A. Schekochihin Stat Phys Lectures, Oxford HT-2012

§16. Degenerate Bose gas

16.1 Bose-Einstein Condensation

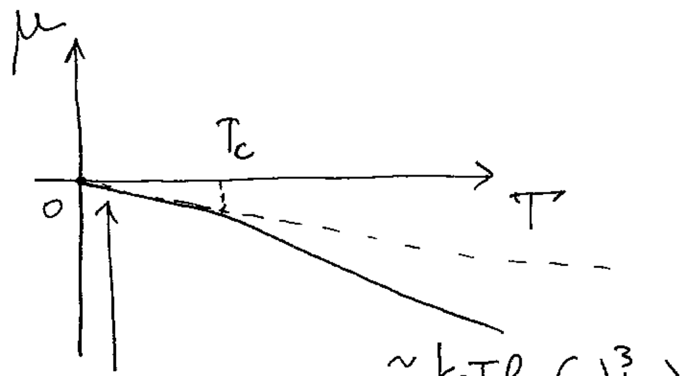
For bosons, we have

$$\boxed{\bar{n}_i = \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1}}$$

and there is no prohibition on multiple particles occupying the same state. Thus, as $T \to 0$ $(\beta \to \infty)$, we expect all the particles to be in the lowest energy state, which we will consider to be $\varepsilon_0 = 0$.
$(\vec{p} = \hbar \vec{k} = 0)$

Thus,
$$\bar{n}_0 = \frac{1}{e^{-\beta\mu} - 1} \to \bar{N} \text{ as } \beta \to \infty$$

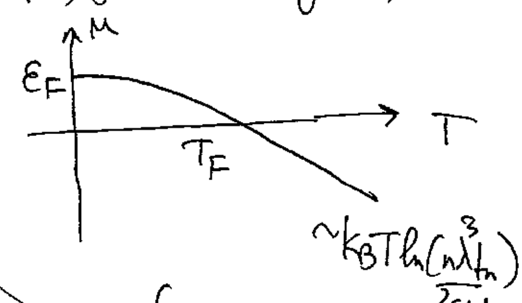
or
$$\mu(T \to 0) \approx -k_B T \ln\left(1 + \frac{1}{\bar{N}}\right) \approx -\frac{k_B T}{\bar{N}} \to 0$$
from below.



$\sim -\frac{k_B T}{\bar{N}}$ degenerate limit (slope very shallow because $\propto \frac{1}{\bar{N}} \ll 1$)

$\sim k_B T \ln\left(\frac{n\lambda_{th}^3}{2s+1}\right)$ classical limit

cf., for Fermi gas,



$\sim k_B T \ln\left(\frac{n\lambda_{th}^3}{2s+1}\right)$

(see p. 139)

NB: Clearly, cannot have $\mu > 0$, otherwise will get $\bar{n}_i < 0$!

Thus, at low temperatures, the lowest-energy state becomes macroscopically occupied – $\bar{n}_0 = \bar{N}$ at $T=0$ and clearly $\bar{n}_0 \sim$ some significant fraction of $\bar{N}$ for temperatures just above zero.

How does this square with our previous calculations in the continuous limit, when we replaced (p.125)

$$\sum_i \to \frac{V(2S+1)}{(2\pi)^3}\int d^3\vec{k} = \frac{V(2S+1)}{2\pi^2}\int_0^\infty dk\,k^2 \underset{k=\frac{\sqrt{2m\varepsilon}}{\hbar}}{=} \frac{(2S+1)Vm^{3/2}}{\sqrt{2}\pi^2\hbar^3}\int_0^\infty d\varepsilon\sqrt{\varepsilon}$$

The $\varepsilon=0$ state actually gives a vanishing contribution to this integral,

! so the continuous approximation of the sum $\sum_i$ was only justified, provided the # of particles in each particular discrete state was small compared to the total N.

This is patently wrong in the limit $T\to 0$, so we have to make special arrangements.

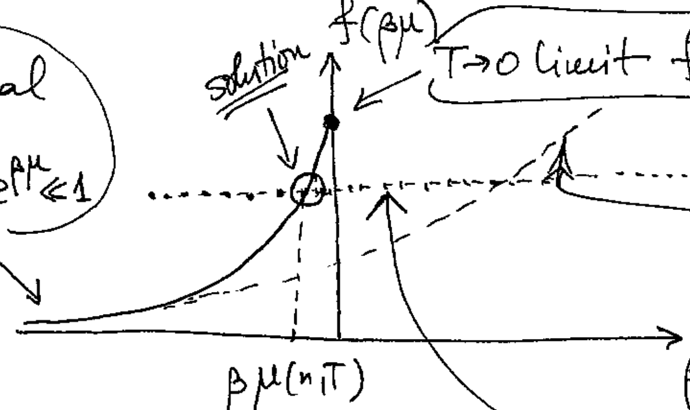
Mathematically, this problem manifests itself in the following way: from (1) (p.126), we are supposed to calculate $\mu(n,T)$ from the equation

$$N = \frac{2(2S+1)}{\sqrt{\pi}}\frac{V}{\lambda_{th}^3}\underbrace{\int_0^\infty \frac{dx\sqrt{x}}{e^{x-\beta\mu}-1}}_{=f(\beta\mu)} \qquad (1)$$

(upon change of variables $x=\beta\varepsilon$)

$$\lambda_{th} = \hbar\sqrt{\frac{2\pi}{mk_BT}}$$

The integral can be calculated – numerically or analytically [see App C.5 of B&B]. Result:



$T \to 0$ limit $f(0) = \int_0^\infty \frac{dx\sqrt{x}}{e^x - 1} = \frac{\sqrt{\pi}}{2} \underbrace{\zeta\left(\tfrac{3}{2}\right)}_{\approx 2.612}$ Riemann zeta fn

classical limit $f \approx \frac{\sqrt{\pi}}{2} e^{\beta\mu} \ll 1$ (see p. 129)

$\frac{\sqrt{\pi}}{2} \frac{n\lambda_{th}^3}{2S+1}$

cf., for Fermi gases, with ⊕,
$f(\beta\mu) \approx \int_0^{x_F} dx\sqrt{x} = \frac{2}{3}(\beta\mu)^{3/2}$
(see p. 135)

To get μ, we must solve

$$f(\beta\mu) = \frac{\sqrt{\pi}}{2} \frac{n\lambda_{th}^3}{2S+1} \propto \frac{n}{T^{3/2}}$$

As we decrease T, the rhs will increase until there is no longer a solution: this happens at $T = T_c$ such that

$$\cancel{\frac{\sqrt{\pi}}{2}} \frac{n\lambda_{th}^3}{2S+1} = f(0) = \int_0^\infty \frac{dx\sqrt{x}}{e^x - 1} = \cancel{\frac{\sqrt{\pi}}{2}} \cdot 2.612$$

$$n\lambda_{th}^3 = 2.612\,(2S+1)$$

or $$\boxed{T_c = \frac{2\pi\hbar^2}{m k_B}\left[\frac{n}{2.612\,(2S+1)}\right]^{2/3}}$$

For $T > T_c$ all is well and we can find $\mu(n,T)$, which will be negative and approaching 0 as $T \to T_c$.

For $T < T_c$, we can just set $\mu = 0$ in (1), but then (1) determines not μ, but rather

The # of particles left in the excited states:

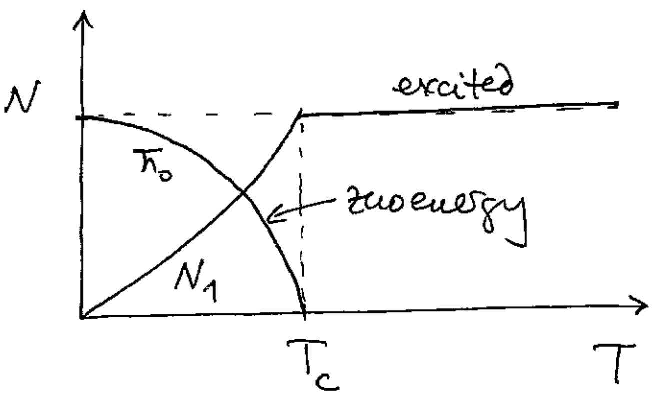
$$N_1 = \frac{2(2S+1)}{\sqrt{\pi}} \frac{V}{\lambda_{th}^3} f(0) = 2.612 \cdot (2S+1) \frac{V}{\lambda_{th}^3} < N$$

because $T<T_c$

The rest of the particles are in the zero-energy state, which the continuous approximation failed to capture. We can calculate how many that is:

Indeed, $$\frac{N_1}{N} = \frac{2.612\,(2S+1)}{n \lambda_{th}^3} = \left(\frac{T}{T_c}\right)^{3/2}$$

So $$\boxed{\frac{\bar{n}_0}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2}}$$



This phenomenon of a macroscopic # of particles collecting in the zero-energy state is called Bose-Einstein condensation (in $\vec{k}$ space!)

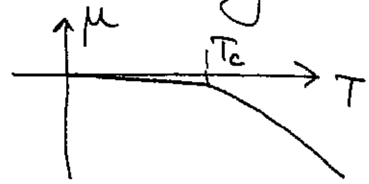
When the system is in this state ($T<T_c$), this is somewhat similar to the situation where the # of particles is not conserved – because particles can always leave the excited population (N_1) and drop into the zero-energy condensate [cf. photon gas – also $\mu=0$!]

Numerically, T_c is same order as the degeneration temperature, $T_c \sim \frac{\hbar^2}{m k_B} n^{2/3} \sim$ a few K under normal conditions (e.g., for ^4He, $T_c \simeq 3K$).

Cornell, Wieman and Ketterle got the 2001 Nobel Prize for experimental observation of the BE condensation.

Notes.

1) As we saw on p. 140, μ is not exactly zero in the condensed state ($T<T_c$), but it is extremely small because $\mu \propto \frac{1}{N} \lll 1$. So:



2) You might ask whether a few states above the lowest-energy one are also macroscopically occupied. This is easy to estimate:

$$\bar{n}_1 = \frac{1}{e^{\beta(\varepsilon_1-\mu)}-1} \quad \text{where} \quad \varepsilon_1 = \frac{\hbar^2 k_{min}^2}{2m}, \quad k_{min} = \frac{2\pi}{L} = \frac{2\pi}{V^{1/3}}$$

size of box

So,

$$\varepsilon_1 = \frac{2\pi^2\hbar^2}{mV^{2/3}} = \frac{2\pi^2\hbar^2 n^{2/3}}{m}\frac{1}{N^{2/3}} \sim \frac{k_BT_c}{N^{2/3}}$$

$$\beta\varepsilon_1 \sim \frac{T_c}{T}\frac{1}{N^{2/3}} \quad \text{whereas} \quad \beta\mu \sim -\frac{1}{N} \ll \beta\varepsilon_1$$

$$\bar{n}_1 \sim \frac{T}{T_c} N^{2/3}$$ – can be quite large ($\gg 1$), but always $\ll \bar{n}_0 \sim N$

So it's ok only to make a special calculation for the condensation into the zero-energy state.

16.2 Thermodynamics of Degenerate Bose Gas

Let's now follow the procedure we always follow and calculate energy, the equ. of state etc.
Since the condensate is in the zero-energy state, it does not contribute to energy and we do not have to worry about discreteness of the sums $\sum_i$.
From (2) (p. 126), we get

$$U = \frac{2(2S+1)}{\sqrt{\pi}} \frac{V}{\lambda_{th}^3} k_B T \underbrace{\int_0^\infty \frac{dx\, x^{3/2}}{e^{x-\beta\mu}-1}}_{\text{as } T<T_c \text{, approximate}}$$

$$\int_0^\infty \frac{dx\, x^{3/2}}{e^x - 1} = \frac{3\sqrt{\pi}}{4} \underbrace{\zeta\left(\frac{5}{2}\right)}_{=1.341}$$

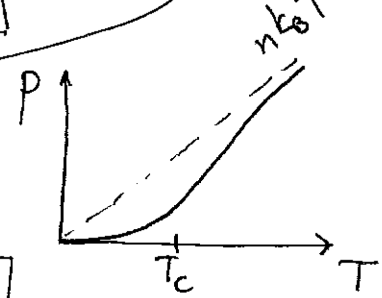
$$\frac{1}{2.612}\left(\frac{T}{T_c}\right)^{3/2} = \frac{(2S+1)}{n\lambda_{th}^3}$$

$$\approx \frac{3}{2} \cdot 1.341 \frac{(2S+1)}{n\lambda_{th}^3} N k_B T \approx 0.128(2S+1) \frac{m^{3/2}(k_B T)^{5/2}}{\hbar^3} V$$

So,

$$\boxed{U = 0.77\, N k_B T_c \left(\frac{T}{T_c}\right)^{5/2}}$$

Equation of state:



$$\Phi = -PV = -\frac{2}{3}U,$$

whence

$$\boxed{p \approx 0.085(2S+1) \frac{m^{3/2}(k_B T)^{5/2}}{\hbar^3}} \propto T^{5/2}$$

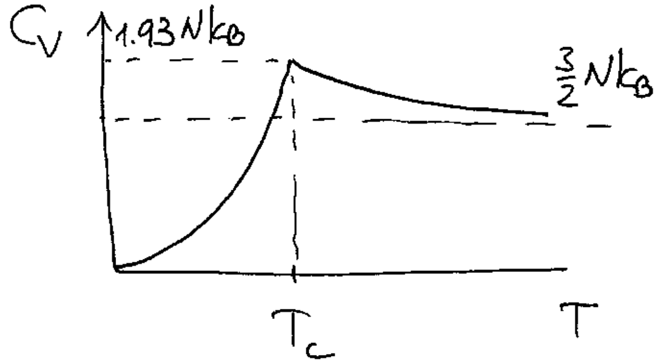
(cf. p. 129)

NB: Pressure is independent of volume (or density)!
This is again because the # of particles with non-zero energy is not conserved, so pressure is a function of T only (cf. photon gas).

Heat capacity:

$$\boxed{C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{5}{2}\frac{U}{T} \approx 1.93\, N k_B \left(\frac{T}{T_c}\right)^{3/2}}$$

Note that $1.93 > \frac{3}{2}$, so C_V will have an interesting shape:



At $T = T_c$, it has a maximum and a discontinuous derivative.

One can calculate the jump in the derivative of C_V at $T = T_c$ by expanding around $T = T_c$ (see LL§62).

The answer is
$$\left(\frac{\partial C_V}{\partial T}\right)_{T=T_c-0} \approx 2.89\, N k_B / T_c$$

$$\left(\frac{\partial C_V}{\partial T}\right)_{T=T_c+0} \approx -0.77\, N k_B / T_c$$

Such is the weird and wonderful quantum world.

Enjoy!

Lecture 7 ended here.