Honors undergraduate seminar, Spring 2004
Introduction to emergent properties of many-particle systems
Lecture 1: course webpage at http://socrates.berkeley.edu/˜jemoore

Many of the most spectacular phenomena of modern physics involve the collective behavior of systems of many interacting particles (electrons, photons, atoms, quarks ...). Our success in understanding such systems since the 1940s has influenced much of the development of high-energy physics, condensed matter physics, and even astrophysics. However, the standard undergraduate curriculum concentrates either on problems of one or two interacting particles, or else on statistical problems where the interactions between particles are neglected entirely.

This course aims to give an introduction, at a moderate level of technical detail, to a few of the exotic effects that appear in many-particle systems. Note that our current understanding of quantum field theory (the synthesis of quantum mechanics and special relativity) is such that **every** system is a many-particle system: even Maxwell's equations of electromagnetism really describe coherent quantum-mechanical states of an enormously large number of photons. Along the way, we will come across many of the major developments in postwar physics, and also understand some of the current trends in physics research.

The prerequisites for this course are a solid undergraduate education (at least one semester each) in nonrelativistic quantum mechanics and in statistical mechanics. A second semester of quantum mechanics will be very helpful. This first lecture rapidly reviews some ingredients from quantum mechanics and introduces the main "paradoxes" confronting physics in the 1940s. Just as many of the most dramatic problems in 1890s physics were stunningly resolved by special relativity and quantum mechanics, some of the 1940s paradoxes were resolved by the methods we will see in this course. Others have been solved but by methods that are a little too technical for these lectures, while a significant number of problems, such as the marriage of quantum mechanics and gravity, survive for future generations.

Our course will cover three main examples of emergent phenomena: superconductivity and other collective quantum states; chaos and the microscopic origin of irreversibility; and phase transitions. Another example of a 1940s problem that was resolved by many-particle physics is "quantum electrodynamics": for example, the electron g-factor, which determines the ratio of its magnetic moment to the Bohr magneton,

$$g = \mu_e/\mu_B \approx 2.002319314, \quad \mu_B = \frac{e\hbar}{2m} \tag{1}$$

has now been calculated to 9 decimal places by including many virtual electron-photon processes, even though g seems like a single-electron property.

Now we do a brief review of a method for solving the quantum harmonic oscillator that will also help us understand many-particle quantum systems.

Raising and lowering operators for the harmonic oscillator

The following short sections on the harmonic oscillator and Slater determinants can be found in any standard quantum mechanics textbook. Consider the good old harmonic oscillator for a single particle moving in one dimension:

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}. \tag{2}$$

We can use a trick to get the whole energy spectrum without having to go through the work of solving the Schrodinger equation to get wavefunctions. Our convention is that the single-particle eigenstate of momentum $\hbar k$ is proportional to $\exp(i(kx-Et))$ with $E=\hbar^2k^2/2m$. The momentum operator is

$$p \equiv -i\hbar\frac{\partial}{\partial x}. \tag{3}$$

Introduce the non-Hermitian operator

$$a = \frac{1}{\sqrt{2\hbar}}\sqrt{m\omega}(x+ip(m\omega)^{-1}) \tag{4}$$

whose adjoint is

$$a^\dagger = \frac{1}{\sqrt{2\hbar}}\sqrt{m\omega}(x-ip(m\omega)^{-1}). \tag{5}$$

Note first that the commutator

$$[a,a^\dagger] = aa^\dagger - a^\dagger a = im\omega(px-xp)(m\omega)^{-1}/\hbar = 1, \tag{6}$$

where we have used the Heisenberg uncertainty relation

$$[x,p] = i\hbar. \tag{7}$$

We can use these commutation relations to generate the entire spectrum of eigenstates for this particular problem. The key is the commutation relation of $a^\dagger$ with H:

$$[H,a^\dagger] = \frac{1}{\sqrt{2\hbar}}\sqrt{m\omega}\left([p^2/(2m),x] - i[m\omega^2x^2/2,p](m\omega)^{-1}\right). \tag{8}$$

Now $[x^2,p] = xxp - pxx = xxp - xpx + xpx - pxx = x[x,p] + [x,p]x = 2i\hbar x$, and $[p^2,x] = -2i\hbar p$. We thus have

$$[H,a^\dagger] = \sqrt{\frac{m\omega}{2\hbar}}\,(-2i\hbar p/(2m) + \hbar x\omega) = \hbar\omega a^\dagger. \tag{9}$$

The assumptions we will need to make are that there is a "ground state" $|0\rangle$ of energy E_0 (you can show that $E_0 = \hbar\omega/2$, the famous zero-point energy of the harmonic oscillator) and that this state is annihilated by a:

$$a|0\rangle = 0. \tag{10}$$

Now consider the state $a^\dagger|0\rangle$. The action of the Hamiltonian on this state can be deduced by the above commutation relation:

$$Ha^\dagger|0\rangle = a^\dagger H|0\rangle + [H,a^\dagger]|0\rangle = a^\dagger(E_0|0\rangle) + \hbar\omega a^d agger|0\rangle = (E_0+\hbar\omega)|0\rangle. \tag{11}$$

Hence the state $a^\dagger|0\rangle$ is an eigenstate of increased energy $E_0+\hbar\omega$. (We haven't bothered to normalize this eigenstate, but the eigenvalue is not altered by normalization.) By the same process of acting with the raising operator $a^\dagger$, we generate a family of eigenstates of energies $E_0+n\hbar\omega$ for integer n, which we label $|n\rangle$. The number operator

$$N = a^\dagger a \tag{12}$$

counts which state the particle is in, and for the harmonic oscillator,

$$H = \hbar\omega(\frac{1}{2} + a^\dagger a), \tag{13}$$

where $E_0 = \hbar\omega/2$ is the zero-point energy.

From your quantum mechanics course, you should be familiar with states that are superpositions of eigenstates of different energies, such as

$$\psi = \frac{1}{\sqrt{3}}|0\rangle + \frac{1}{\sqrt{3}}|1\rangle + \frac{1}{\sqrt{3}}|2\rangle. \tag{14}$$

We are now going to develop a more interesting interpretation of the above algebra of raising and lowering operators (now called "creation" and "annihilation" operators): rather than viewing a state like ψ as a superposition of different energy eigenstates, we can view it as a superposition of states of different particle number.

Second quantization and states with variable particle number

Let us consider the algebra of raising and lowering operators without reference to any particular Hamiltonian H. All we will assume is that there is a vacuum or ground state labeled by $|0\rangle$ which is annihilated by a, and we think of this state as containing zero particles. Acting with $a^\dagger$ increases the number of particles in the state, and each particle contains an energy $\hbar\omega$. Note that this is very different from what we did previously: we are now talking about different occupation numbers of a single quantum-mechanical state, while before we were talking about different states, with different wavefunctions. We are also talking specifically about **bosonic** particles (like photons, for example), since only a single fermion can be in any one quantum-mechanical state, by the Pauli principle. The convenient notation we develop is historically referred to as "second quantization", where first quantization refers to ordinary single-particle wavefunctions.

In a real system, we want to be able to consider many single-particle eigenstates, each of which may have any number of bosons. For example, in your study of black-body radiation in statistical mechanics, you had to consider the electromagnetic modes of a cavity, each of which contained some number of photons. For simplicity let us consider plane waves labeled by momentum $\mathbf{k}$

$$\psi_k = e^{ikx - iEt} \tag{15}$$

and ignore spin. Now the creation operator $a^\dagger_{\mathbf{k}}$ acts to add one boson in the state of momentum $\hbar\mathbf{k}$, and the annihilation operator acts to subtract one boson. The commutation relations of the many-particle system are

$$[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = \delta_{k,k'}. \tag{16}$$

Here the δ-function means that if $\mathbf{k} = \mathbf{k}'$, so that we are looking at creation and annihilation operators in the same quantum-mechanical state, then the operators do not commute; otherwise they are independent of each other. Two creation operators and two annihilation operators always commute:

$$[a^\dagger_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = [a_{\mathbf{k}}, a_{\mathbf{k}'}] = 0. \tag{17}$$

In this Hilbert space of states of all different particle numbers, called a **Fock space**, the same concepts of normalization and superposition apply as in ordinary single-particle Hilbert spaces. To make this a bit more understandable, let us make a quick detour to connect these states to other states you have seen for multiple particles. We will then give some examples of the power of this new notation.

Before proceeding, let's try to make a version of the above for **fermionic** particles. This is not very difficult: a single-particle state of well-defined momentum $\hbar k$ and spin σ should have either zero fermions or one fermion. For fermions we use c for the annihilation operator and $c^\dagger$ for the creation operator. If there are no fermions in a state, then the number operator $N = c^\dagger c$ has expectation value 0 since c annihilates the state, and we assign the operator $cc^\dagger$ the value 1. If there is one fermion in the state, then $c^\dagger$ annihilates the state (since it cannot hold two fermions), $cc^\dagger$ has expectation value 0, and N has expectation value 1. Hence in both states $c^\dagger c + cc^\dagger = 1$: we define this as the **anticommutation** relation

$$\{c^\dagger, c\} = 1. \tag{18}$$

To generalize this to multiple fermions in multiple states, let us go back to the notion of Slater determinants.

You probably remember Slater determinants for states of multiple identical fermions. A convenient way to write an overall wavefunction of three electrons, all with spin up, in single-particle states $\psi_{k1}, \psi_{k2}, \psi_{k3}$ is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \begin{vmatrix} \psi_{k1}(\mathbf{r}_1) & \psi_{k1}(\mathbf{r}_2) & \psi_{k1}(\mathbf{r}_3) \\ \psi_{k2}(\mathbf{r}_1) & \psi_{k2}(\mathbf{r}_2) & \psi_{k2}(\mathbf{r}_3) \\ \psi_{k3}(\mathbf{r}_1) & \psi_{k3}(\mathbf{r}_2) & \psi_{k3}(\mathbf{r}_3) \end{vmatrix}. \tag{19}$$

This satisfies the requirement of asymmetry (by the Pauli principle, since electrons are fermionic their overall wave function must be antisymmetric, and we are assuming that all have the same spin so the orbital part must be antisymmetric); note that the wavefunction vanishes if any two of the positions $\mathbf{r}_i$ or wavefunctions ψ_i are equal. In our second quantization notation, this state is described compactly as

$$\Psi = c^\dagger_{k3,\uparrow} c^\dagger_{k2,\uparrow} c^\dagger_{k1,\uparrow} |0\rangle, \tag{20}$$

where $|0\rangle$ is again the vacuum (the state with no particles). This notation means that starting from the vacuum, we add one electron with wavenumber $k1$ and spin up; then one with wavenumber $k2$ and spin up; then one with wavenumber $k3$ and spin up. The creation operator can be thought of as adding a row at the bottom of the Slater determinant.

With this interpretation of the creation operator, it is natural to extend the anticommutation relation to

$$\{c^\dagger_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\} = \{c_{\mathbf{k}}, c_{\mathbf{k}'}\} = 0. \tag{21}$$

Here the idea that creation operators **anticommute** for different states makes sense since flipping rows in the Slater determinant flips the overall sign. The anticommutator is equal to 1 only if the c and $c^\dagger$ operator act on the same momentum (and spin) state.

The real value of the second quantization notation will become apparent in our discussion of superconductivity. Superconductivity was discovered experimentally in 1911, but the theoretical explanation of superconductivity was only resolved in 1957 (the "BCS" theory of Bardeen, Cooper, and Schrieffer). The success of this theory is that it explains the remarkable phenomenological fact that a superconductor is well described by single-particle quantum mechanics of bosons of charge $2e$. The remainder of this lecture explains one idea of what is so unique about a superconductor: the superconductor is not "perturbative" or "adiabatically continuous" with the Fermi gas of noninteracting electrons.

Adiabatic continuity and discontinuity: superfluidity and superconductivity

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 the great physicist Lev 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 $e^2 n^{-1/3}$ 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

$$T_c \sim D e^{-1/\lambda N(0)}, \tag{22}$$

where D is a bandwidth or Fermi energy, λ is the energy of the attractive electron-electron interaction, and $N(0)$ is the electron density of states (the number of eigenstates per energy) 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

$$T_c \sim 0 + \lambda 0 + \frac{\lambda^2}{2!} 0 + \dots. \tag{23}$$

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.