sequences create the same many-body state but with a sign difference. As you might expect, this sign difference is only there for fermions, and will not be present for bosons. Finally, restoring the spin variable σ , we write the full anticommutation relation as

$$\{c_{\sigma_1 k_1}^\dagger, c_{\sigma_2 k_2}\} = \delta_{k_1, k_2} \delta_{\sigma_1, \sigma_2}. \quad (14)$$

Hence these operators just anticommute unless both the momentum and the spin are the same, in which case there is a number 1 on the right side, expressing the idea that the fermionic state should have probability 1 of being occupied or empty.

Now let’s see how the above need to be modified for bosons. The main examples of bosonic operators that will appear in this course are the modes of the electromagnetic field, or of phonon excitations in a solid. For bosonic operators, we have a commutation relation instead of an anticommutation relation:

$$[b_{k_1}, b_{k_2}^\dagger] = \delta_{k_1, k_2}. \quad (15)$$

From this you can show that the number of quanta in mode k , i.e., the expectation value of the number operator $n_k \equiv b_k^\dagger b_k$, is increased by 1 by the creation operator b_k^\dagger , and decreased by 1 by the annihilation operator

We are now in a position to understand the simplest example of coherent states, which are useful in taking the classical limit of a harmonic oscillator or in setting up Feynman path integrals over classical configurations.

Let’s return to fermions. We can write the filled Fermi sea as

$$\prod_{|k| \leq k_F} c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger |0\rangle. \quad (16)$$

Here all states of momentum below the Fermi momentum are filled by the creation operators, while all those above the Fermi momentum are empty. We could equally well have written this state as a Slater determinant, of course.

As motivation for next time, consider the following famous example of a strongly correlated wavefunction:

$$\Psi_{BCS} = \prod_k (u_k + v_k c_{k\downarrow}^\dagger c_{-k\uparrow}^\dagger) |0\rangle, \quad |u_k|^2 + |v_k|^2 = 1. \quad (17)$$

Here u_k and v_k are some k -dependent complex numbers satisfying the normalization constraint above. Now this will just give the filled Fermi sea above for a particular choice of the u_k, v_k : the filled Fermi sea results from

$$u_k = \begin{cases} 0 & \text{if } k \leq k_f \\ 1 & \text{if } k > k_f \end{cases}, \quad v_k = \begin{cases} 1 & \text{if } k \leq k_f \\ 0 & \text{if } k > k_f \end{cases}. \quad (18)$$

However, suppose we smear out the sharp boundary at the Fermi level by an energy Δ , so that now over some interval, u_k and v_k are both between 0 and 1. This might seem to be similar to the Fermi gas at finite temperature, because then the occupancy is also smeared out over a distance kT near the Fermi level.

However, the smeared BCS state is very different on a fundamental level because it has perfect pair correlations. For every momentum k , even in the smeared state, if the spin-up orbital is occupied then the spin-down orbital at momentum $-k$ is automatically also occupied. This does not occur in the Fermi gas at finite temperature, where the spin-up and spin-down orbitals are independent. The next lecture will begin the discussion of how this amazing state winds up as the ground state of a semi-realistic Hamiltonian.