Degenerate Bose-Gas

For bosons, $\quad n_k = \dfrac{1}{e^{\beta(\epsilon_k - \mu)} - 1}$.

At $T=0$, all bosons will pile into $\min(\epsilon_k) \rightarrow k=0$. So $\quad (F = E - TS)$

$$(T=0) \qquad n_0 = N$$

$$n_k = 0 \quad (k \neq 0)$$

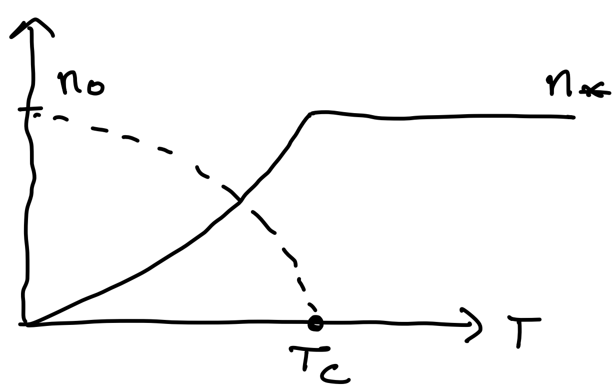
This is a trivial example of "Bose-Einstein" condensate (BEC): all particles in <u>single</u> quantum state! Does it survive to $T>0$?

Writing $\quad N = n_0 + n^*, \quad n^* = \sum_{k \neq 0} n_k$, ~~B.E.C.~~

we say we have a BEC

if $\displaystyle\lim_{V \to 0} n_0/V$ = finite at fixed N/V (or μ)

Remarkably, in 3D this occurs at finite T_c



To proceed, first note we can assume $\mu \leq \min(\epsilon_k)$, otherwise $n_B(\epsilon_k - \mu)$ becomes non-sensical (a more physical understanding will come from looking at limit $\mu \longrightarrow \min(\epsilon_k) - 0^+$: the particle # $N \to \infty$ at fixed V, T.

To start, assume $\mu < \min(\epsilon_k) = 0$ with $\epsilon_k = \dfrac{\hbar^2 k^2}{2m}$ in $D=3$

$$\frac{N}{V} = \int \frac{d^3k}{(2\pi)^3} \frac{\overbrace{1}^{\text{spherically symm.}}}{z^{-1} e^{\beta \epsilon_k} - 1} \qquad z = e^{\beta\mu}$$

Now let $\beta\epsilon_k =: x$ $\quad k = \sqrt{2m/\beta}/\hbar \; x^{1/2} = \dfrac{2\sqrt{\pi}}{\lambda} x^{1/2}$

$$dk = \frac{\sqrt{\pi}}{\lambda} x^{-1/2} dx$$

$$n = 4\pi \int_0^\infty \frac{dk\,k^2}{\underbrace{(2\pi)^3}_{\substack{\text{volume element}\\ \text{after integrating over angles}}}} \frac{1}{z^{-1}e^x - 1} = \frac{1}{\lambda^3} \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2}\,dx}{z^{-1}e^x - 1}$$

Defining $\quad f^{+/-}_m(z) = \dfrac{1}{\Gamma(m)} \displaystyle\int_0^\infty \frac{x^{(m-1)}\,dx}{z^{-1}e^x - 1}$

where $\Gamma(m+1) = m! = \displaystyle\int_0^\infty dx\, x^m e^{-x}$

$$\Gamma(3/2) = \frac{\sqrt{\pi}}{2} = \left(\frac{3}{2} - 1\right)!$$

$$\boxed{\lambda^3 n = f^+_{3/2}(z)} \qquad \frac{2}{\sqrt{\pi}}$$

This gives $n(\mu, \beta) \xleftrightarrow[\text{correspondence}]{} \mu(n, \beta)$

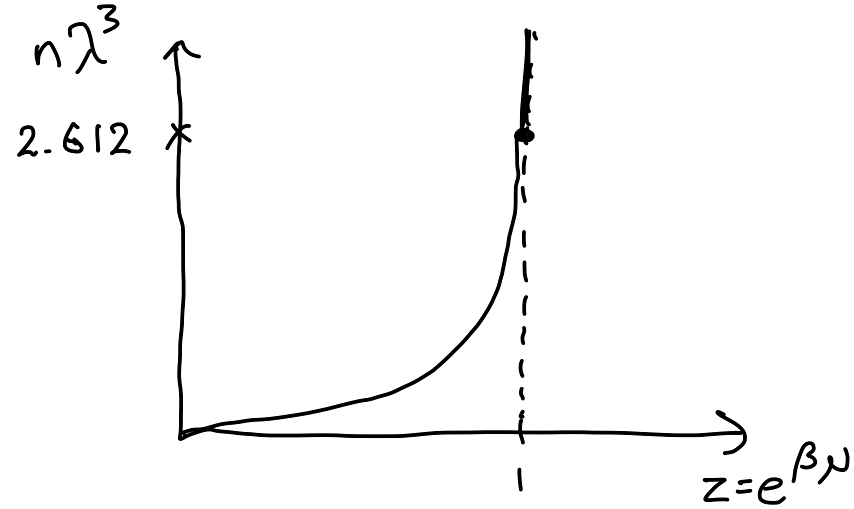
For $\mu < 0 \Rightarrow 0 \le z \le 1$,

$$\lambda n^3 = \overbrace{\frac{1}{(\frac{3}{2}-1)!}}^{\frac{2}{\sqrt{\pi}}} \int_0^\infty \frac{dx\, x^{1/2}}{z^{-1} e^x - 1} \quad \text{is}$$

finite because it is regular at $x \to 0$ and decays as $e^{-x} x^{1/2}$. Right at $z = 1 - 0^+$,

$$\lambda n_x^3 = \overbrace{\frac{1}{(\frac{3}{2}-1)!}}^{2/\sqrt{\pi}} \int_0^\infty \frac{dx\, x^{1/2}}{e^x - 1} \equiv \zeta_{3/2} \simeq 2.612$$

This is finite since $\displaystyle\int_0^X \frac{dx\, x^{1/2}}{(1+x+\dots)-1} \overset{\le}{=} \int_0^X dx\, x^{-1/2} \sim X^{1/2}$



The grand-canonical formalism then breaks down for $\mu > 0$ (in reality, interactions between particle lead to μ-behaviour which well-defined for all μ)

work done on system

$dE = dQ + dW$; $dW = \mu \cdot dN \Rightarrow dQ = dE - \mu\, dN$

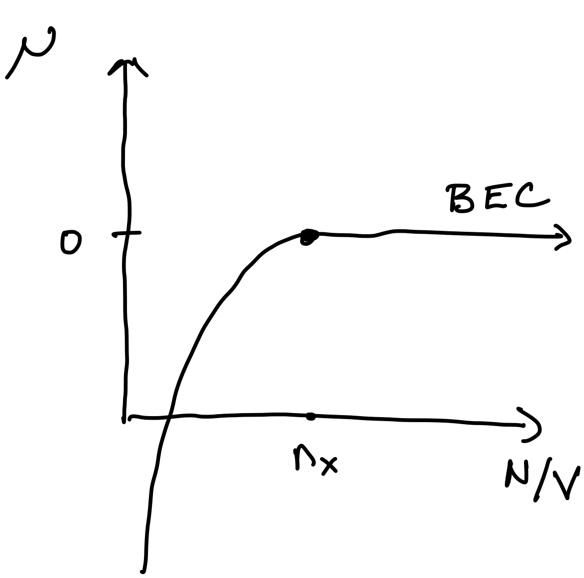
But physically, we can certainly put $n > n_*$ bosons into the box!

The interpretation is that for $n > n_*$, we need to switch to the canonical ensemble. When $\mu = 0$, adding/removing a boson from $k=0$ state has no impact on $F = E - TS = F_0 + F_{k>0}$. This is because $E_{k=0} = 0$, and $S_{k=0} = 0$? because only one quantum state irrespective of n_0! So to minimize F at fixed $\langle N \rangle$, we can adjust n_0 as needed!

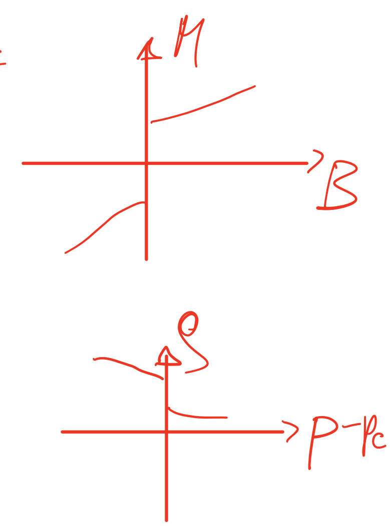
$$\langle n_k \rangle = \begin{cases} \dfrac{1}{e^{\beta E_k} - 1} & \text{for } k \neq 0 \\ n_0 = N - V n_* & \text{for } k = 0 \end{cases}$$

This ensures $\sum_k n_k = N$

Viewed sideways, $\mu(n, \beta)$ "pins" to $\mu = 0$ for $n > n_*$:



c.f.



This kink implies non-analytic behaviour in quantities like C_V, e.g., it is a <u>phase transition</u>. Viewed as function of T at fixed N, $\lambda = \sqrt{2\pi\hbar^2/mk_BT}$,

$$\lambda^3 n_x = \zeta_{3/2}$$

$$\hookrightarrow \left(\frac{2\pi\hbar^2}{mk_BT_c}\right)^{3/2} \frac{N}{V} = \zeta_{3/2}$$

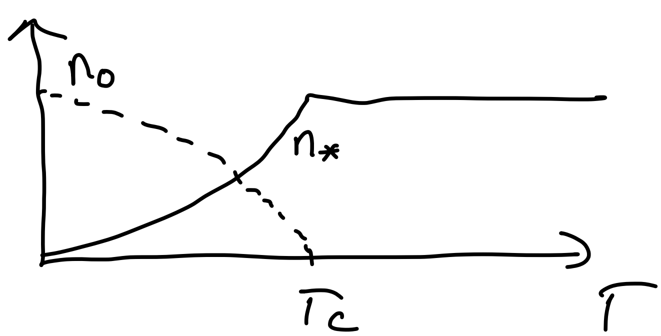
$$\hookrightarrow \quad k_B T_c = \left(\frac{N}{V}\zeta_{3/2}^{-1}\right)^{2/3} \cdot 2\pi\hbar^2/m$$

$$T_c = 3.31\left(\frac{N}{V}\right)^{2/3}\frac{\hbar^2}{k_B \cdot m}$$

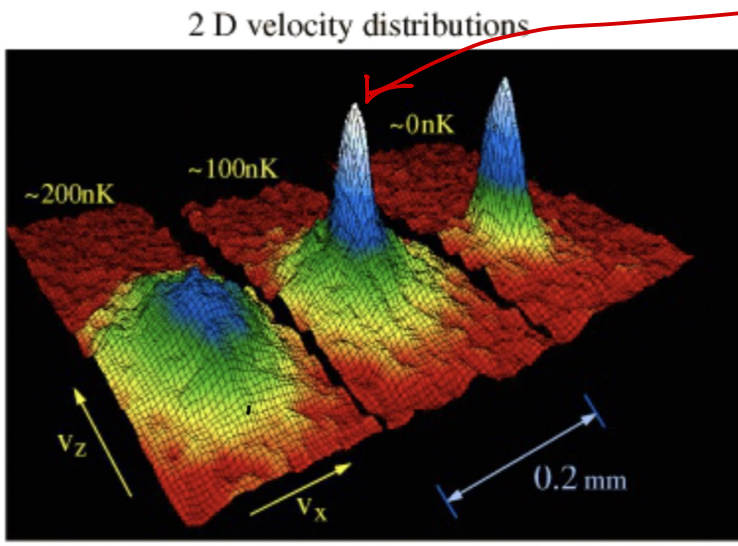
For $T < T_c$, $\frac{N_{ex}}{N} = \zeta_{3/2} \cdot \frac{V}{N}\frac{1}{\lambda^3} \propto \left(\frac{T}{T_c}\right)^{3/2}$

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

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



$$\underbrace{P(\vec{k})}_{n_k} \text{ from free expansion}$$



Weimann + Cornell, JILA: $T_c = 170\,nK$!

Because μ is independent of N for $T < T_c$, we can obtain $P = \frac{\partial \Omega}{\partial V}$ easily in the grand-canonical formalism,

$$\beta P = -\int \frac{d^3k}{(2\pi)^3} \ln\left(1 - e^{-\beta(\epsilon_k - \mu)}\right) = \frac{1}{\lambda^3} \frac{4}{3\sqrt{\pi}} \int_0^\infty \frac{dx\, x^{3/2}}{z^{-1}e^x - 1}$$

$$\beta P(\mu = 0) = \frac{1}{\lambda^3} \zeta_{5/2} = 1.341 / \lambda^3 \qquad [T < T_c]$$

So P depends only on T, not $\frac{N}{V}$!

Very different than $P = \frac{N}{V} k_B T$: only n_{ex} contributes since the n_0 are still!

and $P \to$ const for Fermi!

For heat capacity,