Phys.	344
-------	-----

Fri. 4/10	8.2 Ising Model of Ferromagnets	HW30 66, 74	
Mon. 4/13	Review		HW
Sat. 4/18	3pm Exam 3		

Monday: Review for Test 3. See on-line practice test "lecture-prep" is to bring in questions

7.6 Bose-Einstein Condensation / **Bosons with** $m \neq 0$

This is kind of tricky stuff. **Conceptually:** it appeals to the heart of the difference between distinguishable and indistinguishable particles and what we mean by "temperature." **Quantitatively:** The math doesn't let us come up with a single, perfect model. So, we'll talk some about the concepts and then we'll go about building some mathematical tools that do what we need. If you feel like the mathematical model is kind of cobbled-together, you're absolutely right. It isn't perfect; our goal is just to see that the qualitative behavior we expect is in there.

7.6.1 Why Does it Happen

Okay, what's special about Bosons is that a) their indistinguishable and b) they can occupy the same single-particle state as each other.

T = 0

• So, obviously, if you take away all the energy you can, every particle will happily cohabitate in the single-particle ground state – they have completely degenerated, *condensed* into a single state.

Low T

- As you add energy / raise the temperature, some of the particles will rise to lowlying energy states, but there will still be a large population in the ground state, a large population in the 'condensate,' for higher temperatures than one would classically expect.
- In point of fact, there will always be *some* particles sharing the ground state; however, as T increases, it becomes an insignificant fraction of the population.
- First, why does the ground-state population eventually become insignificant?
 - Think of the distribution of particles in terms of *energy*: The average occupancy of a particular state depends on the energy/kT of that state:

 $n = \frac{1}{e^{(e-m)b} - 1}$. That obviously tells us that a given high energy state is less populated than a given low energy state. Meanwhile, the average number of particles with a given *energy* also depends on how many states have the same energy, i.e., the density of states: $n_{w/e} = g(e)de = g_o e^{\frac{1}{2}}de$. This of course grows with energy – at higher energies, there are more states with the same energy. So the product of these two determines how many particles have a given energy. So, while the ground state will

always be the most popular *single state*, the most popular *energy level* will be where ever $g(\mathbf{e})n = \frac{g_o \mathbf{e}^{\frac{1}{2}}}{e^{(\mathbf{e}-\mathbf{m})\mathbf{b}} - 1}$ is peaked, so the ground state quickly becomes not so popular an *energy level*, and the condensate becomes insignificant.

The peak should occur at

$$\frac{dg(\mathbf{e})n}{d\mathbf{e}} = \frac{g_o \frac{1}{2} \mathbf{e}^{-\frac{1}{2}}}{e^{(\mathbf{e}-\mathbf{m})\mathbf{b}} - 1} - \frac{g_o \mathbf{e}^{\frac{1}{2}} \mathbf{b} e^{(\mathbf{e}-\mathbf{m})\mathbf{b}}}{\left(e^{(\mathbf{e}-\mathbf{m})\mathbf{b}} - 1\right)^2} = 0$$
$$\frac{\mathbf{e}^{-\frac{1}{2}} \left(\left(\frac{1}{2} - \mathbf{e}\mathbf{b}\right) e^{(\mathbf{e}-\mathbf{m})\mathbf{b}} - \frac{1}{2} \right)}{\left(e^{(\mathbf{e}-\mathbf{m})\mathbf{b}} - 1\right)^2} = 0 \Longrightarrow \left(1 - e^{-(\mathbf{e}-\mathbf{m})\mathbf{b}}\right) = 2\mathbf{e}\mathbf{b}$$

- That said, why does the ground-state remain significant for low-ish temperatures?
 - Let's think about the other two kinds of particles for comparison.
 - Fermions
 - Okay, these can't have multiply occupied states, so the lowest energy / zero-temperature configuration for a system of them is simply the first N single-particle states being full.
 - Distinguishable Particles vs. Bosons
 - Like indistinguishable bosons, the lowest energy configuration of the system has all of the particles being in the lowest energy level the difference is that each particle is distinguishable, so while they all have the same energy, they are in distinct states.
 - Another difference is that this situation more rapidly fades into obscurity as temperature rises. Here's why: their distinguishability means that there are a lot more unique states available when you add just a little energy: will particle Bob be excited, or will Alice, or will Carol, or will Doug,... the most popular energy level (where $g(e)n = g_o e^{\frac{1}{2}} e^{-(e-m)b}$ peaks) shifts up higher faster with increasing temperature it does for is Bosons.
 - To get deeper into this, we need to recall just what "temperature" means. If you're in the habit of directly associating temperature with average energy, this may

be a little hard to swallow, but remember: $\frac{1}{T} \equiv \frac{\partial S}{\partial U}$ So

the *temperature* of a system depends not just on how much energy you put in it, but also *how much disorder* it induces (quantified in the entropy).

• **Distinguishable system.** Imagine you have an N-particle system of distinguishable particles and another N-particle system of bosons. If you add, say 2 units of energy to the distinguishable system, then there are

$$\Omega_{Dist}(N,q=2) = \binom{N+2-1}{2} = \frac{(N+1)!}{(N-1)!2} = \frac{(N+1)(N)}{2}$$

. So, the temperature associated with adding one unit is roughly

$$T_{dist} = \frac{\Delta U}{\Delta S} = \frac{2q}{k \ln \left((N+1)N/2 \right)}$$

Also note that of all these possibilities, N of them have N-1 particles remaining in the ground state; the remaining possibilities have only N-2 particles remaining in the ground state. Put another way, the probability of having N-1 particles in the ground state is

$$\Pr(N-1) = \frac{\Omega_{N-1}}{\Omega_{total}} = \frac{N}{(N+1)N/2} = \frac{2}{(N+1)}$$

• **Boson System.** In contrast, if you add two units of energy to a Boson system, there are only two ways they can be distributed: all to one particle, or one to one, and one to another.

 $\Omega_{Bose}(N, q=2) = 2$. So the temperature

associated with adding one unit is roughly

 $T_{Bose} = \frac{\Delta U}{\Delta S} = \frac{2q}{k\ln(2)}$ which is a significantly

higher temperature!

- Also, even at this higher temperature, the probability of having N-1 particles (rather than N-2) in the ground state is ¹/₂ *far* larger than for distinguishable particles.
- **Conclusion.** It takes a higher temperature to force the same amount of energy into a Bose system, and even the n, there's a greater population in the ground state.
- **Density of states effect.** Something that isn't addressed in this simple illustration is a higher energy level generally has a greater degeneracy, but this effects distinguishable particles and bosons equally.
- Pulling back a bit and summarizing: There's the competition between the *probability* of being in a

particular state (higher probability for lower energy states) and the *number* of states with a particular energy. The higher the energy, the less probable a particular state, but the more individual states available. For Distinguishable particle, not only are there more states available for individual particles at higher energies, but there are even more ways of choosing *which* particles will be in which of the occupied states. For distinguishable particles then, it is preferable to have E energy accounted for by having N particles in *different*, medium energy states. For Bosons on the other hand, you're a little more likely to have E energy accounted for by having fewer excited particles in higher energy states – leaving more particle back in the ground state.

Okay, let's get quantitative

- 3 Regimes: T = 0, T very low/moderate, T high (classical)
- We're interested in what fraction of the particles in our system are in the ground state. In the Condensation regime, it's startlingly large.
- Ground State

• The average occupancy of the ground state is $\overline{n}_o = \frac{1}{e^{(e_o - \mathbf{m})b} - 1}$. Since there is only one ground state (degeneracy of 1), the number of particles with this lowest energy is simply $N_o = \overline{n}_o = \frac{1}{e^{(e_o - \mathbf{m})b} - 1}$.

- (**Prep for Pr. 66**) **Question:** For that matter, what would be the average occupancy of one of the 1st excited states? $\overline{n}_1 = \frac{1}{e^{(e_1 m)b} 1}$ For a spin=0 particle, how many 1st excited states are there? – look in p(or n) space. 3. So the number in the first *energy level* is $N_1 = 3\overline{n}_1 = \frac{3}{e^{(e_1 - m)b} - 1}$
- N_{o} \sim \sim N_{o}
- What's mduring condensation, i.e. Low T?
 - We see it in $N_o = \overline{n}_o = \frac{1}{e^{(e_o m)b} 1}$.
 - At low T, we *know* that $N_o \rightarrow N$ where N is generally on order of

10²³. Looking at $N_o = \frac{1}{e^{(e_o - \mathbf{m})\mathbf{b}} - 1}$, N_o can get quite large only if the denominator gets quite small, i.e., $e^{(e_o - \mathbf{m})\mathbf{b}}$ approaches 1. So, expanding $e^{(e_o - \mathbf{m})\mathbf{b}}$ around 1 gives $e^{(e_o - \mathbf{m})\mathbf{b}} \approx 1 + (e_o - \mathbf{m})\mathbf{b}$.

• Note: at first blush, you might think 'what the heck are you doing with a Taylor series, **b** is huge', but for physical

reasons we *know* that the exponent must be tiny for N_0 to be huge, so we can find what **m** does that for us.

•
$$N_o \approx \frac{1}{1 + (\boldsymbol{e}_o - \boldsymbol{m})\boldsymbol{b} - 1} = \frac{kT}{(\boldsymbol{e}_o - \boldsymbol{m})}$$

• (Prep for Pr. 66) So, $\boldsymbol{m} \approx \left(\boldsymbol{e}_o - \frac{kT}{N_o}\right)$

• Now, as T drops and N_o grows, μ clearly approaches ε_o from below. So it approaches the ground state energy from below. So, what's e_o ?

- Energy
- For an order of magnitude calculation, imagine a simple cube of dimensions L. The smallest momentum available is $p_x = 1 \frac{h}{2L}$,

ditto for the y and z components of momentum. So the smallest

energy available is
$$\mathbf{e}_{o} = \frac{1}{2m} \left(\left(\frac{h}{2L} \right)^{2} + \left(\frac{h}{2L} \right)^{2} + \left(\frac{h}{2L} \right)^{2} \right) = \frac{3h^{2}}{8mL^{2}}$$

This is on order of $\mathbf{e}_{o} \propto \frac{3(6.626 \times 10^{-34} Js)^{2}}{8 \cdot (1.673 \times 10^{-27} kg) Im^{2}} = 9.86 \times 10^{-41} J$,

really small! A corresponding temperature would be 10^{-18} K! • Note: for a spin = 0 particle, there is only one ground state.

• (**Prep for Pr. 66**) **Question:** For that matter, what would be the energy of the 1st excited state?

$$\boldsymbol{e}_1 = \frac{1}{2m} \left(\left(\frac{2h}{2L} \right)^2 + \left(\frac{h}{2L} \right)^2 + \left(\frac{h}{2L} \right)^2 \right) = \frac{6h^2}{8mL^2} = 2\boldsymbol{e}_0$$

• Since \mathbf{e}_o is quite small, $\mathbf{m} \approx \left(\mathbf{e}_o - \frac{kT}{N_o} \right)$ means that μ is negative for

elevated temperatures // when N_o is small. Only when temperature drops and the population of the ground state grows appreciably will μ approach the *very* small positive value of ε_o .

• Condensation T, N_o dependence on T.

• So, around what temperature do the particles begin 'condensing' into the lowest energy state?

$$\circ \quad N = \sum_{\text{states}} \overline{n}_s = \sum_{\text{states}} \frac{1}{e^{(\mathbf{e}_s - \mathbf{m})\mathbf{b}} - 1} = \frac{1}{e^{(\mathbf{e}_s - \mathbf{m})\mathbf{b}} - 1} + \sum_{\substack{\text{excited} \\ \text{states}}} \frac{1}{e^{(\mathbf{e}_s - \mathbf{m})\mathbf{b}} - 1} = N_o + N_{\text{excited}}$$

Prep. For HW 74: You'll use Excel to do this sum for the first ~ 200 terms. Note that the degeneracy, $n_{w/e}$ and energy structure are both given in the previous problem.

• Here, I've explicitly separated off the term for the ground state population from all the other terms for the excited states.

•
$$N_{excited} = \sum_{\substack{excited \\ states}} \frac{1}{e^{(e_s - \mathbf{m})b} - 1} = \sum_{\substack{excited \\ e}} n_{s.w/e} \frac{1}{e^{(e - \mathbf{m})b} - 1} = \sum_{\substack{excited \\ e}} \frac{dn_{w/e}}{deb} \frac{1}{e^{(e - \mathbf{m})b} - 1} \Delta eb$$

• This last step of course is in preparation for replacing the sum with an integral, but we can only get away with that if $\Delta eb \ll 1$, or in other words $\Delta e \ll kT$. The energy steps between states are on order of e_o which is pretty darned small, so we can get away with this for most temperatures.

$$N_{excited} = \sum_{\substack{excited \\ \mathbf{e}}} \frac{dn_{s.w/e}}{d\mathbf{e}\mathbf{b}} \frac{1}{e^{(\mathbf{e}-\mathbf{m})\mathbf{b}} - 1} \Delta \mathbf{e}\mathbf{b} \approx \int_{\mathbf{e}_{1}}^{\infty} g(\mathbf{e}) \frac{1}{e^{(\mathbf{e}-\mathbf{m})\mathbf{b}} - 1} d\mathbf{e}$$

$$N_{excited} = n_{spin} \frac{2}{\sqrt{p}} \left(\frac{2pm}{h^2}\right)^{3/2} V \int_{e_1}^{\infty} \sqrt{e} \frac{1}{e^{(e-m)b} - 1} de$$

• Look at the competition in the integrand. \sqrt{e} vs. $\frac{1}{e^{(e-m)b}-1}$.

While the low energy states are by far the *most popular* (according to the second factor particles really want to be in those states), they are also the *fewest* (according to the first factor there just aren't that many of these low energy states), in the end, states with energy much less than kT don't really contribute to the sum.

That's good because, it allows us to play a little loose with the lower end of the integration without significantly affecting the result. The two approximations are that e₁ and m are much smaller than the energy where the integrand becomes significant, i.e., e₁, m≈0.

$$N_{excited} = n_{spin} \frac{2}{\sqrt{p}} \left(\frac{2pm}{h^2}\right)^{3/2} V_0^{\infty} \sqrt{e} \frac{1}{e^{(e)b} - 1} de$$

$$N_{excited} = n_{spin} \frac{2}{\sqrt{p}} \left(\frac{2pmkT}{h^2}\right)^{3/2} V_0^{\infty} \sqrt{x} \frac{1}{e^x - 1} dx$$

$$N_{excited} = n_{spin} \frac{2}{\sqrt{p}} \left(\frac{2pmkT}{h^2}\right)^{3/2} V 2.315 = n_{spin} 2.612 \left(\frac{2pmkT}{h^2}\right)^{3/2} V$$

• The integral was $\Gamma(\frac{3}{2}) \mathbf{Z}(\frac{3}{2}) = 2.612...$

- Limit of Approximation: As we've already seen at very low temperatures, m grows increasingly negative with increasing T. So the approximation $m \approx 0$ is only good for small and moderate temperatures. At high temperatures we can't neglect the chemical potential.
- **Threshold:** Clearly, the approximation breaks down by the time it predicts that the number of particles in excited states *exceeds* the total number of particles in the system. So we can define a threshold by



$$N_{excited} = N$$

$$n_{spin} 2.612 \left(\frac{2\mathbf{p}mkT_c}{h^2}\right)^{3/2} V = N \Rightarrow \frac{V}{N} = v_Q \frac{1}{n_{spin} 2.612}$$

$$T_c = 0.527 \frac{h^2}{k2\mathbf{p}m} \left(\frac{N}{V}\right)^{2/3}$$

- Note: this is roughly when the volume per particle is the quantum volume when wavefunctions must just overlap.
- This can be rephrased in terms of the ground state energy: $kT_c = 0.22 e_o N^{3/2}$, so it can be considerably more than the ground state energy (which itself is quite small and is about $\Delta \varepsilon$ between states).
- With this definition in hand, we can re-write the excited number of particles as

•
$$N_{excited} = \left(\frac{T}{T_c}\right)^{3/2} N$$

• Roughly speaking, the population of excited states goes like:



$$e^{(\mathbf{e}_{o}-\mathbf{m})/kT} = 1 + \frac{1}{N\left(1 - \left(\frac{T}{T_{c}}\right)^{3/2}\right)}$$

$$\mathbf{m} = \mathbf{e}_{o} - kT \ln\left(1 + \frac{1}{N\left(1 - \left(\frac{T}{T_{c}}\right)^{3/2}\right)}\right)$$

• Assuming that N is quite large, L_T

$$\boldsymbol{m} \approx \boldsymbol{e}_o - \frac{kT}{N \left(1 - \left(\frac{T}{T_c} \right)^{3/2} \right)}$$

- This has the same low T behavior as we'd already predicted. Clearly, this gets ill-behaved as T approaches T_c.
- mat $T>T_c$

• Above T_c, The population of the ground state is negligible, so

•
$$N \approx N_{excited} = n_{spin} \frac{2}{\sqrt{p}} \left(\frac{2pm}{h^2}\right)^{3/2} V \int_{0}^{\infty} \sqrt{e} \frac{1}{e^{(e-m)b} - 1} de$$
 is the

defining equation for μ . One can use this to verify the basic form in Figure 7.33.

7.6.2 Real World Examples

It's readily observed in liquid ⁴He. It takes some doing, but it's also observed in Rubidium gas.