

Simple applications of 2<sup>nd</sup>  
quantization

Simple applications of Law

of Newton's

## Ground - states of non - interacting systems

Consider a gas of Bosons in a box. The Hamiltonian will be

$$\mathcal{H} = \sum_{\mathbf{k}} E_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \quad (1)$$

where

$$E_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} \quad k_i = \frac{2\pi l_i}{L}, \quad l_i = 0, \pm 1, \pm 2, \dots \quad (2)$$

The eigenstates of (1) are the Fock states

$$|\vec{m}\rangle = |m_1, m_2, \dots, m_{\mathbf{k}}, \dots\rangle \quad (3)$$

with corresponding energies

$$\mathcal{E}(\vec{m}) = \sum_{\mathbf{k}} E_{\mathbf{k}} m_{\mathbf{k}} \quad (4)$$

The ground state is the configuration with the smallest possible energy. Thus, if we have  $N$  particles, the ground-state will be simply the Fock space with  $N$  particles in the  $\mathbf{k}=0$  state. We can construct this state from the vacuum as

$$|gs\rangle = \frac{(a_0^{\dagger})^N}{\sqrt{N!}} |0\rangle \quad (5)$$

where  $1/\sqrt{N!}$  is just a normalization factor.

Now let's see how to construct the ground-state of a Fermion system or, more specifically, the electron gas. In this case we should include spin and write

$$\mathcal{H} = \sum_{\mathbf{k}, \sigma} E_{\mathbf{k}} a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} \quad (6)$$

where  $\sigma = \pm 1$ . Now the  $a_{\mathbf{k}\sigma}$  are Fermion operators, so the occupation numbers will be  $n_{\mathbf{k}\sigma} = 0, 1$ . The ground-state will then be the Fermi sphere, where we fill all states up to the Fermi momentum

$$k_F = (3\pi^2 N/V)^{1/3} \quad (7)$$

(which was discussed in a previous set of notes). The ground-state may then be written as

$$\begin{aligned} |gs\rangle = |F\rangle &= \left[ \prod_{\mathbf{k}}^{k < k_F} a_{\mathbf{k}\uparrow}^{\dagger} a_{\mathbf{k}\downarrow}^{\dagger} \right] |0\rangle \\ &= | \text{"all states up to } k_F \text{ occupied"} \rangle \end{aligned} \quad (8)$$

this is the Fermi state. Note that we have a sign ambiguity related to the order with which we create the Fermions. This ambiguity is not a problem, but you must be consistent with your calculations.

## The tight-binding model

Recall that, given an arbitrary single-particle operator  $A$ , its second quantized version is

$$A = \sum_{ij} \langle i|A|j \rangle a_i^\dagger a_j \quad (9)$$

consider then the tight-binding Hamiltonian

$$H = - \sum_{m,m'} g(x_m - x_{m'}) |m\rangle \langle m'| \quad (10)$$

Then  $\langle m|H|m \rangle = -g(x_m - x_m)$ . Thus, we may write

$$\mathcal{H} = - \sum_{m,m'} g(x_m - x_{m'}) a_m^\dagger a_{m'} \quad (11)$$

which is the way we write the tight-binding model in 2<sup>nd</sup> quantization. Now the operator  $a_m^\dagger$  creates an electron at site  $m$ . If we have additional degrees of freedom  $\alpha$ , like spin, other orbitals or multiple atoms per unit cell, then the operators become  $a_{m,\alpha}^\dagger$ .

The diagonalization of a tight-binding Hamiltonian can be done in 1<sup>st</sup> or 2<sup>nd</sup> quantization. It does not matter.

Recall that in first quantization we write

$$|m\rangle = \frac{1}{\sqrt{N}} \sum_k e^{ikx_m} |k\rangle \quad (12)$$

But creation operators transform like kets so, in 2<sup>nd</sup> quantization, we use instead

$$a_m^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ikx_m} a_k \quad (13)$$

If we substitute this in Eq (11) we will get

$$\mathcal{H} = \sum_k E_k a_k^\dagger a_k \quad (14)$$

where

$$\begin{aligned} E_k &= - \sum_n g(x_n) e^{ikx_n} \\ &= -2g \cos ka \quad (\text{for nearest neighbor}) \end{aligned} \quad (15)$$

The procedure is identical to the one we did in 1<sup>st</sup> quantization.

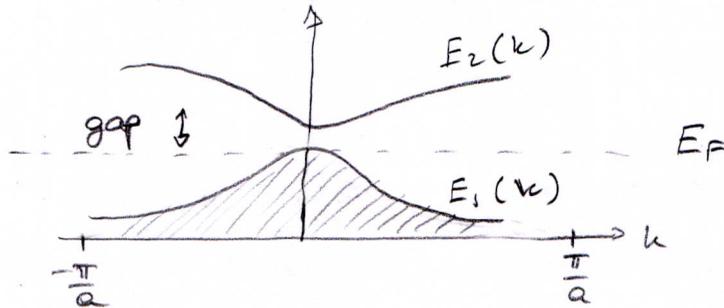
Another thing you should bear in mind is that transformations like (13) preserve the algebra

$$\{a_m, a_m^\dagger\} = \delta_{mm} \quad \mapsto \quad \{a_k, a_k^\dagger\} = \delta_{kk} \quad (16)$$

this is true for any unitary transformation.

## Electrons and holes

Suppose we have a semiconductor, with 2 bands like this:



The Hamiltonian may be written as (I'm ignoring spin)

$$H = \sum_{k, \lambda} E_{\lambda}(k) a_{k\lambda}^{\dagger} a_{k\lambda} \quad (17)$$

where  $\lambda = 1, 2$  distinguishes the 2 bands. We also assume that the first band is completely filled. Thus the ground state will be

$$|F\rangle = \left[ \prod_k a_{k,1}^{\dagger} \right] |0\rangle \quad (18)$$

Now comes a naughty idea: we define

$$c_k^{\dagger} = a_{k,2}^{\dagger} = \text{operator, which creates an electron in the conduction band } (\lambda=2)$$

(19)

But for the valence band, we define the annihilation of an electron as the creation of a hole:

$$b_k^\dagger = a_{k,1} = \text{operator that creates a hole in the valence band } (\lambda=1) \quad (20)$$

↑  
no dagger!

Instead of talking about electrons in 2 bands, we say the conduction band is inhabited by electrons, but the valence band is inhabited by holes.

Note that

$$c_k |F\rangle = 0 \quad (\text{because all states in } \lambda=2 \text{ are already empty})$$

$$b_k |F\rangle = 0 \quad (\text{because all states in } \lambda=1 \text{ are filled})$$

thus, the Fermi state functions like an effective vacuum " $|0\rangle$ " for both electrons and holes. This is the Fermi sea.

Now we can write the Hamiltonian (17) as

$$\mathcal{H} = \sum_{\mathbf{k}} E_1(\mathbf{k}) b_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} + \sum_{\mathbf{k}} E_2(\mathbf{k}) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}$$

In the first term we use the anti-commutation relation

$$\{b_{\mathbf{k}}, b_{\mathbf{k}}^{\dagger}\} = 1 \quad \text{implies} \quad b_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} = 1 - b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}$$

we then get

$$\mathcal{H} = \sum_{\mathbf{k}} E_1(\mathbf{k}) [1 - b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}] + \sum_{\mathbf{k}} E_2(\mathbf{k}) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}$$

But  $\sum_{\mathbf{k}} E_1(\mathbf{k}) = E_{gs}$ , is the ground-state energy. Thus

$$\mathcal{H} = E_{gs} - \sum_{\mathbf{k}} E_1(\mathbf{k}) b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \sum_{\mathbf{k}} E_2(\mathbf{k}) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \quad (20)$$

thus, the holes are particles with negative energy.

Similarly

$$\begin{aligned} \hat{N} &= \sum_{\mathbf{k}, \lambda} a_{\mathbf{k}\lambda}^{\dagger} a_{\mathbf{k}\lambda} = \sum_{\mathbf{k}} b_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} + \sum_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \\ &= \sum_{\mathbf{k}} (1 - b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}) + \sum_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \end{aligned}$$

or

$$\hat{N} = N - \sum_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \sum_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \quad (21)$$

The holes therefore count as negative particles. In this sense, the holes are therefore the "anti-particles" of the electrons.

In fact, if electrons and holes meet, they annihilate and release energy as a photon. This is how a LED works.

Similarly, an incident photon may create an electron-hole pair. This is the idea of a solar panel.

These processes are described in 2<sup>nd</sup> quantization by terms like

$$M_{k,k',q} (c_{k'}^{\dagger} b_{k'}^{\dagger} \alpha_q + \alpha_q^{\dagger} b_{k'} c_k)$$

where  $\alpha_q^{\dagger}$  creates a photon with momentum  $q$  and  $M_{k,k',q}$  are the amplitudes for each process to occur. To make good solar panels and LEDs, we must therefore optimize the  $M_{k,k',q}$ . For instance, we want to build devices where this amplitude is a maximum for  $k+k'=q$ . If this is not true then part of the photon momentum will be dissipated, making our device less efficient.

## Finite temperatures and the grand canonical ensemble

Now let's talk about finite temperatures. In this case the state of the system is described by a density matrix  $\rho$  (see my PDF notes). If the system is in thermal equilibrium, the density matrix will be given by the

Gibbs state

$$\rho = \frac{e^{-\beta \mathcal{H}}}{Z} \quad (22)$$

where

$$Z = \text{tr} (e^{-\beta \mathcal{H}}) \quad (23)$$

is the partition function. To compute  $Z$  we need a sum over all states of the system. In this case, these are the Fock states

$$Z = \sum_{m_1, m_2, \dots} \langle m_1, m_2, \dots | e^{-\beta \mathcal{H}} | m_1, m_2, \dots \rangle \quad (24)$$

where the sum is over each  $m_i$ , either taking the values  $0, 1, 2, \dots$  (for Bosons) or  $0, 1$  (for Fermions).

For certain systems, like photons, phonons, magnons, etc., the number of particles is free to fluctuate, we may then compute the sums in (24) with no difficulty. However, if we are talking about electrons or atoms, the number of particles is fixed at some value  $N$ . Thus, when computing the sum (24) we need to include only those terms for which  $\sum_{\alpha} m_{\alpha} = N$ . The correct way to write (24) would then be

$$Z = \sum_{m_1, m_2, \dots} \langle m_1, m_2, \dots | e^{-\beta H} | m_1, m_2, \dots \rangle \delta\left(\sum_{\alpha} m_{\alpha} = N\right) \quad (25)$$

where  $\delta(a=b)$  is the Kronecker  $\delta$ .

Computing a sum like this, in practice, is an extremely difficult task.

Lucky for us, we can take on a different approach. Instead of working with a fixed number of particles, we allow it to fluctuate, but impose that  $\langle \hat{N} \rangle = N$ . Thus, we work with systems which only have, an average  $N$  particles. When  $N$  is large, the fluctuations become unimportant, so fixing  $\hat{N}$  an average becomes a very good approximation.

when we allow the number of particles to fluctuate, we are in the grand canonical ensemble. the way we fix  $\langle \hat{N} \rangle$  is by introducing a Lagrange multiplier  $\mu$ , called the chemical potential, which is to be adjusted in order to fix  $\langle \hat{N} \rangle = N$ . the Lagrange multiplier is introduced by changing

$$\mathcal{H} \rightarrow \mathcal{H} - \mu \hat{N} \quad (26)$$

thus, the Grand canonical Gibbs state will be

$$\rho = \frac{e^{-\beta(\mathcal{H} - \mu \hat{N})}}{\mathcal{Z}} \quad (27)$$

where

$$\mathcal{Z} = \text{tr} (e^{-\beta(\mathcal{H} - \mu \hat{N})}) = \sum_{m_1, m_2, \dots} \langle m_1, m_2, \dots | e^{-\beta(\mathcal{H} - \mu \hat{N})} | m_1, m_2, \dots \rangle \quad (27)$$

This sum is now unrestricted, so each  $m_i$  can run through all its allowed values.

the Hamiltonian always conserves the number of particles so

$$[\mathcal{H}, \hat{N}] = 0 \quad \rightsquigarrow \quad e^{-\beta(\mathcal{H} - \mu \hat{N})} = e^{-\beta \mathcal{H}} e^{\beta \mu \hat{N}}$$

All thermodynamic information can be extracted from  $Z$  or the thermodynamic potential

$$\boxed{\Phi = -T \ln Z} \quad (28)$$

For instance, the average number of particles  $N = \langle \hat{N} \rangle$  is

$$N = - \frac{\partial \Phi}{\partial \mu} \quad (29)$$

the entropy is

$$S = - \frac{\partial \Phi}{\partial T} \quad (30)$$

and the average energy  $U = \langle \mathcal{H} \rangle$  is

$$U = - \frac{\partial}{\partial \beta} \ln Z \quad (31)$$

I borrowed all these formulas from thermodynamics. But you can also demonstrate them directly from (27) and (28). For instance,

$$\begin{aligned} - \frac{\partial \Phi}{\partial \mu} &= \frac{\partial}{\partial \mu} [T \ln Z] = T \frac{1}{Z} \frac{\partial Z}{\partial \mu} = \frac{T}{Z} \frac{\partial}{\partial \mu} \text{tr} \{ e^{-\beta \mathcal{H}} e^{\beta \mu \hat{N}} \} \\ &= \frac{1}{Z} \text{tr} \{ \hat{N} e^{-\beta \mathcal{H}} e^{\beta \mu \hat{N}} \} \\ &= \text{tr} \{ \hat{N} \rho \} = \langle \hat{N} \rangle \end{aligned}$$

which is (29)

## Example: the free electron gas

the free electron gas has

$$\mathcal{H} - \mu \hat{N} = \sum_{k, \sigma} (E_{k\sigma} - \mu) a_{k\sigma}^\dagger a_{k\sigma} \quad (32)$$

This Hamiltonian is diagonal so

$$\begin{aligned} \langle \vec{n} | e^{-\beta(\mathcal{H} - \mu \hat{N})} | \vec{n} \rangle &= \prod_{k, \sigma} \langle m_{k\sigma} | e^{-\beta(E_{k\sigma} - \mu) a_{k\sigma}^\dagger a_{k\sigma}} | m_{k\sigma} \rangle \\ &= \prod_{k, \sigma} e^{-\beta(E_{k\sigma} - \mu) m_{k\sigma}} \end{aligned}$$

thus, the partition function factors as

$$\begin{aligned} Z &= \prod_{k, \sigma} \sum_{m_{k\sigma}=0,1} e^{-\beta(E_{k\sigma} - \mu) m_{k\sigma}} \\ \therefore Z &= \prod_{k, \sigma} \{ 1 + e^{-\beta(E_{k\sigma} - \mu)} \} \quad (33) \end{aligned}$$

the thermodynamic potential will then be a sum

$$\Phi = -T \sum_{k, \sigma} \ln \{ 1 + e^{-\beta(E_{k\sigma} - \mu)} \} \quad (34)$$

We may now compute the average number of particles

$$N = \langle \hat{N} \rangle = - \frac{\partial \Phi}{\partial \mu} = T \sum_{\mathbf{k}, \sigma} \frac{\beta e^{-\beta(E_{\mathbf{k}} - \mu)}}{1 + e^{-\beta(E_{\mathbf{k}} - \mu)}}$$

or

$$N = \sum_{\mathbf{k}, \sigma} \frac{1}{e^{\beta(E_{\mathbf{k}} - \mu)} + 1} \quad (35)$$

From this formula we may readily recognize

$$\bar{n}_{\mathbf{k}\sigma} = \langle a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} \rangle = \frac{1}{e^{\beta(E_{\mathbf{k}} - \mu)} + 1} \quad (36)$$

which is the Fermi-Dirac distribution [If you want you can also compute  $\bar{n}_{\mathbf{k}\sigma}$  as  $\text{tr}\{a_{\mathbf{k}\sigma}^{\dagger} a_{\mathbf{k}\sigma} \rho\}$ ].

We may also convert the sum in (35) into an integral by introducing the density of states

$$D(E) = \frac{3}{2} \frac{N}{E_F^{3/2}} \sqrt{E} \quad (37)$$

where

$$E_F = \frac{k_F^2}{2m} = \frac{(3\pi^2 N/V)^{2/3}}{2m} \quad (38)$$

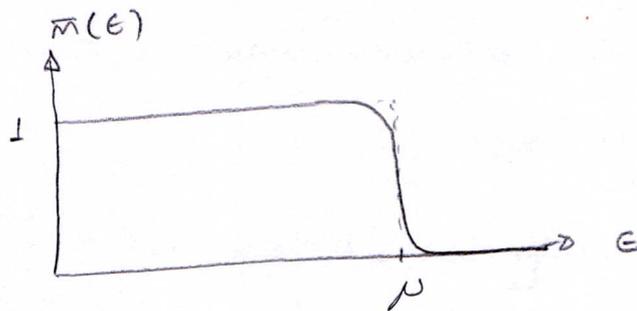
we then get

$$N = \sum_{n,\sigma} \bar{n}_{n,\sigma} = \int_0^{\infty} d\epsilon D(\epsilon) \bar{n}(\epsilon) \quad (39)$$

where

$$\bar{n}(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \quad (40)$$

this function looks like this



It is almost a Heaviside function, except in the vicinity of  $\epsilon = \mu$ .

From looking at this function we see that, at  $T=0$ , the chemical potential will be exactly the Fermi energy  $E_F$ :

$$\mu = E_F \quad (T=0) \quad (41)$$

[Recall that  $E_F$  is such that everything below is occupied and everything above is empty. That is exactly what the figure above looks like]. Thus

$$\bar{n}(\epsilon) = \Theta(\mu - \epsilon) \quad (T=0) \quad (42)$$

For  $T \neq 0$ ,  $\mu$  will differ from  $E_F$ . To find out how, we must solve Eq (39) for  $\mu(N, T)$ . That is in general a difficult task. But for Fermions, the scale of temperature is determined by

$$T_F = \frac{E_F}{k_B} \sim 10^4 - 10^5 \text{ K}$$

thus, for Fermions any reasonable temperature, like  $T = 300 \text{ K}$ , is already a very low temperature. Thus, all finite temperature calculations may be done approximately with great accuracy.

In doing so, the only result we need is the Sommerfeld expansion

$$\int_{-\infty}^{\infty} d\epsilon f(\epsilon) \bar{n}(\epsilon) = \int_{-\infty}^{\mu} d\epsilon f(\epsilon) + \frac{\pi^2}{6} \frac{f'(\mu)}{\beta^2} + \mathcal{O}\left(\frac{1}{\beta\mu}\right)^4 \quad (43)$$

where  $f(\epsilon)$  is an arbitrary function.

Let's see how to use this. we start with (39) so  $f = D$ .

then

$$\begin{aligned} N &= \int_0^{\mu} dE D(E) + \frac{\pi^2 T^2}{6} D'(\mu) \\ &= \frac{3}{2} \frac{N}{E_F^{3/2}} \frac{2}{3} \mu^{3/2} + \frac{\pi^2 T^2}{6} \frac{3}{2} \frac{N}{E_F^{3/2}} \frac{1}{2\sqrt{\mu}} \\ &= N \left\{ \left( \frac{\mu}{E_F} \right)^{3/2} + \frac{\pi^2 T^2}{8} \frac{1}{E_F^{3/2} \sqrt{\mu}} \right\} \end{aligned}$$

thus

$$\mu^{3/2} + \frac{\pi^2 T^2}{8} \frac{1}{\sqrt{\mu}} = E_F^{3/2}$$

we can now solve this equation for  $\mu$ . the solution only needs to be approximate, of order  $T^2$ . It will be

$$\mu \approx E_F - \frac{\pi^2 T^2}{12 E_F} \quad (44)$$

thus,  $T$  lowers  $\mu$  by a factor of order  $T^2/E_F$ .

Now we can do the same for the average energy

$$U = \sum_{k, \sigma} E_{k\sigma} \bar{n}_{k\sigma} = \int_0^{\infty} d\epsilon \epsilon D(\epsilon) \bar{n}(\epsilon) \quad (45)$$

So now we apply (43) with  $f(\epsilon) = \epsilon D(\epsilon)$ . The result will depend on  $\mu$  but we can then use (44) to eliminate it. I will skip the details. The result is

$$\frac{U}{N} = \frac{3}{5} \epsilon_F + \frac{\pi^2 T^2}{4 \epsilon_F} \quad (46)$$

From the energy we may now compute the specific heat

$$C = \frac{1}{N} \frac{\partial U}{\partial T} = \gamma T \quad (47)$$

where  $\gamma = \pi^2/2 \epsilon_F$ . Thus, the specific heat of the electrons is linear in  $T$  and the coefficient is proportional to  $\epsilon_F$ .

This is a popular way of inferring  $\epsilon_F$  from experiment. This  $\gamma$  is called the Sommerfeld coefficient.

A slightly more general calculation gives

$$\gamma = \frac{\pi^2 k_B^2}{3} \frac{D(\epsilon_F)}{N} \quad (48)$$

This formula is useful because it depends on a general density of states, which may be different from (37) [I also plugged  $k_B$  back for future reference].

## Example: Bose - Einstein condensation

Consider now a gas of Bosons. In this case

$$\hat{H} - \mu \hat{N} = \sum_n (E_n - \mu) a_n^\dagger a_n \quad (49)$$

so, similarly to Eq (33), we get

$$Z = \prod_n \sum_{m_n=0}^{\infty} e^{-\beta(E_n - \mu)m_n} \quad (50)$$

the sum is now for  $m_n = 0, 1, 2, 3, \dots$ . Let  $x = e^{-\beta(E_n - \mu)}$ .

then

$$\sum_{m_n=0}^{\infty} e^{-\beta(E_n - \mu)m_n} = \sum_{m_n=0}^{\infty} x^{m_n} = \frac{1}{1-x}$$

thus

$$Z = \prod_n \frac{1}{1 - e^{-\beta(E_n - \mu)}} \quad (51)$$

the thermodynamic potential will then be

$$\Phi = T \sum_n \ln(1 - e^{-\beta(E_n - \mu)}) \quad (52)$$

The average number of particles will then be

$$N = - \frac{\partial \Phi}{\partial \mu} = T \sum_{\mu} \frac{(-1)^{\beta} e^{-\beta(E_{\mu} - \mu)}}{1 - e^{-\beta(E_{\mu} - \mu)}}$$

or

$$N = \sum_{\mu} \frac{1}{e^{\beta(E_{\mu} - \mu)} - 1} \quad (53)$$

thus, we readily recognize the average boson occupation

$$\bar{n}_{\mu} = \langle a_{\mu}^{\dagger} a_{\mu} \rangle = \frac{1}{e^{\beta(E_{\mu} - \mu)} - 1} \quad (54)$$

which is called the Bose-Einstein distribution.

If we are talking about a system where the number of particles is not fixed, this same formula still holds, but with  $\mu = 0$ .

We must, of course, always have  $\bar{n}_{\mu} \geq 0$  since this is an occupation number. Since this must be true for all  $\mu$ , it follows that

$$\mu \leq 0 \quad (55)$$

More generally, if we have a different dispersion relation, then the correct statement is

$$\mu \leq \min(E_{1n}) \quad (56)$$

The actual value of  $\mu$  may be determined from the equation

$$N = \sum_n \bar{n}_n = \int_0^{\infty} D(E) \bar{n}(E) dE \quad (57)$$

where, now  $D(E)$  is half of the result (37) since we don't have spin. I will write the result more explicitly as

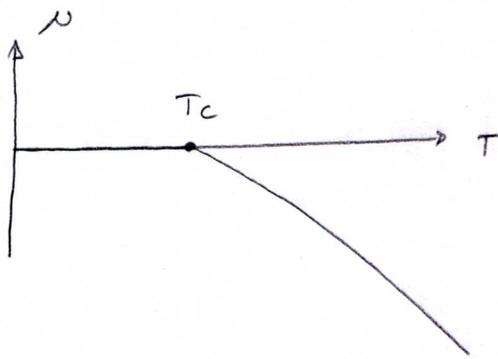
$$D(E) = \frac{V}{4\pi^2} (2m)^{3/2} \sqrt{E} \quad (58)$$

We then get

$$N = \frac{V}{4\pi^2} (2m)^{3/2} \int_0^{\infty} dE \frac{\sqrt{E}}{e^{\beta(E-\mu)} - 1} \quad (59)$$

This equation cannot be solved analytically, but may be done so numerically.

If we solve (59) we will get something like



Recall that  $\mu \leq 0$ . For large  $T$ ,  $\mu$  is very negative. But as we cool down we eventually reach a point  $T_c$  where  $\mu = 0$ . This is the onset of Bose-Einstein condensation

we can determine the critical temperature  $T_c$  by putting  $\mu = 0$  in (59). We then get

$$N = \frac{V}{4\pi^2} (2m)^{3/2} \int_0^{\infty} d\epsilon \frac{\sqrt{\epsilon}}{e^{\beta\epsilon} - 1} \quad x = \beta\epsilon$$

$$= \frac{V}{4\pi^2} (2m)^{3/2} \frac{1}{\beta^{3/2}} \int_0^{\infty} dx \frac{\sqrt{x}}{e^x - 1}$$

the remaining integral is just a number. Thus we conclude that

$$T_c \propto (N/V)^{2/3} \quad (60)$$

what happens below  $T_c$ ? In this region  $\rho$  continues to be zero. what happens is that a macroscopic number of particles begin to accumulate at the state with  $k=0$ . For this reason we need to be careful how we treat Eq (57). when we approximate  $\sum_{k \neq 0} \bar{n}_k$  as an integral, we assume  $\bar{n}_k$  is a smooth function. But for  $T < T_c$  that is no longer true because  $\bar{n}_0$  becomes macroscopically large.

The correct way to treat this is to separate  $N$  as

$$N = \bar{n}_0 + \sum_{k \neq 0} \bar{n}_k$$

Now the last term may be approximated by an integral:

$$N = \bar{n}_0 + \frac{V}{4\pi^2} (2m)^{3/2} \int_0^{\infty} d\epsilon \frac{\sqrt{\epsilon}}{e^{\beta\epsilon} - 1}$$

$$x = \beta\epsilon$$

$$= \bar{n}_0 + \frac{V}{4\pi^2} (2m)^{3/2} \frac{1}{\beta^{3/2}} \int_0^{\infty} dx \frac{\sqrt{x}}{e^x - 1}$$

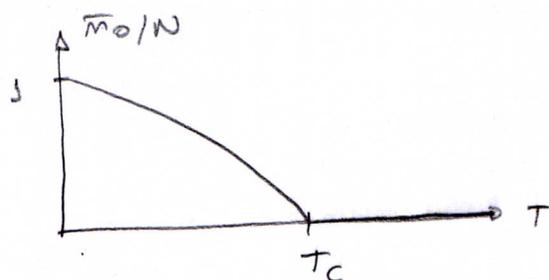
we may write this more neatly as

$$N = \bar{n}_0 + N \left( \frac{T}{T_c} \right)^{3/2}$$

Thus,

$$\boxed{\frac{\bar{m}_0}{N} = J - \left(\frac{T}{T_c}\right)^{3/2}} \quad T < T_c \quad (56)$$

This quantity represents the condensate fraction



It is the fraction of atoms in the  $k=0$  state.

Looking at this, it seems that  $\bar{m}_0$  is the order parameter of this phase transition. But things are a bit more subtle.

The state of the system may be written as

$$\rho = \prod_k \frac{e^{-\beta(E_{1k} - \nu) a_{1k}^\dagger a_{1k}}}{Z_k} \quad (57)$$

But for  $T < T_c$  we get  $\nu = 0$ . Moreover,  $E_0 = 0$ , so the density matrix for the  $k=0$  mode becomes the identity

$$\rho = \mathbb{1}_{k=0} \otimes \prod_{k \neq 0} \frac{e^{-\beta E_{1k} a_{1k}^\dagger a_{1k}}}{Z_k}$$

In general, when dealing with a thermal state

$$\rho = \frac{e^{-\beta \epsilon a^\dagger a}}{Z}$$

we have

$$\langle a^\dagger a \rangle = \bar{n}(\epsilon) \quad \text{but} \quad \langle a \rangle = 0$$

But now, for the  $\kappa = 0$  state, this need not be true. It is therefore possible to have  $\langle a_0 \rangle \neq 0$ . This is the order parameter

$$\text{Order parameter} = \phi = \langle a_0 \rangle$$

(59)

the actual state of the  $\kappa = 0$  mode is undetermined for our model. But there is reason to believe that even a tiny interaction would push the state toward a coherent state

$$\rho_{\kappa=0} = |\phi\rangle\langle\phi|$$

(59)

where  $a|\phi\rangle = \phi|\phi\rangle$ . For a coherent state  $\langle a_0^\dagger a_0 \rangle = |\phi|^2$ . Thus, the condensate occupation  $\bar{n}_0$  is the modulus of the order parameter. But in general,  $\phi$  will be complex. Thus we may write

$$\phi = \bar{n}_0 e^{i\theta}$$

(60)

where  $\theta$  is some phase.

In our model  $S$  is arbitrary. But interactions will cause  $S$  to choose some specific value. This is the spontaneous symmetry breaking. We will learn more about it in the coming lectures.