Physics 4261: Lectures for week 13

Prof. Colin V. Parker (cparker@gatech.edu)
Georgia Institute of Technology

13.1 Density of states

In order to find the total number of bosons in a box, we have to sum over all the energy levels of the box, multiplying by the Bose factor for each level, i.e.

$$N = \sum_{i=0}^{\infty} \frac{1}{e^{(E_i-\mu)/k_B T} - 1} = \int_0^{\infty} \sum_{i=0}^{\infty} \delta(E - E_i) \frac{1}{e^{(E-\mu)/k_B T} - 1}\, dE.$$

Now the quantity

$$g(E) = \sum_{i=0}^{\infty} \delta(E - E_i),$$

is called the density of states, and is very important. To calculate it, note that the number of states of energy less than E is $\int_0^E g(E) dE$. In a box with side L and periodic boundary conditions, the states have energies given by

$$\begin{aligned} E &= \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 \left(n_x^2 + n_y^2 + n_z^2\right), \\ E &= \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 n^2, \\ n &= \sqrt{\frac{2mE}{\hbar^2}\frac{L^2}{(2\pi)^2}}. \end{aligned}$$

where n_x, n_y, and n_z are integers. The number of states up to a maximum level n_{max} can be computed from the volume of a sphere as

$$N = \frac{4\pi}{3} n_{\text{max}}^3.$$

Putting this together,

$$\begin{aligned} N(E) &= \frac{4\pi}{3}\left(\frac{2mE}{\hbar^2}\frac{L^2}{(2\pi)^2}\right)^{3/2}, \\ g(E) &= \frac{\partial N}{\partial E} = 2\pi V \sqrt{E}\left(\frac{2m}{\hbar^2 (2\pi)^2}\right)^{3/2}, \\ g(E)/V &= \sqrt{\frac{m^3}{2\hbar^6 \pi^4}}\sqrt{E}. \end{aligned}$$

Then, the total density of particles is

$$n = \sqrt{\frac{m^3}{2\hbar^6\pi^4}} \int_0^\infty \frac{\sqrt{E}}{e^{(E-\mu)/k_B T} - 1}\, dE,$$

$$n = \sqrt{\frac{m^3}{2\hbar^6\pi^4}} (k_B T)^{3/2} \int_0^\infty \frac{u}{e^{-\mu/k_B T} e^u - 1}\, du.$$

Now, clearly as μ becomes large and negative, this quantity can be as small as we like. And if μ is positive, everything is total nonsense. But what about $\mu = 0$? Then the integral gives,

$$n_0 = \sqrt{\frac{m^3}{2\hbar^6\pi^4}} (k_B T)^{3/2} \int_0^\infty \frac{u^{1/2}}{e^u - 1}\, du.$$

Now, this integral will be some dimensionless number (it's 2.315 BTW). Note, importantly that while the integrand diverges at $u = 0$, the singularity is integrable. For small u we have

$$\frac{u^{1/2}}{e^u - 1} \approx \frac{u^{1/2}}{1 + u + u^2/2 + \cdots - 1} \approx u^{-1/2}.$$

Therefore, there is a finite n_0, where even if $\mu = 0$ we cannot exceed this number. What if $n > n_0$. Then we have the BEC state. The remaining atoms go into the ground state. Why the ground state? Because the approximation that you can replace the sum by an integral breaks down. There is actually only one ground state and the μ becomes arbitrarily close to zero.

13.1.1 Putting in some numbers

If we put in the mass of ^{87}Rb and a density of 10 atoms per cubic micron, I get a transition temperature of 86 nK.

13.2 Interactions

Of course, the above theory predicts finite occupation of the ground state for the non-interacting system only. We would like to introduce interactions, and see how they influence the behavior. However, first we should think a little about how atoms interact, and it is convenient to introduce the concept of partial wave scattering. One striking fact is that the binding energy between two atoms is usually thousands of Kelvin. And the BEC is at nanoKelvin. So how can this be "weakly" interacting? The answer is that the interaction is very short range. Because energy is conserved, any collision between ground state atoms is elastic, and so two colliding particles will not bind, no matter how deep the interaction potential. Of course, three atoms can bind a pair and release the third one at high speed, this is called three-body loss and it is to be avoided by making the density low. What about the two body interactions? We would like to model the interactions as simply as possible, but perturbation theory will break down with the deep potential.

13.2.1 Gross-Pitaevskii equation

Once we have the effect of the interactions under control, we will write an equation for how a BEC behaves. With no interactions, the (pure) BEC is simply N atoms in the ground state. Therefore, it obeys the single-particle Schrödinger equation,

$$\left\{-\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{r})\right\}\psi = E\psi.$$

This can be seen as minimizing an energy functional

$$\mathcal{H}_{\mathrm{s}} = \frac{\hbar^2}{2m}|\nabla\psi|^2 + V(\mathbf{r})|\psi|^2.$$

The Gross-Pitaevskii equation adds a term to the energy functional

$$\mathcal{H}_{\mathrm{GP}} = \frac{\hbar^2}{2m}|\nabla\psi|^2 + V(\mathbf{r})|\psi|^2 + \frac{g}{2}\left(|\psi|^2\right)^2,$$

leading to the Gross-Pitaevskii equation (GPE),

$$\left\{-\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{r}) + g|\psi|^2\right\}\psi = \mu\psi.$$

But how to find g? How to do perturbation theory with deep potentials?

1. Find the scattering length for the deep potential.
2. Find the equivalent shallow potential with the same scattering length.
3. Do perturbation theory on the shallow potential.
4. Conclude that as far as long-range physics is concerned, the answers are the same.

13.2.2 Partial waves

Consider an atom in a plane wave state, incident on a fixed target, whose potential drops to zero at some range. Actually we could also use the concept of reduced mass to consider a pair of atoms incident at some relative wavevector. If we assume the interaction is spherically symmetric, we would very much like to take advantage of the spherical harmonics so that we have only to solve a 1D equation instead of a 3D one. When solving for bound states, this is something we know how to due. However, for an incoming plane wave, we have the state:

$$\psi = e^{ikz} = e^{ikr\cos\theta}.$$

Ideally we would like to expand this in terms of spherical harmonics,

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} c_l R_l(r) Y_{l,0}(\theta).$$

We note there is no need for spherical harmonics with $m \neq 0$, because the incoming state and all properties are symmetric on the z-axis. What can be said about the functions $R_l(r)$. First, because the incoming plane wave satisfies the wave equation,

$$\nabla^2\psi + k^2\psi = 0,$$

we know that the functions $R_l(r)$ can be written as linear combinations of the spherical Bessel functions of the first and second kind $j_l(kr)$ and $\eta_l(kr)$. To find the coefficient, we take the limit $r \to 0$, and evaluate the integral

$$\begin{aligned}
c_l R_l(r) &= 2\pi \int_0^\pi Y^*_{l,0}(\theta) e^{ikr\cos\theta} \sin\theta \, d\theta, \\
c_l R_l(r) &\approx 2\pi \int_0^\pi Y_{l,0}(\theta) \left[1 + ikr - \frac{1}{2}(kr)^2 + \cdots \right].
\end{aligned}$$

This is obviously bounded and hence we reject any component of the spherical Bessel functions of the second kind (or spherical Neumann functions) diverge at the origin, while the plane wave does not. Noting that the first two spherical Bessel functions (of the first kind) and their asymptotic forms are

$$\begin{aligned}
j_0(kr) &= \frac{\sin(kr)}{kr} & j_0(kr) &\approx 1 \quad (r \to 0) & j_0(kr) &\approx \frac{\sin(kr)}{kr} \quad (r \to \infty), \\
j_1(kr) &= \frac{\sin(kr)}{(kr)^2} - \frac{\cos(kr)}{kr} & j_1(kr) &\approx \frac{kr}{3} \quad (r \to 0) & j_1(kr) &\approx \frac{\sin(kr - \pi/2)}{kr} \quad (r \to \infty),
\end{aligned}$$

we can write out the first few terms and guess the result

$$\begin{aligned}
e^{ikr\cos\theta} &\approx \sqrt{4\pi} Y_{0,0}(\theta) + i\sqrt{12\pi}\frac{kr}{3} Y_{1,0}(\theta) + \cdots, \\
e^{ikr\cos\theta} &= \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)} j_l(kr) Y_{l,0}(\theta).
\end{aligned}$$

Now, we can solve each angular momentum "channel" or "partial wave" separately. As we'll see in a minute, then we can use the long-range asymptotic forms to determine how much probability amplitude was scattered. But note now the equation in each channel is

$$-\frac{\hbar^2}{2m}\frac{d^2 u_l}{dr^2} + V(r) u_l + \frac{\hbar^2 l(l+1)}{2mr^2} u_l = k^2 u_l,$$

where $u = r\psi$. For those channels with $l > 0$, if we take the limit of $k \to 0$, we see that the centrifugal barrier becomes large compared with the incident energy at a large distance, before the potential even starts to matter! This is in line with a classical description of impact parameter. Therefore, most of the time, we only have to carry out the expansion to the first term! But let's go ahead and see what happens. Suppose we solve the full Schrödinger equation and produce a wavefunction u_l. We know that u at large r has to satisfy the simple wave equation (because the potential is zero). Therefore u_l can be written

$$\begin{aligned}
u_l(r) &= A_l r j_l(kr) + B_l r \eta_l(kr), \\
u_l(r) &\underset{r\to\infty}{\longrightarrow} \frac{A_l}{k}\sin(kr - l\pi/2) - \frac{B_l}{k}\sin(kr - l\pi/2), \\
u_l(r) &\underset{r\to\infty}{\longrightarrow} \frac{C_l}{k}\sin(kr - l\pi/2 + \delta_l), \\
u_l(r) &\underset{r\to\infty}{\longrightarrow} \frac{C_l}{2ik}\left[e^{i(kr - l\pi/2 + \delta_l)} - e^{-i(kr - l\pi/2 + \delta_l)}\right].
\end{aligned}$$

If we denote the incoming wave as $v_l(r)$, then from the above (still at large r)

$$v_l(r) \underset{r\to\infty}{\longrightarrow} \frac{i^l\sqrt{4\pi(2l+1)}}{2ik}\left[e^{i(kr-l\pi/2)} - e^{-i(kr-l\pi/2)}\right].$$

Since we'd like to set boundary conditions such that there is no incoming spherical wave, all the incoming waves must come from the incident wave, so that

$$C_l = i^l\sqrt{4\pi(2l+1)}e^{i\delta_l}.$$

This in turn implies

$$u_l(r) - v_l(r) \underset{r\to\infty}{\longrightarrow} \frac{i^l\sqrt{4\pi(2l+1)}}{2ik}e^{i(kr-l\pi/2)}\left[e^{2i\delta_l} - 1\right],$$
$$u_l(r) - v_l(r) \underset{r\to\infty}{\longrightarrow} \sqrt{4\pi(2l+1)}\frac{e^{i\delta_l}}{k}\sin(\delta_l)e^{ikr}.$$

Therefore, the outgoing wave (with the incident wave subtracted) is given by

$$\left[\sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}\frac{e^{i\delta_l}}{k}\sin(\delta_l)Y_{l,0}\right]e^{ikr}.$$

Then the total cross section is (summing over all of the $Y_{l,0}$)

$$\sigma = \sum_{l=0}^{\infty}\sigma_l = \sum_{l=0}^{\infty}\frac{4\pi}{k^2}(2l+1)\sin^2\delta_l.$$

The quantities δ_l are called the phase shifts, and e.g. δ_0 is called the s-wave phase shift, δ_1 is called the p-wave phase shift, etc. Again remember we will only work with $l = 0$. Notice that in this quantum treatment, the only thing that matters to the long-range physics is the phase shift for scattering. Therefore, many different potentials might exist, but all potentials leading to the same s-wave phase will look identical at low energy. Thus, the behavior of our BEC is determined by the s-wave phase shift exclusively, and we can ignore the thousand-Kelvin scale physics going on when two atoms get very close.

13.3 The finite square well

Let's work the best example, which is a square well (i.e. spherical well) of potential $-V_0$ and radius a. Outside the well we have the asymptotic form

$$u_2 = B\sin(kr + \delta_0),$$

Inside the well the s-wave solution is given by

$$u_1 = C\sin(k_0 r), \qquad k_0 = \sqrt{k^2 + \frac{2m}{\hbar^2}V_0}.$$

Setting values and derivatives equal gives

$$\begin{aligned}
C\sin(k_0 a) &= B\sin(ka+\delta_0),\\
k_0 C\cos(k_0 a) &= kB\cos(ka+\delta_0),\\
\tan(ka+\delta_0) &= \frac{k}{k_0}\tan(k_0 a) = \frac{ka}{k_0 a}\tan(k_0 a).
\end{aligned}$$

Now let us take the low energy limit $ka \to 0$, and get

$$\begin{aligned}
ka+\delta_0 &\approx ka\frac{tan(k_0 a)}{k_0 a},\\
\delta_0 &\approx ka\left(\frac{tan(k_0 a)}{k_0 a} - 1\right).
\end{aligned}$$

If we also take the limit $k_0 a \to 0$, then

$$\begin{aligned}
\delta_0 &\approx k\frac{k_0^2 a^3}{3},\\
\delta_0 &\approx k\frac{2mV_0 a^3}{3\hbar^2},\\
\delta_0 &\approx k\frac{2mV_0 V}{4\pi\hbar^2}.
\end{aligned}$$

For geometric reasons, the quantity $-\delta_0/k$ is called the "scattering length". In this case the outgoing wave has the form

$$u_{\text{out}} = \sin\left[k(a-a_s)\right].$$

Note that a_s can be positive if $V_0 > 0$ $k_0^2 < 0$, which makes perfect sense actually. It is typical for a_s to converge to a particular value as $k \to 0$. From the above, for a spherical well,

$$a_s = \frac{2mV_0 V}{4\pi\hbar^2}.$$

If we take $m = M/2$ (the reduced mass), we arrive at a formula,

$$V_0 V = \frac{4\pi\hbar^2 a_s}{M}.$$

What is the quantity $V_0 V$. Well, it has units of energy per unit density, or energy density per unit density squared. Thus it is appropriate to be the interaction energy in the Gross-Pitaevskii equation. Furthermore, it makes sense. If the potential V_0 is small, the first perturbative correction to the energy will be

$$\Delta E = \int |\psi|^2 V_0\, dV = V_0 V|\psi|^2.$$

This suggests an effective interaction of V_0 times the probability of finding two atoms within V_0 of each other. In total this makes the interaction energy density equal to $\frac{1}{2}V_0 V|\psi|^4$.

13.4 Why is a BEC a superfluid?

Let's review so far on BEC:

1. Depending on the density of states, the BE distribution can be finite at $\mu = 0$.
2. If this occurs, have to go to more details of the states, and put all extra particles in the ground state
3. Extra ground state particles interact and obey GPE
4. Excitations in the GPE follow a linear dispersion

$$\begin{aligned}
\begin{pmatrix} \epsilon_k + \mu - \hbar\omega & g\psi_0^2 \\ g(\psi_0^*)^2 & \epsilon_k + \mu - \hbar\omega \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} &= 0, \\
(\epsilon_k + \mu)^2 &= \hbar^2\omega^2 + g^2(|\psi^2|)^2, \\
\hbar^2\omega^2 &= (\epsilon_k + \mu)^2 - \mu^2, \\
\hbar\omega &= \sqrt{(\epsilon_k + \mu)^2 - \mu^2}.
\end{aligned}$$

For large ϵ_k, we have $\hbar\omega \sim \epsilon_k + \mu$, and for small ϵ_k we have $\hbar\omega \sim \sqrt{2\mu\epsilon_k}$. Since $\epsilon_k \sim k^2$, we have a linear k-dependence for the sound waves. Note that these are the only type of excitations.

13.4.1 Landau's criteria

Note that no excitations exist with a phase velocity, that is, a ratio of $v_c = \omega/k = E/p$, less than some critical value (normally equal to $\sqrt{\mu/m}$. Let us see the implications for a body moving in the fluid. Suppose a very heavy object moves through the BEC. Now, the object would like to slow down by giving some of it's energy to the fluid. But as the energy is kinetic energy, it must also transfer some momentum. The energy and momentum on slowing from v_0 to v_1

$$\begin{aligned}
\Delta E &= \frac{1}{2}M\left[v_0^2 - v_1^2\right] = \frac{1}{2}M\left[-2\mathbf{v}_0 \cdot \delta\mathbf{v} - \delta\mathbf{v}^2\right], \\
\Delta\mathbf{p} &= M\delta\mathbf{v}, \\
\left|\frac{\Delta E}{\Delta p}\right| &\leq v_0 - \frac{1}{2}|\delta v| \leq v_0.
\end{aligned}$$

Now, the argument of Landau is that if $v_0 < v_c$, no excitation is possible, because no excitation, or set of excitations in the fluid can possibly carry momentum δp with less energy than $v_c\delta p$.