

Bose & Fermi Gases - A Summary

1 Einstein Solids

An atom can oscillate in 3 independent directions. Hence, if we model a lattice as being made up of N oscillators, we actually have $\frac{N}{3}$ atoms. The energy of each oscillator is given by $\epsilon_i = (n_i + \frac{1}{2})\hbar\omega$. We make the assumption that every oscillator has the same angular frequency ω of vibration. If we rescale the energy axis, we have:

$$\epsilon_i = n_i\hbar\omega$$

Hence, the total energy of the lattice is given by:

$$U = \sum_i \epsilon_i = n\hbar\omega$$

Now, let $g(n, N)$ be the number of ways of arranging a system of N particles into a state with energy $n\hbar\omega$. Standard permutation theory then gives us:

$$g(n, N) = \frac{(N + n - 1)!}{n!(N - 1)!}$$

Thus, we have that $g(n, N)$ is the number of microstates in a given macrostate.

We define equilibrium to be where:

$$dg = \frac{\partial g}{\partial n}dn + \frac{\partial g}{\partial N}dN = 0$$

Notice, a differential w.r.t n is basically that of the internal energy U . The system may be a composite of a number of different types of oscillators (e.g. different atoms). So that must be taken into account. For example, if $g(n, N) = g_a(n_a, N_a)g_b(n_b, N_b)$, then we will have that, in equilibrium:

$$g_a \frac{\partial g_b}{\partial n_b} dn_b + g_b \frac{\partial g_a}{\partial n_a} dn_a + g_a \frac{\partial g_b}{\partial N_b} dN_b + g_b \frac{\partial g_a}{\partial N_a} dN_a = 0$$

We notice that $dN = dN_a + dN_b = 0$, hence we are able to eventually define a couple of quantities that are constant in equilibrium: temperature and chemical potential. Infact, if we also let the volume of the system vary as well, so that $g(n, N, V)$, we are also able to define the pressure. We end up having the following quantities fall out:

$$\frac{1}{T} = \frac{k_B}{g} \frac{\partial g}{\partial U} \tag{1.1}$$

$$\mu = -T \frac{\partial S}{\partial N} \tag{1.2}$$

$$p = T \frac{\partial S}{\partial V} \tag{1.3}$$

After using the following expression for entropy:

$$S = k_B \ln g \tag{1.4}$$

Now, using Stirling's approximation, we are able to get $n(T)$, from putting the expression for g into the above for S :

$$n(T) = \frac{N}{e^{\frac{\hbar\omega}{k_B T}} - 1} \quad (1.5)$$

Now, we define the heat capacity in the usual way, but rewriting the differential into a more useful form:

$$C = \frac{\partial U}{\partial T} = \hbar\omega \frac{\partial n}{\partial T}$$

2 Probability Distributions

We are able to write the probability to find the system in a state with N particles, and energy ϵ :

$$P(N, \epsilon) \propto e^{\frac{N\mu - \epsilon}{k_B T}}$$

This comes from Taylor expanding g . To normalise this probability, we must sum over all particle occupancies in all energy states, to give the grand partition function:

$$\mathcal{Z} = \sum_N \sum_{\epsilon} e^{\frac{N\mu - \epsilon}{k_B T}}$$

Hence, giving us the Gibbs probability distribution:

$$P(N, \epsilon) = \frac{e^{\frac{N\mu - \epsilon}{k_B T}}}{\mathcal{Z}} \equiv p_i \quad (2.1)$$

So, using the probability function, we are able to compute the average value of a quantity x :

$$\langle x \rangle = \sum_i p_i x_i$$

Notice, in \mathcal{Z} , we have an expression for $N\mu$. This is present as it is assumed not to be constant. If the particle number of the system is constant, we end up with the partition function:

$$Z = \sum_{\epsilon} e^{-\frac{\epsilon}{k_B T}}$$

With p_i changing accordingly, and being known as the Maxwell-Boltzmann distribution.

3 Identical Particles

Bosons have symmetric wavefunctions;

Fermions have anti-symmetric wavefunctions. One consequence of the anti-symmetry is that no two identical fermions may be in the same state.

We are able to go from the above general probability distributions, to writing the average number of particles in a particular energy state $\langle n(\epsilon) \rangle$. These expressions are different for fermions and bosons:

3.1 Fermi-Dirac Distribution

We can only sum for there being zero or one particle in each energy state:

$$\langle n(\epsilon) \rangle_{FD} = \sum_{i=0,1} n_i p_i \quad (3.1)$$

$$= \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1} \quad (3.2)$$

3.2 Bose-Einstein Distribution

We can sum for there being any number of particles in a given energy state:

$$\langle n(\epsilon) \rangle_{BE} = \sum_{i=0}^{\infty} n_i p_i \quad (3.3)$$

$$= \frac{1}{e^{(\epsilon-\mu)/k_B T} - 1} \quad (3.4)$$

3.3 Spin Corrections

If the particle is spin s , then the particle distributions are modified thus:

$$\langle n(\epsilon) \rangle = \frac{2s + 1}{e^{(\epsilon-\mu)/k_B T} \pm 1} \quad (3.5)$$

4 Classical Limit

In the classical limit, we say that the average particle occupancy of a given state is very much less than one: $\langle n \rangle \ll 1$. Hence, from just looking at the equations, we are able to write:

$$\langle n(\epsilon_i) \rangle \approx e^{(\mu-\epsilon_i)/k_B T} \equiv n_i$$

We can compute $\langle N \rangle \equiv N$, the mean number of particle in the system, by summing over all possibilities for probabilities of there being particles in a particular energy state:

$$\begin{aligned} N &= \sum_i n_i \\ &= e^{\mu/k_B T} \left(\frac{1}{2} \sqrt{\frac{2mL^2 k_B T}{\hbar^2 \pi}} \right)^3 \end{aligned}$$

From which we can get the following expression for the chemical potential:

$$\mu = k_B T \ln \frac{n}{n_Q} \quad (4.1)$$

Where we have defined the number density n and quantum density n_Q :

$$n = \frac{N}{L^3} \quad (4.2)$$

$$n_Q = \left(\frac{mk_B T}{2\pi\hbar^2} \right)^{3/2} \quad (4.3)$$

The quantum density n_Q has the interpretation as being the density of particles at which they occupy boxes the size of their de Broglie wavelength.

This is modified if there is spin, via:

$$\mu = k_B T \ln \frac{n}{(2s+1)n_Q}$$

If there are internal quantum numbers (e.g. orbital angular momentum):

$$\mu = k_B T \ln \frac{n}{Z_{int} n_Q}$$

We are able to write down the average internal energy of the system and heat capacity:

$$U = \sum n_i \epsilon_i = \frac{3}{2} N k_B T$$

$$C = \frac{\partial U}{\partial T} = \frac{3}{2} N k_B$$

Hence, we have calculated the classical internal energy and heat capacity, via quantum mechanical ideas of identical particles and quantised energy states.

The general expression for the entropy of a system, described by some probability distribution function p_i is given by:

$$S = -k_B \sum_i p_i \ln p_i$$

If we do this, in the classical limit, we end up with the Sackur-Tetrode equation:

$$S = N k_B \left(\frac{5}{2} + \ln \frac{n_Q}{n} \right)$$

From which we can compute the equation of state $pV = Nk_B T$ and $C_p = \frac{5}{2} N k_B T$.

5 Fermi Gases

We say that quantum effects are important for $n \geq n_Q$.

Considering a Fermi gas at $T = 0$, we use the step function approximation of the average particle occupancy: all particles are in the states $\epsilon < \epsilon_F$, and are nowhere else. Thus, the system is in its ground state when all of the lowest possible energy states are full, and none above. From the previous expression for $\langle n \rangle_{FD}$, we have that the Fermi energy ϵ_F is the value of the chemical potential μ at $T = 0$.

For non-relativistic particles, we have the general expression for the link between wavevector k and energy ϵ , where we use Fermi-values:

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} \quad (5.1)$$

And, for ultra-relativistic particles we have:

$$\epsilon_F = p_{FC} = \hbar c k_F \quad (5.2)$$

We define the Fermi temperature thus:

$$\epsilon_F = T_F k_B \quad (5.3)$$

5.1 Density of States

In 3D, we want to compute the number of states residing in the positive annulus $k \rightarrow k + dk$. We can find this by finding the volume of the annulus $\frac{1}{8}4\pi k^2 dk$ and divide by the volume taken up by a single state $(\frac{\pi}{L})^3$. Hence, for spinless particles:

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

Hence, we define the density of states:

$$\frac{dn}{dk} = \frac{k^2 L^3}{2\pi^2} \quad (5.4)$$

If the particles have a spin s , then this needs to be multiplied by the spin multiplicity factor:

$$\frac{dn}{dk} = (2s + 1) \frac{k^2 L^3}{2\pi^2}$$

Now, we can compute the number of particles under the Fermi wavevector k_F :

$$N = \int_0^\infty dn \langle n \rangle = \int_0^{k_F} \frac{dn}{dk} dk = \frac{k_F^3 L^3}{6\pi^2}$$

Resulting in $k_F = (6\pi^2 n)^{1/3}$. Hence, we can write down the Fermi energy for spinless particles:

$$\epsilon_F = \frac{\hbar^2}{2m} (6\pi^2 n)^{2/3}$$

This has been done for $T = 0$; thus $\langle n \rangle = 1$ for $k < k_F$ and zero above. To compute N generally, or indeed compute the average value of any quantity of the system as a whole:

$$X = \int_0^\infty \frac{dn}{dk} \langle n \rangle x dk$$

Or, if the average value of a quantity, of a single particle, is wanted:

$$Y = \frac{1}{N} \int_0^\infty \frac{dn}{dk} \langle n \rangle y dk$$

To compute the average energy of the system, it is easier to redefine the density of states to be in energy-space, as opposed to k -space:

$$U = \int_0^\infty \frac{dn}{d\epsilon} \langle n \rangle \epsilon d\epsilon$$

These integrals, in general, are very hard to do, and we will always be given the integral.

To compute the average velocity of a particle, we write:

$$V = \frac{1}{N} \int_0^\infty \frac{dn}{dk} \langle n \rangle v dk$$

Where we get v from $\epsilon = \frac{\hbar^2 k^2}{2m} = \frac{1}{2} m v^2$. Hence $v = \frac{\hbar k}{m}$.

To compute the variance in a quantity, we need only compute:

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$$

To find the equation of state of a fermi gas, we need to initially compute U , then via $dU = TdS - pdV$ at $T = 0$, we have $p = -\frac{dU}{dV} = \frac{2}{5} n \epsilon_F$.

Now, at $T = 0$, we find that U is independent of T . Hence, $C = \frac{\partial U}{\partial T} = 0$. So, to find the heat capacity, we must do some sort of low-temperature corrections. We do this estimate by saying that particles within $k_B T$ of ϵ_F move. Hence, the fraction of particles which are excited is $\frac{k_B T}{\epsilon_F} N$. Hence, additional energy is of the order $\frac{k_B T}{\epsilon_F} N k_B T$. Hence:

$$U = \frac{3}{5} N \epsilon_F + \alpha \frac{(k_B T)^2}{\epsilon_F} N$$

For low temperature, particle distributions look like a crumbling cliff-face. The examples we have considered are electrons in metals and white dwarfs.

6 Bose Gases

Recall:

$$\langle n \rangle_{BE} = \frac{1}{e^{(\epsilon - \mu)/k_B T} - 1} \tag{6.1}$$

If N is fixed, μ rises as T drops. But, for physical systems, $\mu \leq 0$; if we have defined $\epsilon_0 = 0$. So, at some $T = T_c$, we have that $\mu = 0$ is a really good approximation:

$$N \equiv \int_0^\infty \frac{dn}{d\epsilon} \frac{1}{e^{\epsilon/k_B T_c} - 1} d\epsilon$$

From this, we are able to calculate T_c . Now, we have for $T < T_c$, a modified BE distribution:

$$\langle n \rangle = \frac{1}{e^{\epsilon/k_B T} - 1}$$

So that we now have:

$$N = N_0 + \int_0^\infty \frac{dn}{d\epsilon} \langle n \rangle d\epsilon$$

Putting all this together, allows us to write the fraction of particles in the ground state, at temperatures close to the critical:

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

Formulated for non-relativistic bosons. We are able to end up showing that $N_0 \approx N$, for $T < T_c$; where we have macroscopic occupation of the ground state. This leads into the condition that $n < n_Q$. Hence, we see that for a bose gas, when quantum effects become important, all particles jump into the ground state.

6.1 Blackbody Radiation

This is for a gas of photons in thermal equilibrium. We can find that $\mu = 0$, as the number of particles in the system is not constant. We can calculate the energy U , and hence energy density $\frac{U}{V}$ of the gas:

$$\frac{U}{V} = \int_0^\infty 2 \frac{dn}{d\epsilon} \langle n \rangle \frac{1}{V} \epsilon d\epsilon$$

Where the 2 comes from there being 2 polarisation states: a multiplicity factor. Where:

$$\langle n \rangle = \frac{1}{e^{\epsilon/k_B T} - 1}$$

We can compute the power radiated per unit area by such a body:

$$P = \frac{1}{4} c \frac{U}{V}$$

Which will lead us to Stefan's Law: $P = \sigma T^4$. We can then find out how this energy is distributed over wavelengths.

We say that $u(\lambda)d\lambda$ is the energy per unit volume, in the range $\lambda \rightarrow \lambda + d\lambda$. That is:

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

Which we can compare to a previous expression, to leave us with:

$$u(\lambda)d\lambda = 2 \frac{dn}{d\epsilon} \langle n \rangle \frac{1}{V} \epsilon d\epsilon$$

This is solved, to find Planck's distribution curve; using $\epsilon = \hbar\omega = \frac{hc}{\lambda}$. We find that the wavelength which has maximum power is just determined by the temperature of the blackbody. To find the pressure exerted by such a body, we calculate S , then use:

$$p = T \left(\frac{\partial S}{\partial V} \right)_U$$

Being careful about making $S(V)$. We find $p = \frac{1}{3} \frac{U}{V}$. In adiabatic expansion, $dS = 0$.