Bose and Fermi Gases

Timothy Head
tim.head@student.manchester.ac.uk

15th December 2006

Introduction

This lecture is about Bose and Fermi gases, mainly statistical physics. It is lectured by J. Forshaw(email address??).

Textbooks, he recommends, tho subject to personal taste.

- "Introductory Statistical Mechanics", Bowley&Sanchez
- "Thermal Physics", Kittel&Kroemer
- "An Introduction to thermal physics", Schroeder
- "Lectures on Statistical Mechanics", Bowler, this is a special little booklet

For syllabus see the blue book.

1 Counting quantum states: entropy&temperature

Generally interested in systems in equilibrium. A system is not necessarily a gas that is, rather a collection of elements. Elements of a system don't interact with each other. We want to be able to count the number of quantum states accessible to a particle system. Once you can do that you make a huge progress in understanding the system as a whole.

So how do we count then? Consider hydrogen atom in a box. To completely specify the state of that system we need the set of quantum numbers:

- n, m_l, m_s will do to first approximation
- n_x, n_y , n_z these specify translational motion of the atom

The box is specified by

$$V = 0 \text{ for } \begin{cases} 0 < x < L \\ 0 < y < L \\ 0 < z < L \end{cases}$$

and $V = \infty$ everywhere else. Wave-function is

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

Figure 1: Represent each quantum state of energy by a X and delineate between oscillators using a | (see figure 29-09–1)

with a solution like $\psi \propto \sin(\frac{n_x \pi x}{L})\sin(\frac{n_y \pi y}{L})\sin(\frac{n_z \pi z}{L})$ and energy is given by

$$E = \frac{\hbar^2\pi^2}{2m^2}(n_x^2 + n_y^2 + n_z^2)$$

.

Einstein's Model of a solid This is a simple model, it assumes that every molecule is a SHO independent of other molecules surrounding it(independent harmonic oscillators). Furthermore we assume that all molecules oscillate at the same frequency. In a 3D solid each atom can oscillate in 3 independent directions. So if there are N oscillators then there are $\frac{N}{3}$ atoms. Energy of the i$^{\text{th}}$ oscillator is:$(n_i + \frac{1}{2})\hbar\omega$, where n_i is quantum number of i$^{\text{th}}$ oscillator. Safe to measure all energies relative to ground state so we will call $\epsilon_i = n_i\hbar\omega$ the energy of the i$^{\text{th}}$ oscillator. Our N oscillators have energy

$$U = \underbrace{(n_1 + n_2 + ... + n_N)}_{=n}\hbar\omega$$

The system as a whole can be specified by $(n_1,\ n_2,\ n_3,\ ...\ ,\ n_N)$. Clearly there are several quantum states(microstates) corresponding to the same total energy(macrostate). Let $g(n,\ N)$ (sometimes called $\Omega(n,\ N)$) be the number of possible quantum states of the system when the total energy is $n\hbar\omega$.

n	g(n, N)	list of quantum states
0	1	(0, 0, 0, ..., 0)
1	N	(1, 0, 0, ..., 0), (0, 1, 0, ... , 0), ... , (0, 0, ... ,1)
2	$N + \frac{N(N-1)}{2}$	(2, 0, 0, ..., 0), (0, 2, 0, ... , 0), ... , (0, 0, ... ,2), (1, 1, 0, ..., 0), (0, 1, 1, ... , 0) etc

Generally $g(n,\ N) = \frac{(N+n-1)!}{n!(N-1)!}$. This is called the statistical weight of the macrostate. Proof for this goes like this:

We want the total number of ways of arranging n crosses and N-1 vertical lines. Now comes the crucial assumption: If a system is *closed* and in *equilibrium* then it is equally likely to be in any one of the accessible quantum states.

So the probability our Einstein Solid is in any particular quantum state is just $\frac{1}{g(n,\ N)}$. This idea leads us immediately to a definition of *temperature* and the concept of *entropy*.

Temperature To get the idea of temperature we ought to consider two Einstein solids in contact such that they can exchange energy between them. Two solids A and B each with energy $U_A = n_A\hbar\omega$ and $U_B = n_B\hbar\omega$ respectively. The number of quantum states of the system A + B is

$$g_{A+B}(N,\ n) = \sum_{n_A=0}^{n} g(N_A,\ n_A)g(N_B,\ n - n_A) \tag{1}$$

where $n = n_A + n_B$. Intuition tells us that (provided system(N) is big enough) the system will settle down into an *equilibrium* state, i.e. a macrostate with $n_A = \tilde{n}_A$. Remarkable the notion of a "unique" equilibrium macrostate is present in our analysis so far. If the following is true there will be one preferred state.

$$g_{A+B}(N,\ n) = \sum_{n_A \approx \tilde{n}_A} g(N_A,\ n_A) g(N_B,\ n - n_A) \tag{2}$$

where we sum "around" $\tilde{n}_A$, a little bit to the left a bit to the right. If equation 2 is the "same" as equation 1 then we need not bother about all those microstates "far" away from $\tilde{n}_A$, they have no or almost no statistical weight. Later we will see that this is true, see figure in week three's lecture notes `http://www.hep.man.ac.uk/u/forshaw/BoseFermi/lect3.pdf` for a plot.

For simplicity consider a system so that $N_A = N_B = \frac{1}{2}N$. We expect $\tilde{n}_A \approx \frac{1}{2}n \approx \tilde{n}_B$. For large N and n the following approximation of the product in equation 2 is true(derivable with Sterling's approximation)

$$g(\frac{N}{2},\ n_A) g(\frac{N}{2},\ n_B) \propto \exp(-\frac{(n_A - \frac{n}{2})^2}{\sigma^2}) \tag{3}$$

where $\sigma^2 = \frac{n(N+n)}{2N}$. If $n,\ N \gg 1$ then $\sigma \ll \frac{1}{2}n$. As σ controls the width of the Gaussian in equation 3 this tells us that the distribution has a very narrow peak, hence a preferred macrostate. The statistical weight of very few microstates is much bigger than that of all the others. This proves that what we were just assuming in equation 2 is actually true.

Insert fig 2-10–1. For a real solid with $N \approx 10^{22}$ then $\sigma = 10^{11}$, this is more like a Dirac-delta than a Gaussian. If we measured the energy of Einstein solid A we would measure that $n_A = \frac{1}{2}n(1 \pm 10^{-11})$.

We can locate the equilibrium configuration by differentiating equation 3 and setting it to zero.

$$\frac{\partial(g_A g_B)}{\partial n_A} dn_A = 0$$

applying the product rule we obtain

$$g_B \frac{\partial g_A}{\partial n_A} dn_A + g_A \frac{\partial g_B}{\partial n_B} dn_B = 0$$

requiring that $dn_A = -dn_B$ since $n = n_A + n_B$ is fixed.

$$(g_B \frac{\partial g_A}{\partial n_A} - g_A \frac{\partial g_B}{\partial n_B}) dn_A = 0$$

which gives

$$\frac{1}{g_A} \frac{\partial g_A}{\partial n_A} = \frac{1}{g_B} \frac{\partial g_B}{\partial n_B} = \frac{\partial(\ln g_B)}{\partial n_B} \tag{4}$$

from this it is easy to define temperature as

$$\frac{1}{k_B T} = \frac{\partial \ln g}{\partial U}$$

with this definition equation 4 becomes $\frac{1}{k_B T_A} = \frac{1}{k_B T_B}$. We absorbed the constants needed to make the transition from ∂n to ∂U in k_B. This definition satisfies desire to have a definition where "energy" flows from a hotter body to a colder one. Let hot body lose heat ΔK then

$$\Delta \ln g_{hot} \approx -\Delta u / k_b T_{hot}$$

$$\Delta \ln g_{cold} = +\Delta u / k_B T_{cold}$$

net change increases in $\Delta \ln g$ since $|\Delta \ln g_{hot}| < \Delta \ln g_{cold}$, this makes sense as $\Delta \ln g$ must increase since equilibrium is at a maximum of $g_A g_B$. Energy flows from the hotter to the colder body as system moves towards equilibrium.

Second law of thermodynamics follows straight forwardly from this

$$S = k_B \ln g$$

Although we talked about an Einstein solid it should be clear this is much more general. WE can define temperature the following way $\frac{1}{T} = (\frac{\partial S}{\partial U})_{V,N}$. We can calculate the specific heat capacity of a solid given by

$$C = \frac{\partial U}{\partial T}$$

In order to get U let's compute $U = n\hbar\omega$. Will use the fact that $\frac{\partial S}{\partial U} = \frac{1}{k_B T}$ to fix n. So we can write

$$\frac{S}{k_B} = (N+n)\ln(N+n) - N\ln N - n\ln n$$

using Sterling's approximation. Which allows us to write

$$\frac{1}{k_B}\frac{\partial S}{\partial N} = \frac{\hbar\omega}{k_B T}$$

as $\ln(N+n) - \ln n = \frac{\hbar\omega}{k_B T}$. Solve for n giving

$$n = \frac{N}{\exp(\frac{\hbar\omega}{k_B T}) - 1}$$

which gives

$$U = \frac{N\hbar\omega}{\exp(\frac{\hbar\omega}{k_B T}) - 1}$$

so writing heat capacity

$$C = N k_B \frac{x^2 e^x}{(e^x - 1)^2}$$

where $x = \frac{\hbar\omega}{k_B T} = \frac{\Theta_E}{T}$. If $x \ll 1$ $C \approx N k_B$. This is exactly what one would expect from the equipartition theorem. Look at lecture four notes for a plot of heat capacity for diamond.

If $x \gg 1$ $C \approx N k_B x^2 e^{-x} \to 0$ (this is at low T).

2 The Gibbs Factor

What is the probability that a particular system is in a particular quantum state? In this section we will answer this question. For a isolated system this is easy, Probability $= \frac{1}{g}$. We are going to consider more general systems which are not isolated form their environment. Lets consider a system S which forms part of a larger system R. (Sketch of big box(system R) and inside a little box(system S) R is isolated.) At equilibrium the number of quantum states available to S+R is simply $g_T = g_S \times g_R$. If U_S is the energy of system and N_S is the number of particles in system, then equilibrium implies

$$dg_T = (\frac{\partial g_T}{\partial U_S})_{N_S,V_S} dU_S + (\frac{\partial g_S}{\partial U_S})_{N_S,V_S} dN_S = 0$$

substituting for g_T

$$g_S \frac{\partial g_R}{\partial U_S} dU_S + g_R \frac{\partial g_S}{\partial U_S} dU_S ....$$

using $dU_S = -dU_R$ and $dN_S = -dN_R$

$$\frac{1}{g_R}\frac{\partial g_R}{\partial U_R} = \frac{1}{g_S}\frac{\partial g_S}{\partial U_S} \Rightarrow T_R = T_S$$
$$\frac{1}{g_R}\frac{\partial g_R}{\partial N_R} = \frac{1}{g_S}\frac{\partial g_S}{\partial N_S} \Rightarrow \frac{\partial \ln g_R}{\partial N_R} = \frac{\partial \ln g_S}{\partial N_S}$$

this implies that something else other than temperature is equal in equilibrium. We define $\mu \equiv -T\frac{\partial S}{\partial N}$ (the chemical potential). This allows us to say that $\mu_R = \mu_S$ in equilibrium.

Aside if V_S varied then would also

$$\frac{\partial \ln g_R}{\partial V_R} = \frac{\partial \ln g_S}{\partial V_S}$$

so if we define $p \equiv T\frac{\partial S}{\partial V}$(pressure) then $p_R = p_S$.

Our goal is to find probability $P(N_S, U_S)$ to find S to be in a *single* quantum state with N_S particles & energy U_S. This implies $g_S = 1$, we want to know when it is in exactly one microstate. Thus $P(N_S, U_S) \propto g_R(N_T - N_S, U_T - U_S) \times 1$. We can rewrite this using entropy S (do not confuse with system S).

$$P(N_S, U_S) \propto \exp(\frac{S_R(N_T - N_S,\ U_T - U_S)}{k_B}) \tag{5}$$

we can Taylor expand about N_T, U_T.

$$S_R(N_T - N_S,\ U_T - U_S) \simeq S_R(N_T, U_T) - N_S\frac{\partial S_R}{\partial N}|_{N_T,U_T} - U_S\frac{\partial S_R}{\partial U}|_{N_S,U_S} + O()$$

where $O()$ is terms of second and higher order.

$$\simeq S_R(N_T, U_T) + \frac{\mu N_S}{T} - \frac{U_S}{T} \tag{6}$$

we are finished.

Lets have a closer look at higher order terms O, they depend on the derivatives of μ and U. If the reservoir is big enough then neither depends on N_S and U_S.

We can now sub 6 into 5 which gives

$$P(N_S, U_S) \propto \exp(\frac{S_R(N_T, U_T)}{k} + \frac{\mu N_S}{kT} - \frac{U_S}{kT})$$

by moving S_R into the constant of proportionality we get $P(N_S, U_S) \propto \exp(\frac{\mu N_S}{kT} - \frac{U_S}{kT})$, this is the Gibbs distribution.

We write this a bit more neatly as

$$\begin{aligned} P(N,\ \epsilon) &\propto \exp\left(\frac{\mu N - \epsilon}{k_B T}\right) \\ P(N,\ \epsilon) &= \frac{\exp\left(\frac{\mu N - \epsilon}{k_B T}\right)}{\mathcal{Z}} \\ \mathcal{Z} &\equiv \sum_{all\ states} \exp\left(\frac{\mu N - \epsilon}{k_B T}\right) \end{aligned} \quad (7)$$

Equation 7 gives the probability of finding system in a *particular* quantum state containing N particles and energy ϵ. We call $\mathcal{Z}$ the Grand Partition Function.

Averages can be computed as usual

$$< x >= \sum_{N,\ S} P(N,\ \epsilon) X(N,\ \epsilon)$$

here we find the average value of x.

Note that if there is more than one type of particle in system then we can write $\mu N = \mu_1 N_1 + \mu_2 N_2 + ... + \mu_i N_i$, where N_i is number of particles of type i and μ_i chemical potential of particle type i. Prove it!

As an example we look at carbon monoxide poisoning. A hemoglobin(Hb) can bind either a carbon monoxide or an oxygen. What is the probability that a Hb is bound with a CO or O_2 or is unbound? System is either

- 1×Hb, ϵ(unbound) $= 0$
- 1×Hb + O_2, $\epsilon(O_2) = -0.7$eV
- 1×Hb + CO, ϵ(CO) $= -0.85$eV

We do not need the chemical potential of Hb, as it would just cancel when we use equation 7. A constant in both $\mathcal{Z}$ and P just cancels. Grand Partition function is given by

$$\begin{aligned} \mathcal{Z} &= e^0 + \exp\left(\frac{\mu(CO) - \epsilon(CO)}{kT}\right) + \exp\left(\frac{\mu(O_2) - \epsilon(O_2)}{kT}\right) \\ &= 1 + 120 + 40 = 161 \end{aligned}$$

at $T = 310$K. So the probability of the Hb being unbound is just $P = \frac{1}{\mathcal{Z}} = \frac{1}{161} \approx 0.6\%$. For a 1% concentration of CO

$$\begin{aligned} \mu(CO) &= -0.7\text{eV} \\ \mu(O_2) &= -0.6\text{eV} \end{aligned}$$

these are the chemical potentials. The probability for it to be bound $P = \frac{40}{161} \approx 25\%$ and probability for bound with CO $P = \frac{120}{161} \approx 75\%$. If there is no CO around then $P(\text{unbound}) = \frac{1}{41}$ and $P(\text{O}) = \frac{40}{41}$.

Figure 2: Two distinguishable particles with two accessible states have four states.

Figure 3: Two indistinguishable particles(boson) have only three states, for fermions there is only one states as no two fermions are allowed in the same state(Pauli principle)

3 Identical Particles

16.10.2006

We are going to be interested in system containing a bunch of particles. We need to be sure we can count quantum states for such systems. Consider a system of 2 particles and 2 accessible quantum states. If the particles are *distinguishable* then there are 4 possible quantum states for the system.

In order to enumerate quantum states we need to know if our particles are distinguishable or indistinguishable. We will now attempt to derive the Pauli principle.

Consider a two particle system. Let $\phi_n(x)$ be an energy eigenstate for a *single* particle. so that $\hat{H}(x)\phi_n(x) = E_n\phi_n(x)$ is true. Assume the two particles do not interact with each other, the Hamiltonian of the two particle system is $\hat{H}(x) + \hat{H}(y)$ and $\phi_n(x)\phi_m(y)$ is an energy eigenstate

$$[\hat{H}(x) + \hat{H}(y)]\phi_n(x)\phi_m(y) = (E_n + E_m)\phi_n(x)\phi_m(y)$$

but $\phi_m(x)\phi_n(y)$ is by same reasoning also an energy eigenstate of energy $E_n + E_m$. Now if particles are identical no observable can depend upon whether particle at x has energy E_n or E_m. This implies that all observable should be unchanged if we swap the locations $x \leftrightarrow y$. Prove it!

So the correct energy eigenstate for two identical particles, $\psi_{nm}(x,\ y)$ must be that linear combination of $\phi_n(x)\phi_m(y)$ and $\phi_m(x)\phi_n(y)$ which satisfies

$$|\psi_{nm}(x,\ y)|^2 = |\psi_{nm}(y,\ x)|^2 \tag{8}$$

equation 8 implies that

$$\psi_{nm}(x,\ y) = e^{i\alpha}\psi_{nm}(y,\ x)$$

swapping this back gives $\psi_{nm}(x,\ y) = e^{i\alpha}e^{i\alpha}\psi_{nm}(x,\ y)$. This implies that $e^{2i\alpha} = 1$ from which it follows that $e^{i\alpha} = \pm 1$. Thus

$$\psi_{nm}(x,\ y) = \pm\psi_{nm}(y,\ x)$$

These we only have two linear combinations of $\phi_n(x)\phi_m(y)$ and $\phi_n(y)\phi_m(x)$ which which satisfy Eqn X

$$\begin{aligned}\psi_{nm}(x,y) &= \phi_n(x)\phi_m(y) + \phi_n(y)\phi_m(x)\\ &= \phi_n(x)\phi_m(y) - \phi_n(y)\phi_m(x)\end{aligned}$$

these are equations A and B. A is even under $x \leftrightarrow y$, B is odd under $x \leftrightarrow y$. Particle described by wavefunction A are bosons and particles described by wavefunction B are fermions. The Pauli principle "drops out" for free, if we try to put two fermions in the same state

$$\psi_{nm}(x,\ y) = \phi_i(x)\phi_i(y) - \phi_i(y)\phi_i(x) = 0$$

no two fermions can be in the same quantum state.

Fermions carry $\frac{1}{2}$ integer spin, bosons carry integer spin(0,1,2,3,...all times hbar). In order to derive this we need called "spin & statistics theory". ^4He boson or fermion? ^3He boson or fermion? 20.10.2006

4 Bose-Einstein & Fermi-Dirac distributions

We are now ready to use the Gibbs factor to figure out properties of a system of bosons or fermions. Let's consider a system S in a reservoir R, a (ideal) gas of identical particles. Here n_i says how many particles are in state i and have energy ϵ_i. Gibbs tells us that the probability to find S in a single quantum state

$$P\left(\{n_i,\ \epsilon_i\}\right) = \frac{\exp\left[\frac{\mu(n_1+n_2+...)}{k_bT} - \frac{(n_1\epsilon_1+n_2\epsilon_2+...)}{k_bT}\right]}{\sum_n \exp\left[\frac{\mu(n_1+n_2+...)}{k_bT} - \frac{n_1\epsilon_1+n_2\epsilon_2+...}{k_bT}\right]}$$

this function factorises to

$$\begin{aligned} P\left(\{n_i,\ \epsilon_i\}\right) &= \frac{\exp\left[\frac{n_1(\mu-\epsilon_1)}{k_bT}\right]}{\sum \exp\left[\frac{n_1(\mu-\epsilon_1)}{k_bT}\right]} \times \frac{\exp\left[\frac{n_2(\mu-\epsilon_1)}{k_bT}\right]}{\sum \exp\left[\frac{n_2(\mu-\epsilon_1)}{k_bT}\right]} \times ... \\ &= P_1\left(n_1\right) \times P_2\left(n_2\right) \times ... \end{aligned}$$

where P_1 gives probability to find n_1 particles in ϵ_1.

We could have derived $P_i(n_i)$ directly if we had considered S to be a single energy level ϵ_i. This is sensible since a system needs to have a well defined occupancy, a well defined energy&be in equilibrium with a large reservoir(all the other energy levels).

Now we can figure out the mean number of particles in a particular state. For a system of identical(all spin *up*) *fermions*. Occupancy of a given energy level is 0 or 1. So the mean number of fermions in a state ϵ is just

$$< n(\epsilon) >_{FD} = \frac{0 + 1 \times \exp((\mu-\epsilon)/k_bT)}{e^0 + \exp((\mu-\epsilon)/k_bT)}$$

Now do this for *bosons*, any occupancy is allowed so

$$\begin{aligned} < n >_{BE} &= \frac{0 + \exp\left(\frac{\mu-\epsilon}{k_bT}\right) + 2\exp\left(\frac{2(\mu-\epsilon)}{k_bT}\right) + 3\exp\left(\frac{3(\mu-\epsilon)}{k_bT}\right) + ...}{e^0 + \exp\left(\frac{\mu-\epsilon}{k_bT}\right) + \exp\left(\frac{2(\mu-\epsilon)}{k_bT}\right) + \exp\left(\frac{3(\mu-\epsilon)}{k_bT}\right) + ...} \\ &= \frac{a + 2a^2 + 3a^3 + ...}{1 + a + a^2 + a^3 + ...} \end{aligned}$$

where $a=\exp(\frac{\mu-\epsilon}{k_bT})$ using the geometric series we get

$$\begin{aligned}1+a+a^2+a^3+... &= \frac{1}{1-a}\\ a+2a^2+3a^3+... &= a(1+2a+3a^2+...)\\ &= a\frac{d}{da}(a+a^2+a^3+...)\\ &= \frac{a}{(1-a)^2} \Rightarrow <n(\epsilon)>=\frac{a}{1-a}\end{aligned}$$

so substituting back in our final result is

$$<n(\epsilon)>_{BE}=\frac{1}{\exp(\frac{\epsilon-\mu}{k_bT})-1}$$

This is the Bose-Einstein distribution function. We now look at a plot of Fermi-Dirac, Bose-Einstein and Classical distributions. These should be on the website.

In a gas of particles of spin S the mean number of particles in ϵ is

$$\begin{aligned}<n(\epsilon)> &= \frac{2S+1}{\exp\left(\frac{\epsilon-\mu}{k_bT}\right)\pm 1}\\ &= <n(\epsilon)>_{-S}+<n(\epsilon)>_{-S+1}+<n(\epsilon)>_{-S+2}+\\ &\quad +...+<n(\epsilon)>_S\end{aligned}$$

this works for electrons but for photons it does not hold. Photons have spin ±1 which is OK but s=0 is not allowed.

5 The classical limit

23.10.2006

Before turning to quantum gases let's first look at the classical limit. This is the limit where $<n(\epsilon)>\ll 1$ is a good approximation&there is no significant difference between bosons&fermions. We want to find:

- chemical potential
- entropy
- heat capacity
- derive pVT relation

Chemical potential has so far not had a very physical interpretation. We can always(in principle) compute it by calculating the mean number of particles in our system, $N\equiv<N>$.

$$N=<N>=\sum_i <n(\epsilon_i)>\approx\sum_i \exp\left(\frac{\mu-\epsilon_i}{kT}\right)$$

as we are in the classical limit Bose-Einstein and Fermi-Dirac distributions are essentially the same. If we can perform this sum over i we have an expression for μ in terms of N.The single particle energy levels are those of a particle in a box. We know that in an infinite square well $\epsilon_i = \epsilon(n_1,\ n_2,\ n_3) = \frac{\hbar^2\pi^2}{2mL^2}\left(n_1^2+n_2^2+n_3^2\right)$ so we could write equation X as

$$N = \sum_{n_1,n_2,n_3} \exp\left(\frac{\mu - \epsilon(n_1,\ n_2,\ n_3)}{kT}\right)$$

exploiting fact that we must sum over very large number of energy levels.

What is the typical value of $(n_1,\ n_2,\ n_3)$ for a gas of hydrogen in a box of side $1m$ at room temperature? It is about $n_1^2+n_2^2+n_3^2 \approx kT\frac{mL^2}{\hbar^2\pi^2} \approx 10^{19}$. This means we can employ the following result

$$\sum \exp\left(\frac{\mu - \epsilon(n_1,\ n_2,\ n_3)}{kT}\right) \approx \int dn_1 dn_2 dn_3 \exp\left(\frac{\mu - \epsilon(n_1,\ n_2,\ n_3)}{kT}\right)$$

treat n_i as continuous variables&integrate over them. We define $\alpha = \frac{\hbar^2\pi^2}{2mL^2kT}$ so our integral becomes

$$\begin{aligned} N &= \int_0^\infty dn_1 \int_0^\infty dn_1 \int_0^\infty dn_1 e^{\frac{\mu}{kT}} e^{-\alpha n_1} e^{-\alpha n_2} e^{-\alpha n_3} \\ &= e^{\frac{\mu}{kT}} \left[\int_o^\infty e^{-\alpha n^2} dn\right]^3 \end{aligned}$$

using $\int dx e^{-\alpha x^2} = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}$ we get

$$\begin{aligned} N &= \exp\left(\frac{\mu}{kT}\right)\left(\frac{1}{2}\sqrt{\frac{2mL^2kT}{\hbar^2\pi}}\right)^3 \\ &= k_bT \ln\frac{n}{n_Q} \end{aligned}$$

using $\frac{N}{L^2} = n$ and n_Q the *quantum density* or *quantum concentration*. 27.10.2006

Recall that classical limit is when $\frac{\epsilon-\mu}{kT} \gg 1$ or $< n > \ll 1$. Also consider the fact that $\frac{\epsilon}{kT} \approx 1$ for typical particles, so we want $-\frac{\mu}{kT} \gg 1$. This implies $\ln\frac{n_Q}{n} \gg 1 \Rightarrow n \ll n_Q$. Another way to figure out if quantum effects are important or not involves the de Broglie wavelength, explanation follows.

estimate n_Q by assuming it to equal the concentration when each particle occupies a volume λ_Q^3. De Broglie wavelength is given by $\lambda_Q = \frac{h}{p}$. Using as typical momentum $p = mv,\ v \approx \sqrt{\frac{kT}{m}}$ so $p \approx \sqrt{mkT}$ which gives $\lambda_Q \approx \frac{h}{\sqrt{mkT}}$, we assume concentration $n_Q \approx \left(\frac{1}{\lambda_Q}\right)^3 \approx \left(\frac{mkT}{h^2}\right)^{\frac{3}{2}}$. Which is exactly as expected except for a factor of 2π.

Comments

- Do not forget spin multiplicity. If gas is made of particles with spin S. Consider $n = (2s+1)\exp\left(\frac{\mu}{kT}\right)n_Q$ for spin S particles. This has implications e.g. $\mu = kT\ln\left(\frac{n}{(2s+1)n_q}\right)$(taking log of both sides).

- The actual value of μ depends upon the zero of the energy scale. We are free to choose ϵ but only if μ changes too in order to compensate for this. Consider $\epsilon = \epsilon_0 + (n_1,\ n_2,\ n_3)$, which gives $\mu = \epsilon_0 + \ln \frac{n}{n_q}$.
- We have implicitly assumed the gas is mono-atomic. If the particles have internal energy states we need to account for them. Rotational or vibrational degrees of freedom,

$$N \approx \sum_i \exp\left(\frac{\mu - \epsilon_i}{kT}\right) = \sum_{n_1,n_2,n_3,j} \exp\left(\frac{\mu - \epsilon_{int}^j - \frac{\left(n_1^2+n_2^2+n_3^2\right)\hbar^2\pi^2}{2mL^2}}{kT}\right)$$

so we can write

$$n = e^{\frac{\mu}{kT}} n_Q \underbrace{\sum_j \exp\left(-\frac{\epsilon_j}{kT}\right)}_{= Z_{int}}$$

In the classical limit we could have calculated the mean number of particles $< n >$ in a given state directly, if we assume that the particles occupy states independently of each other. Let us do this now.

$$< n(\epsilon_i) >= (\#\ particles) \times (probability\ of\ finding\ a\ particle\ in\ \epsilon_i)$$

we know how to do this using the Boltzmann factor

$$\begin{aligned} < n(\epsilon_i) > &= N \frac{\exp\left(-\frac{\epsilon_i}{kT}\right)}{\sum_i \exp\left(-\frac{\epsilon_i}{kT}\right)} \\ &= \frac{N \exp\left(-\frac{\epsilon_i}{kT}\right)}{n_Q L^3} \end{aligned}$$

The "error" in this argument(why it is only an approximation) is to assume particles occupy energy levels independently of each other. This will *not* be true for a quantum gas. The internal energy is easy to compute, it is just $U = \sum_i \epsilon_i < n(\epsilon_i) >$,

$$\begin{aligned} U &\approx N \frac{\sum \exp\left(-\frac{\epsilon_i}{kT}\right) \epsilon_i}{\sum \exp\left(-\frac{\epsilon_i}{kT}\right)} \\ &= NkT^2 \frac{\partial \ln Z}{\partial T} \\ &= nkT^2 \frac{\partial}{\partial T} \left(\ln L^3 + \frac{3}{2} \ln\left(\frac{mkT}{2\pi\hbar^2}\right)\right) \\ U &= NkT^2 \times \frac{3}{2}\frac{1}{T} = \frac{3}{2}NkT \end{aligned}$$

6.11.2006

6 Computing the Entropy

We must count all accessible quantum states. But how do we do that for a system with variable energy & particle number?

Figure 4: Grid of systems, we are interested in one little box of these, thats our system. It is surrounded by $M-1$ replica systems. Replica meaning that all macroscopic properties are identical.

Clearly we want the mean entropy. How? We can do it by considering the following situation

Each system is completely disclosed by specifying its quantum state, e.g. for a gas it would be a long list of occupation numbers. So each distinct configuration of "Boxes" constitutes one quantum state of the entire system. So to compute the entropy of the entire system we must count the number of ways of shuffling our M boxes. This is just $W = \frac{M!}{m_1!m_2!m_3!...}$, where m_i is the number of boxes in the i-th quantum state.

$$\begin{aligned} m_1 + m_2 + ... &= M \\ m_1\epsilon_1 + m_2\epsilon_2 + ... &= E \end{aligned}$$

Suppose our system has only two accessible quantum states "1" & "2" and suppose we consider 4 boxes. How many quantum states can there be for the system as a whole? This gives $W = 6 = \frac{4!}{2!2!}$, try counting for yourself by drawing a picture. So entropy of complete system is

$$S_M = k_B \ln W = k_B \left(M \ln M - \sum_i m_i \ln m_i \right) \tag{9}$$

using Sterling's approximation to get second part. Since $M = \sum m_i$ we have $M \ln M = \sum m_i \ln M$, this allows us to rewrite 9 as

$$\begin{aligned} S_M &= k_B \left(\sum_i m_i \ln \frac{M}{m_i} \right) \\ &= -k_B M \sum \frac{m_i}{M} \ln \frac{m_i}{M} \end{aligned}$$

so the entropy per box is $S = \frac{S_M}{M} = -k_B \sum \frac{m_i}{M} \ln \frac{m_i}{M}$. But as $M \to \infty$, $\frac{m_i}{M} \to p_i$ tends to the probability that any one system(ie box) is in the i-th quantum state & this is something we know, it is the Gibbs distribution.

$$\begin{aligned} p_i &= \frac{\exp\left[\frac{(\mu N_i - \epsilon_i)}{kT}\right]}{\sum_{ASN} \exp\left[\left(\frac{\mu N_j - \epsilon_j}{kT}\right)\right]} \\ \Rightarrow S &= -k_B \sum p_i \ln p_i \end{aligned}$$

NB. true for classical or quantum gas. To compute p_i need $\mathcal{Z}$. For bosons

$$\begin{aligned} \mathcal{Z}_{bosons} &= \sum_{\{n_i\}} \exp\left(\frac{n_1(\mu - \epsilon_1)}{kT}\right) \exp\left(\frac{n_2(\mu - \epsilon_2)}{kT}\right) \times ... \\ where \quad n_1\epsilon_1 + n_2\epsilon_2 + ... &= E = \epsilon_{(i)} \\ where \quad n_1 + n_2 + ... &= N = N_{(i)} \end{aligned}$$

this allows us to rewrite $\mathcal{Z}_{bosons}$ as

$$\mathcal{Z}_{bosons} = \prod_i \left[1 + \exp\left(\frac{\mu - \epsilon_i}{kT}\right) + \exp\left(\frac{2(\mu - \epsilon_i)}{kT}\right) + ...\right]$$

which can be written as a sum again by knowing that this product is just a geometric sum.

$$\begin{aligned} \ln \mathcal{Z}_{bosons} &= \sum_i \ln\left(\frac{1}{1 - \exp\left(\frac{\mu-\epsilon_i}{kT}\right)}\right) \\ &= -\sum_i \ln\left(1 - \exp\left(\frac{\mu - \epsilon}{kT}\right)\right) \end{aligned}$$

for fermions this is

$$\begin{aligned} \mathcal{Z}_{fermion} &= \prod \left(1 + \exp\left(\frac{\mu - \epsilon_i}{kT}\right)\right) \\ \ln \mathcal{Z}_{fermion} &= \sum \ln\left(1 + \exp\left(\frac{\mu - \epsilon_i}{kT}\right)\right) \end{aligned}$$

we are in the classical limit $\exp(...) \ll 1$, using $\ln(1+x) \approx x$ if $x \ll 1$. This gives then

$$\begin{aligned} \ln \mathcal{Z}_{bosons} &= \ln \mathcal{Z}_{fermions} = \sum \exp\left(\frac{\mu - \epsilon_i}{kT}\right) \\ \ln \mathcal{Z}_{classical} &= e^{\frac{\mu}{kT}} Z \end{aligned}$$

where Z is the canonical single particle partition function($Z = \sum \exp\left(-\frac{\epsilon_i}{kT}\right)$). 10.11.2006
We know that $S = -k \sum p_i \ln p_i$, where the sum is over all states of the gas i.

$$\begin{aligned} S &= -k \sum \frac{\exp\left(\frac{\mu N_i - E_i}{kT}\right)}{Z_{classical}} \left(\frac{\mu N_i - E_i}{kT} - \exp\left(\frac{\mu}{kT}\right) Z\right) \\ &= -k \left(\frac{\mu}{kT} \sum p_i N_i - \frac{1}{kT} \sum p_i E_i - e^{\frac{\mu}{kT}} Z \sum p_i\right) \\ &= -k \left(\frac{\mu N - U}{kT} - e^{\frac{\mu}{kT}} Z\right) \end{aligned}$$

substitute for $\frac{\mu}{kT} = \ln \frac{n}{n_Q}$ and $Z = n_Q V$,

$$\begin{aligned} S &= -kN \ln \frac{n}{n_Q} + \frac{U}{T} + \frac{n n_Q V}{n_Q} \\ &= -kN \ln \frac{n}{n_Q} + \frac{U}{T} + \frac{NV}{V} \\ &= Nk \left(\ln \frac{n_Q}{n} + \frac{U}{kTN} + 1\right) \end{aligned}$$

for a mono atomic gas we can substitute $U = \frac{3}{2} NkT$ so we get $S = Nk\left(\ln \frac{n_Q}{n} + \frac{5}{2}\right)$. This is the entropy of a classical ideal gas, it is called the SACKUR-TETRODE equation.

Now can determine pressure $p = T\left(\frac{\partial S}{\partial V}\right)_{\mu,U} = NkT\frac{\partial}{\partial V}(\ln V + \ln n_Q)$, leaving out all the things that are fixed in this derivative, now use $n_Q = \left(\frac{mkT}{2\pi\hbar^2}\right)^{3/2}$ and $U = \frac{3}{2}NkT$, so we get $p = NkT\frac{\partial \ln V}{\partial V} = \frac{NkT}{V}$, this is just $pV = NkT$. We can also compute $c_p = T\left(\frac{\partial S}{\partial T}\right)_{p,N}$

$$\begin{aligned} c_p &= NkT\frac{\partial}{\partial T}(\ln n_Q + \ln V) \\ &= NkT\frac{\partial}{\partial T}\left(\ln V + \frac{3}{2}\ln T\right) \end{aligned}$$

now use $pV = NkT$ so we get $c_p = nKT\frac{\partial}{\partial T}\left(\ln T + \frac{3}{2}\ln T\right) = NkT\frac{5}{2T} = \frac{5}{2}Nk_B$.

7 Fermi gases

Now focus on a non-interacting gas of spin 1/2 particles. At "sufficiently low T" quantum effects are *not* negligible.

Show that the free electrons in a metal at room temperature will be in the quantum regime. We are in the quantum regime if $n > n_Q$. Lets work out how many electrons there are per unit volume in a metal. Assume there are ~1 conduction electrons per atom, IE $n \approx \frac{10^3\frac{kg}{m^3}}{10^{-25}kg} = 10^{28}m^{-3}$. This gives us $T \leq \left(10^{28}\right)^{2/3}\frac{2\pi\hbar^2}{mk} \approx 10^5K$. So for all temperatures less than this we need to consider quantum effects.

Show that atomic Nitrogen gas at STP is *not* quantum. We have $n \approx \frac{p}{kT} \approx \frac{10^5}{10^{-23}\times 10^2} \approx 10^{26}m^{-3}$ and this gives $T \leq \left(10^{26}\right)^{3/2}\frac{2\pi\hbar^2}{mk} \approx 10K$. SO only below 10 Kelvin will we see interesting quantum effects. 12.11.2006

Missed lecture about zero temperature things. 17.11.2006

Look up what density of states is and how it is dn/dk or dn/de. What is Fermi energy, degenerate Fermi gas, k space? Fermi energy for a 2D electron gas is

$$\epsilon_F = \frac{\hbar^2\pi N}{mA}$$

Calculate the density of states for a 3D gas of spin less particles & use it to re-derive our earlier results for the chemical potential & energy of an ideal gas in the classical regime.

We want to work out the total number of states within region $k + dk$

$$dn = \frac{dn}{dk}dk = \frac{4\pi k^2 dk}{8} \times \frac{1}{\left(\frac{\pi}{L}\right)^3}$$

total number of "dots" with in spherical shell of volume $\frac{4\pi k^2 dk}{8}$ divided by volume of one "dot" $\left(\frac{\pi}{L}\right)^3$. We get

$$\frac{dn}{dk} = \frac{Vk^2}{2\pi^2}$$

To compute μ we calculate $N = \int \frac{dn}{dk}dk < n(k) >_{classical}$ where $< n(k) >_{classical} = \exp\left(\frac{\mu}{k_BT} - \frac{\epsilon}{k_BT}\right)$. Now do the integral

$$N = \frac{V}{2\pi^2}\int_0^\infty k^2 dk e^{\frac{\mu}{k_BT}}\exp\left(-\frac{\hbar^2k^2}{2mk_BT}\right)$$

where we have used $\epsilon = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$. If we have a ultra relativistic gas we would use $\epsilon = \hbar ck = cp$ with $p = \hbar k$(remember e^2=p^2+m^4). Rewrite the integral in eqn1

$$N = \frac{V}{2\pi^2} e^{\frac{\mu}{k_B T}} \int k^2 \exp\left(-\alpha k^2\right) dk$$

with $\alpha \equiv \frac{\hbar^2}{2mk_B T}$. Given $\int \sqrt{x} e^{-x} dx = \frac{\sqrt{\pi}}{2}$ we can do the integral, requires change of variables though. We let $x = \alpha k^2$ and $dx = 2\alpha k dk$ which gives

$$N = \frac{V}{2\pi^2} e^{\frac{\mu}{k_B T}} \int \frac{x}{\alpha} \frac{dx}{2\alpha} \left(\frac{\alpha}{x}\right)^{\frac{1}{2}}$$

using $n = \frac{N}{v}$ we get

$$n = \frac{1}{2\pi^2} e^{\frac{\mu}{k_B T}} \frac{1}{2\alpha^{3/2}} \int \sqrt{x} e^{-x} dx$$

so we now put α back in, we get

$$\begin{aligned} n &= \frac{1}{8} \left(\frac{1}{\alpha\pi}\right)^{3/2} e^{\frac{\mu}{k_B T}} = \frac{1}{8} \left(\frac{2mk_B T}{\pi\hbar^2}\right) e^{\frac{\mu}{k_B T}} \\ &= n_Q e^{\frac{\mu}{k_B T}} \end{aligned}$$

where we have use quantum concentration, we get $\mu = k_B T \ln \frac{n}{n_Q}$.

We can also compute the energy. Using k space it is easy and integral would be

$$\begin{aligned} U &= \int \frac{dn}{dk} dk < n(k) > \frac{\hbar^2 k^2}{2m} = ... \\ &= \int \frac{dn}{dk} dk < n(\epsilon) > \epsilon \end{aligned}$$

in ϵ space.

We need to work out $dn/d\epsilon = \frac{dn}{dk}\frac{dk}{d\epsilon} = \frac{Vk^2}{2\pi^2} \times \frac{\epsilon^{-1/2}}{2} \left(\frac{2m}{\hbar^2}\right)^{1/2}$ where we used $\epsilon = \frac{k^2\hbar^2}{2m}$. This gives for a non relativistic gas in energy space

$$\frac{dn}{d\epsilon} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2}$$

so for energy U of gas we get

$$U = \int \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{3/2} \exp\left(\frac{\mu}{k_B T} - \frac{\epsilon}{k_B T}\right) d\epsilon$$

use $\exp\left(\frac{\mu}{k_B T}\right) = \frac{n}{n_Q}$ and again doing change of variables

$$\begin{aligned} &= \underbrace{\int x^{3/2} e^{-x} dx}\, \frac{2Nk_B T}{\sqrt{\pi}} \\ &= \frac{3\sqrt{\pi}}{4} \times ... \\ &= \frac{3}{2} k_B N T \end{aligned}$$

Back to the degenerate Fermi gas. What is ϵ_F? We again have $N = \int \frac{dn}{dk} dk < n(k) >_{FD}$ where $< n(k) >_{FD}= 1$ if $\epsilon < \epsilon_F$ and $= 0$ if $\epsilon > \epsilon_F$. The integral is much easier now

$$N = \int_0^{k_F} \frac{Vk^2}{2\pi^2} \times 2 \times 1 dk = \frac{V}{\pi^2}\frac{k_F^3}{3}$$

which gives $k_F = \left(3n\pi^2\right)^{1/3}$ which gives $\epsilon_F = \frac{\hbar^2}{2m}\left(3n\pi^2\right)^{2/3}$. Finding the energy is now easy, just do

$$U = \int \frac{dn}{dk} dk \times 1 \times \frac{\hbar^2 k^2}{2m}$$

Think there is some bits missing here. 20.11.2006

Fermi temperature given by $k_B T_F = \epsilon_F$. If $T \leq T_F$then the gas is a "quantum gas". If $T \gg T_F$ then the thermal energy is sufficiently large that the fermions "don't care" about the Pauli principle & the gas is classical. Let us check this

$$k_B T \gg \epsilon_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{3/2}$$

we can rearrange this to give $n \ll \left(\frac{2mk_BT}{\hbar^2}\right)\frac{1}{3\pi^2} = \frac{8}{3\sqrt{\pi}} n_Q$ which gives $n \ll n_Q$ as before.

Let's finally compute the "equation of state"(at $T = 0$). For that we need the pressure. Usually we would use $p = T\left(\frac{\partial S}{\partial V}\right)_{U,N}$. At $T = 0$ we can work out this expression $dU = TdS - pdV$, as TdS is zero at $T = 0$ we get

$$\begin{aligned} p &= -\left(\frac{\partial U}{\partial V}\right)_N = \frac{3}{5}N\frac{\partial}{\partial V}\epsilon_F \\ &= \frac{3}{5}\left(-\frac{2}{3}\frac{\epsilon_F}{V}\right) \\ p &\Rightarrow \frac{2}{5}n\epsilon_F \end{aligned}$$

Since ϵ_F is independent of T we also have $c_V = \left(\frac{\partial U}{\partial T}\right) = 0$. Ideally we would like to know just how $c_V varies as T \rightarrow 0$. To obtain this wen need to work much harder. We need

$$U = \int_0^\infty \frac{dn}{d\epsilon}\epsilon d\epsilon \frac{1}{\exp\left(\frac{\epsilon-\mu}{k_BT}\right)+1}$$

this time not cheating with the Fermi-Dirac distribution as before. We can show that(see his website)

$$U \approx \frac{3}{5}N\epsilon_F + \frac{\pi^2}{4}N\left(\frac{k_BT}{\epsilon_F}\right)^2\epsilon_F$$

for completeness also state that $\mu \approx \epsilon_F\left[1 - \frac{\pi^2}{12}\left(\frac{k_BT}{\epsilon_F}\right)^2\right]$. We can estimate these results. The number of electrons that are excited at T just over zero is $\approx \left(\frac{k_BT}{\epsilon_F}\right)N$, hence the additional energy $\Delta U \approx N\left(\frac{k_BT}{\epsilon_F}\right) \times k_BT = \frac{N(k_BT)^2}{\epsilon_F}$, this is not that bad. If we use this we get

$$c_V = 2Nk_B\frac{k_BT}{\epsilon_F}$$

8 Electrons in metals

Assume that the electrons in a metal behave as an ideal gas.

- The gas will be degenerate at room temperature
- And the electrons move non-relativistically

24.11.2006

Some predictions he makes

$$C_{electrons} = \frac{\pi^2}{2} N k_B \left(\frac{k_B T}{\epsilon_F} \right) \propto T$$

compare to classical expectation $C_{electrons} = \frac{3}{2} N k_B$. This extra factor (proportionality to T) should be negligible at room temperature. From measurements it was known that the total heat capacity of a conductor was $C_{total} = 3Nk_B$, we would classically expect $C_{total} = 3Nk_B + \frac{3}{2}Nk_B$, this is wrong. From real form of $C_{electrons}$ we can understand why this is so, $C_{electrons}$ becomes negligible for low temperatures.

Consider liquid ^{3}He, this is a fermion. We can work out $\epsilon_F = 4.2 \times 10^{-4}$eV, gives $T_F = 5$K. So we need to cool it below that temperature to get it to behave like a quantum thing. For $T < 5$K we expect quantum effects & $C = aT$, with $a = 1.0K^{-1}$. At very low temperates(<2mK) the helium forms pairs of helium-3 molecules which now are bosons and not fermions anymore.[1] These pairs are called "Cooper pairs".

9 Electrons in stars

As a center of a star consist of protons and electrons whizzing about "on their own", they are not connected, so it is fair to assume it to be a gas of electrons. The core temperature of the sun is $T_\odot = 10^7$K[2]. Do the electrons form a degenerate Fermi gas? electron density is about the same as proton density, given by $n \approx \frac{M_\odot}{m_p} \times \frac{1}{V_\odot} \approx 10^{30}$. We are interested in all this if we have T_F similar to T.

Fermi energy is given by $T_F = \frac{\epsilon_F}{k_B} = \frac{1}{k_B} \left[\frac{\hbar^2}{2m} \left(3\pi^2 n\right)^{2/3} \right] \approx 10^5 K$, so the sun is to hot or number density is not high enough, $T_\odot \gg T_F$.

27.11.2006

White dwarf stars Stars collapsing under gravity to the point where p+p fusion can occur, requires $T \approx 10^7$K. The radius is stabilized against further gravitational collapse by the pressure exerted by the hot gas of ions, electrons&photons.

When all of the proton fuel is exhausted the star collapses again under gravity until either helium nuclei start to fuse($T \approx 10^8$K) or until the electrons become degenerate & exert a pressure which resists any further collapse.

Stars which have stopped burning nuclear fuel & supported by the pressure of degenerate electrons are called white dwarf stars. Given the mass of a white dwarf we can computer its radius. We even have data to compare to, see website.

[1] he gives a big hint that it would make a lot of sense to work these things out for yourself, understand the plot of helium-3 head capacity and such.

[2] $k_B T = 10^7 \times 10^{-23} = 10^{-46} J \approx 10^3 eV \gg 13.6 eV$

Consider a thin shell of thickness dr at radius r inside the star. At equilibrium electron pressure and gravitational force have to balance.

The inward force due to gravity is

$$dF = G \times \frac{4\pi r^2 dr \times \rho(r)}{r^2} \times M(r)$$

where $M(r)$ is total mass of the star inside the shell.

This must be balanced by the outward force due to the electrons, ie pressure at r must be slightly larger then at $r + dr$, saying $p(r) > p(r + dr)$. Electron pressure is given by

$$\begin{aligned} dF &= -4\pi r^2 \left[P(r+dr) - P(r)\right] \\ &= -4\pi r^2 dP(r) \end{aligned}$$

but we know (worked out before) that

$$p = \frac{2}{5} n\epsilon_F = \frac{2}{5} n^{5/3} \frac{\hbar^2}{2m} \left(3\pi^2\right)^{2/3}$$

ie. n must fall as r increases. If we equate these we get

$$-\frac{dP}{dr} = \frac{\rho(r) GM(r)}{r^2}$$

which is true in equilibrium. This is a rather nasty equation(try and differentiate this) but we can make progress if we are happy to make some simplifying assumptions. If we integrate this equation we get

$$-\int_{P(0)}^{P(R)} dP = \int_0^R dr \rho(r) \frac{GM(r)}{r^2}$$

with $M(r) = \int_0^r 4\pi r\prime^2 dr\prime \rho(r\prime)$. This is really really complicated, essentially its the integral of rho inside the integral of rho.

Now we assume $\rho(r)$ is approximately constant, $\rho(r) = \rho_c = \frac{M}{\frac{4}{3}\pi R^3}$, so we are now left with

$$\begin{aligned} -P(R) + P(0) &\approx 4\pi G\rho_c^2 \int_0^R \frac{dr}{r^2} \frac{r^3}{3} \\ P(0) &\approx \frac{4\pi F\rho_c^2}{3} \frac{1}{2} R^2 \end{aligned}$$

assuming also that $P(0) \gg P(R)$. Putting

$$P(0) = P = \frac{2}{5}\left(\frac{\hbar^2}{2m}\right)\left(3\pi^2\right)^{2/3}\left[\frac{M}{\frac{4}{3}\pi R^3}\frac{1}{u}\right]^{5/3}$$

where u is atomic mass constant, M is total mass of star and R is radius of star. We can write $P \propto \frac{M^{5/3}}{R^5}$, hiding all the constants.

Equating gives

$$\begin{aligned} \frac{M^{5/3}}{R^5} &\propto \frac{M^2}{R^4} \\ M^{-1/3} &\propto R \end{aligned}$$

which gives $RM^{1/3} = const.$ We predict this to be $\frac{\hbar^2}{5m} 3^{2/3} \pi^{4/3} \left(\frac{3}{4\pi u}\right)^{5/3} \frac{8\pi}{3G} \approx$ 10^{16}mkg^1/3. This number is in pretty good agreement with data.

We ought to check that at this radius the density is high enough to be degenerate.

$$T_F = \frac{1}{k_B} \frac{\hbar^2}{2m} \left(3\pi^2 n\right)^{2/3}$$

with $n \approx 10^{25}$, so $T_F = 10^9$K. This is bigger than $10^7 - 10^8$K, which we assume to be the temperature of the whole thing. 1.12.2006

What are the speeds of the electrons?

$$v_F = \sqrt{\frac{2k_B T_F}{m}} \approx 10^8$$

which is just about non-relativistic.

But if M is "too big" then T_F could be large enough so that the electrons move relativistically. Must re-visit the calculation of $p_{electron}$ using relativistic ideas

$$\frac{dn}{d\epsilon} = \frac{V\epsilon^2}{\pi^2 \hbar^3 c^3}$$

for an ultra relativistic gas, was $\propto \sqrt{\epsilon}$ for non-relativistic. We have $p = -\left(\frac{\partial U}{\partial V}\right)_{N,}$ at $T = 0$. So we find U from

$$U = \int_0^{\epsilon_F} \epsilon \frac{dn}{d\epsilon} d\epsilon = \frac{V}{\pi^2 \left(\hbar c\right)^3} \frac{\epsilon_F^4}{4}$$

get the Fermi energy, ϵ_F from

$$N = \int_0^{\epsilon_F} \frac{dn}{d\epsilon} d\epsilon = \frac{V}{\pi^2 \left(\hbar c\right)^3} \frac{\epsilon_F^3}{3}$$

so we get U to be

$$U = \frac{V}{\pi^2 \left(\hbar c\right)^3} \frac{1}{4} \left(3\pi^2\right)^{4/3} \left(\hbar c\right)^4 \times \left(\frac{N}{V}\right)^{4/3}$$

this is just $U = AV^{-\frac{1}{3}}$ were all the constants live in A. So for the pressure we get

$$p = -\left(\frac{\partial U}{\partial V}\right) = \frac{1}{3}\frac{U}{V}$$

as the pressure exerted by the electrons. Following exactly same method as in previous lecture we get electron pressure to be

$$\propto \left(\frac{M}{R^3}\right)^{4/3} = \frac{M^{4/3}}{R^4}$$

As this now has the same R dependence as pressure due to gravity we need to look at the M dependence. For small masses electron pressure is bigger than gravity pressure and for big masses gravity wins. M_c, the critical mass at which they exactly balance is determined by all the constants which we should be able to compute!

Putting in the constant of proportionality we get

$$\frac{\hbar c}{12\pi^2}\left(\frac{M}{\frac{4}{3}\pi R^3 u}\right)^{4/3}=\frac{3}{8\pi}\frac{GM}{R^4}$$

solving this for M we get $M_c \approx M_\odot$.

If mass of the star $M < M_c$ then it will start expanding until it becomes non-relativistic and hence is stable again.

If mass $M > M_c$ star collapses, ϵ_F keeps rising, Eventually the electrons have enough energy to initiate $e^- p \to n\nu_e$. All electrons and protons "disappear" leaving behind a gas of neutrons, as the neutrinos just fly off.

10 Bose Gases

What happens to a gas of bosons in the quantum regime? Let's investigate $T \to 0$ limit. First think about a "classical gas" in this limit. How low must T be for the majority of atoms to sit in the ground state? We have

$$\Delta\epsilon = \epsilon_1 - \epsilon_0 = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2\left[\left(2^2+1^2+1^2\right)-\left(1^2+1^2+1^2\right)\right]$$

most particles in ground state if

$$\frac{\langle n(\epsilon_0)\rangle}{\langle n(\epsilon_1)\rangle}=\exp\left(-\frac{\Delta\epsilon}{k_B T}\right)\ll 1$$

where we have $\langle n(\epsilon)\rangle = \exp\left(\frac{\mu-\epsilon}{k_B T}\right)$. If we use $m = 6.6\times 10^{-27}$, this is helium-4 and $L = 1cm$ we get $T \ll 10^{-14}$K. 4.12.2006

Things are very different for an ideal gas of bosons. Recall

$$\langle n(\epsilon)\rangle_{BE}=\frac{1}{\exp\left(\frac{\epsilon-\mu}{k_B T}\right)-1}$$

need $\epsilon-\mu>0$ for all ϵ, if $\epsilon = 0$ then $\mu < 0$. What happens as T is reduced? If μ was fixed then we would end up with $\langle n(\epsilon)\rangle_{BE} = 0$ for all energies at very low temperatures, This makes no sense at all, where have all the particles gone. Formally we have

$$N=\int_0^\infty \frac{dn}{d\epsilon}\frac{d\epsilon}{\exp\left(\frac{\epsilon-\mu}{k_B T}\right)-1}$$

so as T falls, μ rises and N is fixed. Remember the assumption we made at the beginning that all energy levels contribute and are closely spaced and hence we can write the previous formula as a integral instead of a sum that it strictly speaking should be. We will have to go back and do it as a sum probably.

At some $T = T_c$ we will have $\mu = 0$

$$N=\int_0^\infty \frac{dn}{d\epsilon}\frac{d\epsilon}{\exp\left(\frac{\epsilon}{k_B T_c}\right)-1}$$

What happens below T_c? Out equation for N breaks down as $\mu \to 0$. Recall $N=\sum_i \langle n(\epsilon_i)\rangle_{BE}$ and that we approximated this by an integral, which now breaks down. As $\mu \to 0$ so the ground state dominates the sum. TO see this note that as $\mu \to 0$

$$\langle n(0)\rangle_{BE} \approx \frac{1}{1+\left(\frac{\epsilon-\mu}{k_BT}\right)-1} = \frac{k_BT}{-\mu} = N_0$$

this is the mean number of particles in the ground state. We used an "math trick" to rewrite the exponential with an argument of zero as a sum.

So we should write

$$N = N_0 + \underbrace{\int_\delta^\infty \frac{dn}{d\epsilon}\langle n(\epsilon)\rangle_{BE}}_{=N_{excited}}$$

where $\epsilon_0 = 0$ and $\epsilon_1 > \delta$. We can safely take $\delta \to 0$ because $\frac{dn}{d\epsilon} \propto \sqrt{\epsilon}$. T_c is thus the temperature where μ is so small that the ground state is microscopically occupied, ie N_0 is not negligible. We can estimate the number of particles in the ground state for $T < T_c$:

$$N_{excited} = \int_0^\infty \frac{Vm^{3/2}}{\sqrt{2}\pi^2\hbar^3}\underbrace{\frac{\epsilon^{1/2}d\epsilon}{\exp\left(\frac{\epsilon}{k_BT}\right)-1}}_{=}$$

(Eqn 1) assuming $\mu = 0$for $T < T_c$. But $T_c$is defined using

$$N = \int_0^\infty \frac{Vm^{3/2}}{\sqrt{2}\pi^2\hbar^3}\frac{\epsilon^{1/2}d\epsilon}{\exp\left(\frac{\epsilon}{k_BT_c}\right)-1}$$

we can rewrite Eqn 1 to be dimensionless by dividing all energies by k_BT. So we can rewrite

$$N_{excited} = \int_0^\infty \frac{Vm^{3/2}}{\sqrt{2}\pi^2\hbar^3}\underbrace{\frac{xdx}{\exp(x)-1}\times(k_BT)^{3/2}}_{=}$$

and similarly for N.

$$N = \{...\}\times(k_BT_c)^{3/2}$$

where $\{...\} =$

We can now write

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

and hence $N_0 = N\left(1-\left(\frac{T}{T_c}\right)^{3/2}\right)$.

Note that for density of helium we get $T_c = 3K$. Also $T < T_c$ is the regime for which

$$\left(\frac{mk_BT}{\hbar^2}\right) \leq n$$

this looks very similar to n_Q.

Producing a Bose-Einstein Condensate

8.12.2006

4-He is a super fluid at 2K but it is not a weakly interacting gas of bosons. In 1995 we had first observation of BEC in a weakly interacting gas of rubidium 87 atoms. To date also seen in Na, Li, He and K.

How did they do it? We need to get about 1μK. To produce a gas of rubidium we heat it to about 10^3K, then use Laser-Cooling to cool it to about 10μK. Now we trap them in a magnetic trap, with the potential just high enough to trap the slowest/coolest atoms. SO after a while the hot/fast atoms will have "split out" of the trap. The final step is to turn off the trap and let atoms expand. If you take pictures during this process you will see a BEC. Read Anderson et al, "Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor", July 1995, Vol 269, journal unknown.

Black Body Radiation

Consider a gas of photons in thermal equilibrium. This has three interesting features:

- Gas really is ideal
- Gas really is ultra relativistic
- The chemical potential $\mu = 0$

To prove $\mu = 0$. The number of photons N is a system can not be fixed, ever! Even very very low energy photons will interact with the walls of our box and start disappearing or appearing. Equilibrium requires $dS = 0$ for S+R(system plus reservoir). This gives

$$\left(\frac{\partial S}{\partial N}\right)_{U,V} dN = 0$$

previously $dN = 0$(when N could be fixed) but this is not possible now so $\mu \propto \frac{\partial S}{\partial N} = 0$.

We have

$$\langle n\left(\epsilon\right)\rangle = \frac{1}{\exp\left(\frac{\epsilon}{k_B T}\right) - 1}$$

and the density of states

$$\frac{dn}{dk} = \frac{4\pi k^2}{8} \times \frac{1}{\left(\frac{\pi}{L}\right)^3} \times 2$$

where the 2 comes from the spin multiplicity for photons[3]. We can also write down the density of states in energy space

$$\frac{dn}{d\epsilon} = \frac{V}{\pi^2}\frac{\epsilon^2}{\left(\hbar c\right)^3}$$

where we have used $\epsilon = \hbar c k$ and made a change of variables from the previous expression. Remember, this is like for an ultra relativistic gas.

[3]This is the only place where $2s+1$ fails since $s = 1$ for photons.

The internal energy per unit volume is

$$\frac{U}{V}=\frac{1}{V}\int_0^{\infty}\frac{dn}{d\epsilon}\left\langle n\left(\epsilon\right)\right\rangle d\epsilon=\frac{1}{\pi^2\left(\hbar c\right)^3}\int_0^{\infty}d\epsilon\frac{\epsilon^3}{\exp\left(\frac{\epsilon}{k_BT}\right)-1}$$

we rewrite this in dimensionless form as

$$\frac{U}{V}=\frac{1}{\pi^2\left(\hbar c\right)^3}\int d\left(\frac{\epsilon}{k_bT}\right)\frac{\left(\epsilon/k_BT\right)^3}{\exp\left(\frac{\epsilon}{k_BT}\right)-1}\times\left(k_BT\right)^4$$

which is a simple integral now

$$\frac{U}{V}=const\times\int dx\frac{x^3}{\exp\left(x\right)-1}$$

which gives

$$\frac{U}{V}=\left[\frac{\pi^2k_B^4}{15\left(\hbar c\right)^3}\right]T^4$$

To connect with black body radiation image in a box full of photons with a little hole. Inside it there is a photon gas at thermal equilibrium and temperature T. It will absorb everything incident upon it & emits at characteristic temperature T.

From kinetic theory of gases, number of particles escaping through the hole per unit time$=\frac{1}{4}ncA$, where n is unit number of photons in box. So power radiated is just $=\frac{1}{4}\frac{U}{V}cA$. So we can write

$$P=\frac{1}{4}c\left[\frac{\pi^2k_B^4}{15\left(\hbar c\right)^3}\right]T^4=\sigma T^4$$

which is Stefan's law. 11.12.2006

Also interesting is the spectral energy density $u\left(\lambda\right)d\lambda$ energy per unit volume in the wavelength range $\lambda\rightarrow\lambda+d\lambda$. Use

$$\frac{U}{V}=\int u\left(\lambda\right)d\lambda=\frac{1}{\pi^2\left(\hbar c\right)^3}\int\frac{\epsilon^3d\epsilon}{\exp\left(\frac{\epsilon}{kT}\right)-1}$$

using $\epsilon=\frac{hc}{\lambda}$ so we get

$$\frac{1}{\pi^2\left(\hbar c\right)^3}\int\frac{\left(\frac{hc}{\lambda}\right)^3\frac{hc}{\lambda^2}d\lambda}{\exp\left(\frac{hc}{\lambda kT}\right)-1}$$

so we get for the spectral energy density $u\left(\lambda\right)$

$$\begin{aligned}u\left(\lambda\right)&=\frac{\left(2\pi\right)^3}{\pi^2}\times\frac{hc}{\lambda^5}\times\frac{1}{\exp\left(\frac{hc}{\lambda kT}\right)-1}\\&=\frac{8\pi hc}{\lambda^5}\frac{1}{\exp\left(..\right)-1}\end{aligned}$$

This is Planck's formula. Classical limit is $h\rightarrow0$ so we get $\exp\left(\frac{hc}{kT\lambda}\right)\approx1+\frac{hc}{\lambda kT}$ so Planck's formula can be written as

$$u\left(\lambda\right)=\frac{8\pi kT}{\lambda^4}$$

this is the "Rayleigh.Jeans formula". This is badly divergent as $\lambda\rightarrow0$. Which leads to the ultraviolet catastrophe.

Wien's Displacement Law can easily be derived now. The maximum of $u(\lambda)$ occurs at $\lambda T = const$. We can write

$$u(\lambda) = \frac{f(\lambda T)}{\lambda^5}$$

we require that $\frac{du}{d\lambda} = 0$ from which we get

$$\frac{df(x)}{dx}\frac{dx}{d\lambda}\frac{1}{\lambda^5} + f(x)\left(\frac{-5}{\lambda^6}\right) = 0$$

where $x = \lambda T$. We now write

$$\begin{aligned} f'(x)\frac{T}{\lambda^6} &= \frac{5f(x)}{\lambda^6} \\ f'(x)\underbrace{\lambda T}_{=x} &= 5f(x) \end{aligned}$$

this implies that there is a solution for some x, ie x=constant.

Note: sometimes spectral energy density is written in terms of frequency rather than wavelength

$$\int_0^\infty u(\omega)\, d\omega = \frac{U}{V}$$

so here we just use $\epsilon = \hbar\omega$. Go to beginning of lecture and replace all ϵ with hbar c. We get

$$\begin{aligned} u(\omega) &= \frac{1}{\pi^2(\hbar c)^3}\frac{(\hbar\omega)^3\hbar}{\exp\left(\frac{\hbar\omega}{kT}\right)-1} \\ &= \frac{\hbar\omega^3}{\pi^2 c^3\left(\exp\left(\frac{\hbar\omega}{kT}\right)-1\right)} \end{aligned}$$

Finish off by computing S and then p. Recall

$$S = -k_B\sum_{ASN}\frac{\exp\left(\frac{\mu N_s - E_s}{k_B T}\right)}{\mathcal{Z}}\left(\frac{\mu N_s - E_s}{kT} - \ln\mathcal{Z}\right)$$

put $\mu = 0$. Then we can write

$$S = +\frac{k_B U}{kT} - \ln\mathcal{Z}$$

where

$$\ln Z = -\int\frac{dn}{d\epsilon}d\epsilon\ln\left(1 - \exp\left(-\frac{\epsilon}{kT}\right)\right)$$

where you have to sub in dn/de and then make change of variables so we have dimensionless integral, then do lots of maths. If we now collect everything together we get

$$S = \frac{U}{T} + \frac{V(kT)^3\pi^2 k}{45(\hbar c)^3}$$

now put $\frac{U}{V}=\frac{\pi^2 k^4}{15(\hbar c)^3}T^4$ so we get as a final result $S = \frac{4}{3}\frac{U}{T} = \frac{4\pi^2 k^4 T^3 V}{45(\hbar c)^3}$. Can get p now using $p = T\frac{\partial S}{\partial V}$. We need $S\left(U,V\right)$. S=$\frac{4}{3}aVT$ and $U = aVT^4 \Rightarrow \left(\frac{U}{aV}\right)^{1/4}$ which gives

$$S = \frac{4}{3}aV\left(\frac{U}{aV}\right)^{3/4}$$

Now we can differentiate this with respect to V. This gives $p = \frac{1}{3}\frac{U}{V} = \frac{1}{3}aT^3$. Compare this to $pV = nRT$. And see that if we do an adiabatic expansion at constant temperature the entropy is fixed.

11 Lattice vibrations of a solid

15.12.2006

We have just been thinking about a gas of photons . System specified by stating the set of energy levels $\{\epsilon_i\}$ and their occupancy $\{n_i\}$.

There is a totally equivalent way to thinking about what is going on in a solid. Photons in energy level $\epsilon_i = \hbar\omega_i$ can be viewed as the quanta associated with a quantum harmonic oscillator of frequency ω_i. System is a set of harmonic oscillators each “loaded” with quanta.

Making this link we can re-derive the heat capacity of a solid à la Einstein. Suppose we have a solid, with side of length L, with N atoms on a periodic lattice. In 3D there are $3N$ normal modes, ie $3N$ allowed frequencies of vibration, $3N$ harmonic oscillators.

Einstein's assumed that all $3N$ oscillators oscillate with the same frequency. Quantizing the oscillators $\Rightarrow$set of oscillators each “loaded” with quanta. Einstein's solid has $3N$ degenerate energy levels each loaded with phonons.

Any number of quanta can reside on any given oscillator, phonons are bosons. As in the photon gas case the total number of phonons is not fixed, so again the chemical potential $\mu = 0$.

So

$$U_{Einstein} = \sum_{i=1}^{3N} \langle n_i \rangle_{BE} \times \hbar\omega_i$$

where $\omega_i = \omega$, ie only one frequency.

$$= 3N \times \frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

so for the heat capacity of a solid,

$$\frac{\partial U}{\partial T}_{Einstein} = C_{Einstein} = 3Nk_B\frac{x^2 e^x}{\left(e^x - 1\right)^2}$$

with $x = \frac{\hbar\omega}{k_B T}$. This has some success at large T and as $T \to 0$. We assume that the allowed phonon energy levels are exactly as for standing waves in a box. Hence

$$U_{Debye} = \int \frac{dn}{d\omega} d\omega \left\langle n\left(\omega\right)\right\rangle \hbar\omega$$

What is the density of states?

$$\frac{dn}{d\omega} = \frac{dn}{dk}\frac{dk}{d\omega} = \frac{4\pi k^2}{8}\frac{1}{\left(\frac{\pi}{L}\right)^3} \times 3 \times \frac{1}{v_s}$$

where the 3 arises because sound waves can travel longitudinal and twice transversal. We assume $\omega = v_s k$ where v_s is the speed of sound, which gives us $\frac{dk}{d\omega}$. Which finally gives

$$\frac{dn}{d\omega} = \frac{3V\omega^2}{2\pi^2 v_s^3}$$

Going back to the energy we have

$$u_{Debye} = \int_0^{\omega_D} \frac{3V\omega^2}{2\pi^2 v_s^3} \frac{\omega^3 d\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

Note $\omega <_D$ we expect that $\lambda \geq d$, where d is the lattice spacing. We can also argue, because there are only $3N$ oscillators, that

$$3N = \int_0^{\omega_D} \frac{dn}{d\omega} d\omega = \frac{3V}{2\pi^2 v_s^3} \frac{\omega_D^3}{3}$$

this allows us to work out ω_D.

$$\omega_D = v_s \left(6\pi^2 \frac{N}{V}\right)^{1/3}$$

so we can do the energy integral

$$u_{Debye} = \int_0^{\omega_D} \frac{3V\omega^2}{2\pi^2 v_s^3} \frac{\omega^3 d\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1}$$

and then find the heat capacity $\frac{\partial U}{\partial T}$

$$C_{Debye} = \int_0^{\omega_D} \frac{3V\omega^2}{2\pi^2 v_s^3} \frac{\omega^3 d\omega}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} e^{\frac{\hbar\omega}{k_B T}} \frac{\hbar\omega}{k_B T^2}$$

now we let $x = \frac{\hbar\omega}{k_B T}$ and do lots of algebra and we get

$$C_{Debye} = 3Nk_B \left[\frac{3}{x_D^3} \int_0^{x_D} \frac{x^4 e^x}{(e^x - 1)^2} dx\right]$$

where$x_D = \frac{\hbar\omega_D}{k_B T}$. At high T, $x_D \to 0$ we get

$$C \approx 3Nk_B \frac{3}{x_D^2} \int \frac{x^4 dx}{x^2} = 3Nk_B$$

and at low T, $x_D \to \infty$

$$\begin{aligned} C &\approx 3Nk_B \frac{3}{x_D^3} \int_0^\infty x^4 e^{-x} dx \\ &\propto T^3 \end{aligned}$$

as the integral is just a number, and $x_D \propto \frac{1}{T}$.