XIV. Ideal Bose Gas and Bose-Einstein Condensation

This part is a shortened and simplified version focusing on the physics behind BEC. It will be followed by a more detailed and mathematical discussion.

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Background Knowledge (Non-interacting Bosons)†

$$N = \sum_{\substack{\text{single-particle} \\ \text{states } i}} \underbrace{\frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1}}_{f_{BE}(\varepsilon_i)}$$

Physical meaning: # Bosons per single-particle state

$\mu < \varepsilon_i$ for all i (follows from meaning of $f_{BE}(\varepsilon_i)$ and $f_{BE}(\varepsilon_i) \geq 0$)

and thus $\mu < \underbrace{\varepsilon_{\text{lowest}}}$

lowest single-particle state's energy

$(\mu < 0)$

$$E = \sum_{\substack{\text{single-particle} \\ \text{states } i}} \varepsilon_i \cdot \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1}$$

$$Q(T,\mu,V) = \prod_i \frac{1}{1 - e^{-\beta(\varepsilon_i - \mu)}}$$

$$\Omega = -kT \ln Q = kT \sum_i \ln\left(1 - e^{-\beta(\varepsilon_i - \mu)}\right)$$

$$pV = -\Omega = -kT \sum_i \ln\left(1 - e^{-\beta(\varepsilon_i - \mu)}\right) = -kT \sum_i \ln\left(1 - \xi e^{-\beta\varepsilon_i}\right)$$

$\xi \equiv e^{\beta\mu}$

$0 \leq \xi \leq 1$

high-temp. limit; low-temp. [different from Fermi Gas]

† See Chapter XII.

- **Recall**

$$f_{BE}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}-1}$$ is the number of bosons in a single-particle state at the energy ε

$\therefore$ $f_{BE}(\varepsilon) \geq 0$ for all single-particle energy ε

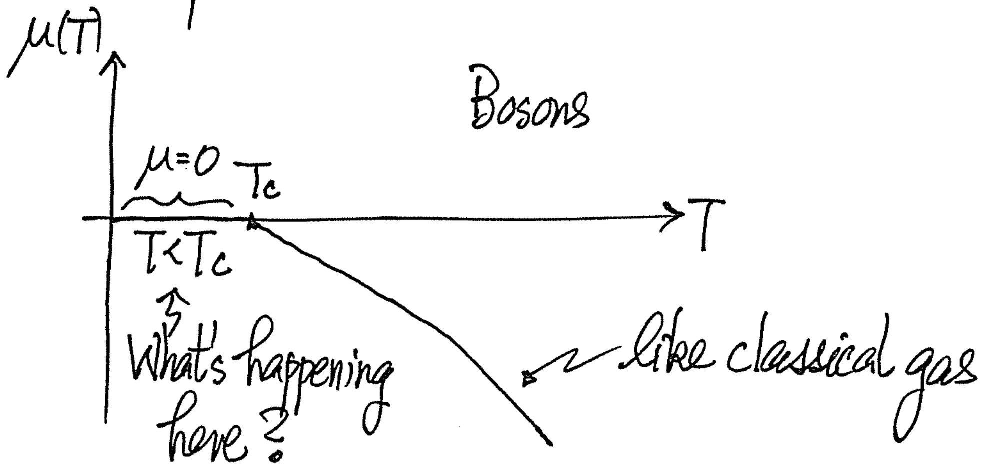
$\Rightarrow$ $\mu \leq \varepsilon$ for all single-particle energy ε

$\Rightarrow$ $\mu \leq \varepsilon_{lowest}$

- $\boxed{\text{Particle-in-a-big-box: } \mu \leq 0}$

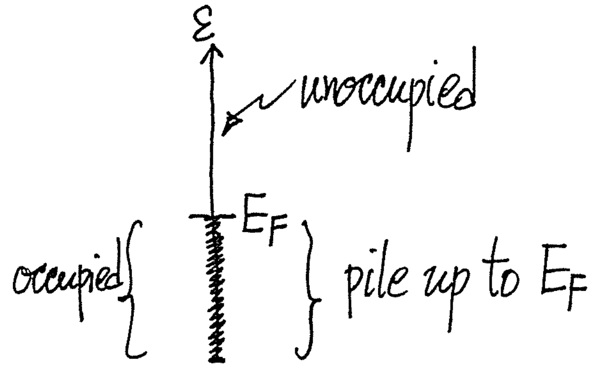
μ is very negative at high temperature ($\because$ Bose gas $\approx$ classical gas)

$\therefore$ Expect something to happen when $\mu \to 0$ as temperature decreases.

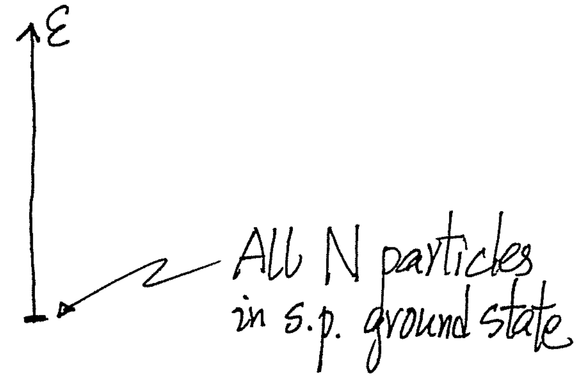


- Getting a sense that Bosons and Fermions are very different at T=0

$\boxed{T=0 \text{ Fermi Gas}}$



$\boxed{T=0 \text{ Bose Gas}}$



$\boxed{\text{Look at } N_0 \equiv \#\text{ particles in "}\vec{k}=0\text{ state"}}$

Fermions

$N_0 = 2$ (up/down spin)

i.e. 2 out of N particles

Key point:

$\begin{cases} N = 10^{22} \text{ particles} \\ N_0 = 2 \end{cases}$

$\begin{cases} N = 10^{32} \text{ particles} \\ N_0 = 2 \text{ (same "2")} \end{cases}$

$\boxed{N_0 \text{ does not scale with } N}$

OR $\frac{N_0}{N} \to 0$ as $N \to \infty$ ($V \to \infty$)

Bosons

$N_0 = N$

(N out of N go to s.p. ground state)

$N = 10^{22}$, $N_0 = 10^{22}$

$N = 10^{32}$, $N_0 = 10^{32}$

Key Point:

$\boxed{N_0 \text{ scales with } N}$

OR $\frac{N_0}{N}$ is a finite number

$\boxed{\text{"}\vec{k}=0\text{ state" is macroscopically occupied!}}$

A. 3D Non-relativistic Bosons in Volume V

[particle-in-a-big-box]

- 3D and $\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}$

$$g(\varepsilon) = G_s \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2} \quad \text{density of states}$$

$$= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2} \quad \text{for spinless } (s=0) \text{ boson}$$

$$G_s = 2s+1 = 1$$

- For particle-in-a-big-box, the lowest single-particle $\varepsilon_{lowest} \to 0$

  $\therefore \mu < 0$ for all temperatures

- Usually call the ε_{lowest} state (the single particle ground state) the "$\vec{k}=0$ state".[+]

[+] In solid state physics, you used the periodic boundary conditions in treating single-particle states, resulting really in a "$\vec{k}=0$ state".

B. Possibility of Bose-Einstein Condensation

- $T=0$, N_0 scales with N for Bosons, i.e. macroscopically occupied

- But do we really need $T=0$ for "$\vec{k}=0$ state" to be macroscopically occupied, will it happen for sufficiently low temperatures $T < T_c$ for some T_c? What is T_c?

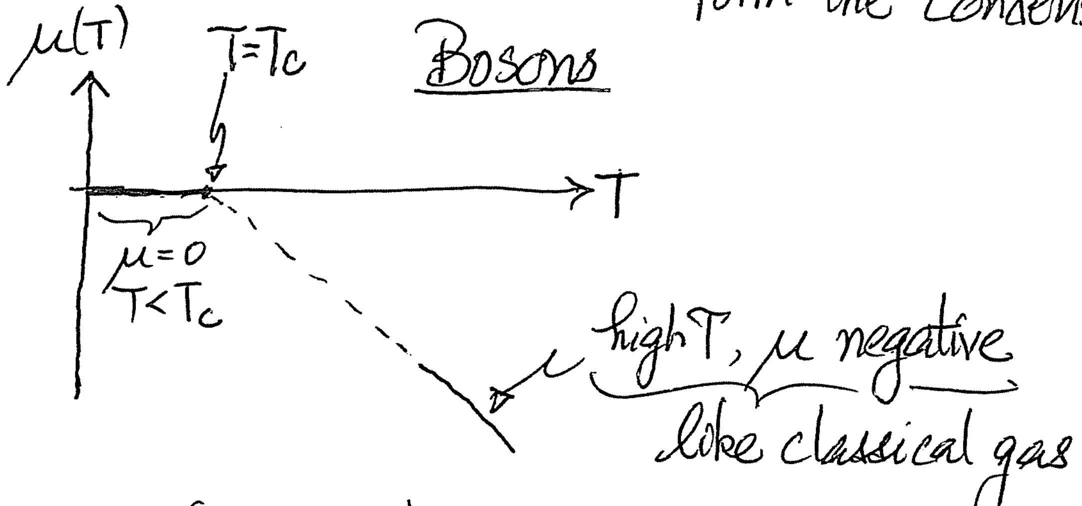
Ans: Depends on dimensionality and dispersion relation.

- If yes, the bosons "condense" into the the $\vec{k}=0$ state with N_0/N being a finite number. It is "Bose-Einstein Condensation" (BEC).

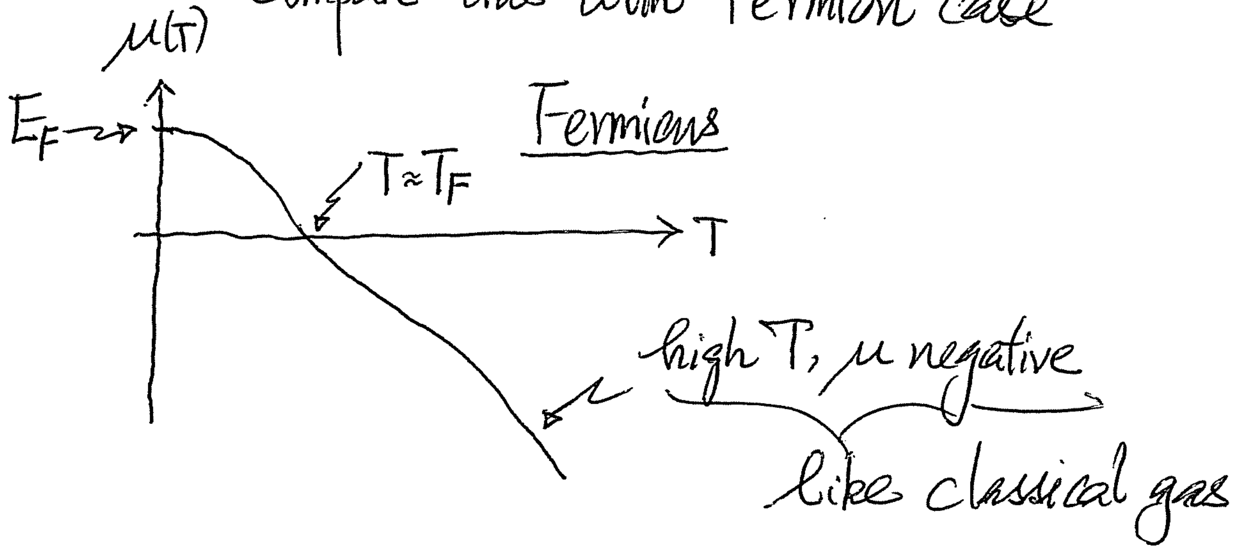
- For 3D non-relativistic bosons in a volume V, the answer is Yes. We use this example to illustrate the key idea.

- What will happen is:
  - high T, $\mu \leq 0$ (similar to classical gas)
  - As T decreases, μ shifts towards zero from below
  - At $T = T_c$, $\mu \to 0$ and μ cannot shift anymore
  - Further lowering the temperature, $\mu = 0$ and cannot shift, particles $\underbrace{\text{go into } \vec{k}=0 \text{ state}}_{\text{single-particle ground state}}$

form the "condensate"



Compare this with Fermion case



We will encounter an integral of the form:

$$\int_0^\infty \frac{x^{1/2}\,dx}{e^x - 1}$$

(i) checking the upper and lower ends of the integral, it is a finite number

(ii) $$\int_0^\infty \frac{x^{1/2}\,dx}{e^x - 1} = \underbrace{\frac{\sqrt{\pi}}{2} \cdot (2.612)}$$

More important is that it is just a finite number. [order-1]

C. The Bose-Einstein condensation temperature T_c

- What do we expect?

The condensation must come from the bosonic nature of the particles, i.e., when quantum nature is important!

Thus, perhaps the criteria is

$$\lambda_{th}^3 \approx \frac{V}{N}$$

OR

$$\left(\frac{h}{\sqrt{2\pi m kT}}\right)^3 \approx \frac{V}{N} \quad \text{defines } T_c$$

[We will see that this is not too far away from the result!]

and when

$$\left(\frac{h}{\sqrt{2\pi m kT}}\right)^3 > \frac{V}{N}, \quad \text{then the condensate appears.}$$

3D Ideal Bose Gas

- Density of states $g(\varepsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2} \propto \varepsilon^{1/2}$
- Equation for N

$$N = \sum_i \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1} \qquad \text{(general)}$$

- Turn it into an integral:

$$N \overset{?}{=} \int_0^\infty \frac{g(\varepsilon)\,d\varepsilon}{e^{\beta(\varepsilon-\mu)}-1} \overset{?}{=} \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}\,d\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}$$

$$\boxed{\text{Q: "?" Anything wrong?}}$$

Note: $\underbrace{g(\varepsilon) \propto \varepsilon^{1/2}}_{g(0)=0}$

$\Rightarrow$ integral does not include number of particles in $\varepsilon = 0$ state!

Formally,

$$N = \underbrace{N_0(T)}_{\substack{\text{particles in}\\ \varepsilon=0\\ \text{state}}} + \underbrace{\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}\,d\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}}_{\text{particles in all other single-particle states}}$$

$$N = N_0 + \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}}{e^{\beta(\varepsilon-\mu)}-1}$$

Valid for all T

- For $T > T_c$:
  - Can adjust μ ($\mu<0$) so that the integral accounts for N
  - N_0 term is negligible!

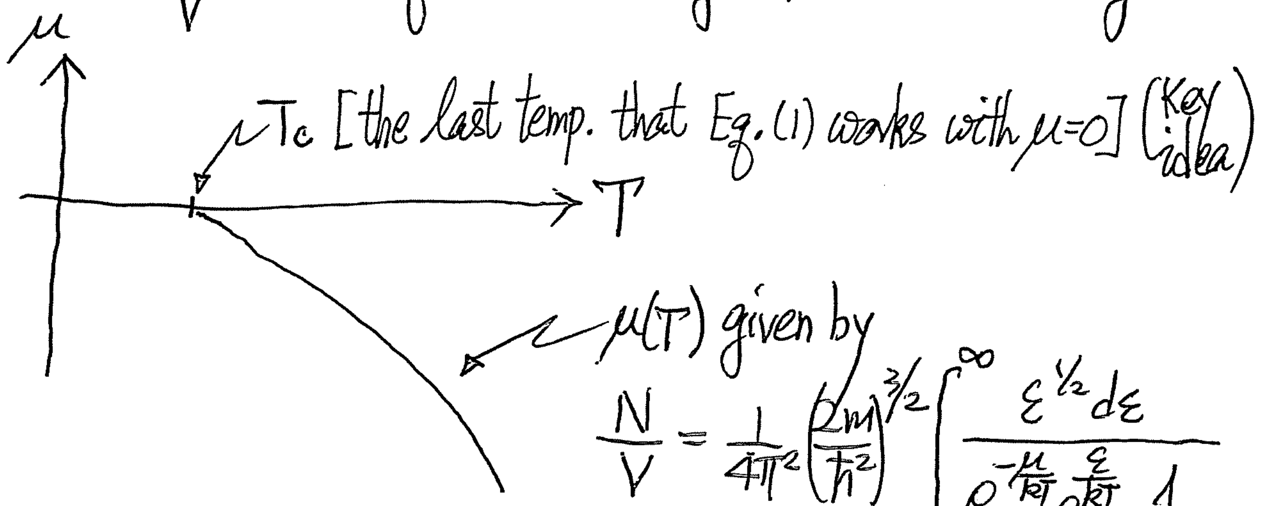
    Meaning: Even $N_0 \neq 0$, the number N_0 does not scale with N for $T > T_c$.

    [Similar to the case of fermionic systems.]

For $T > T_c$:

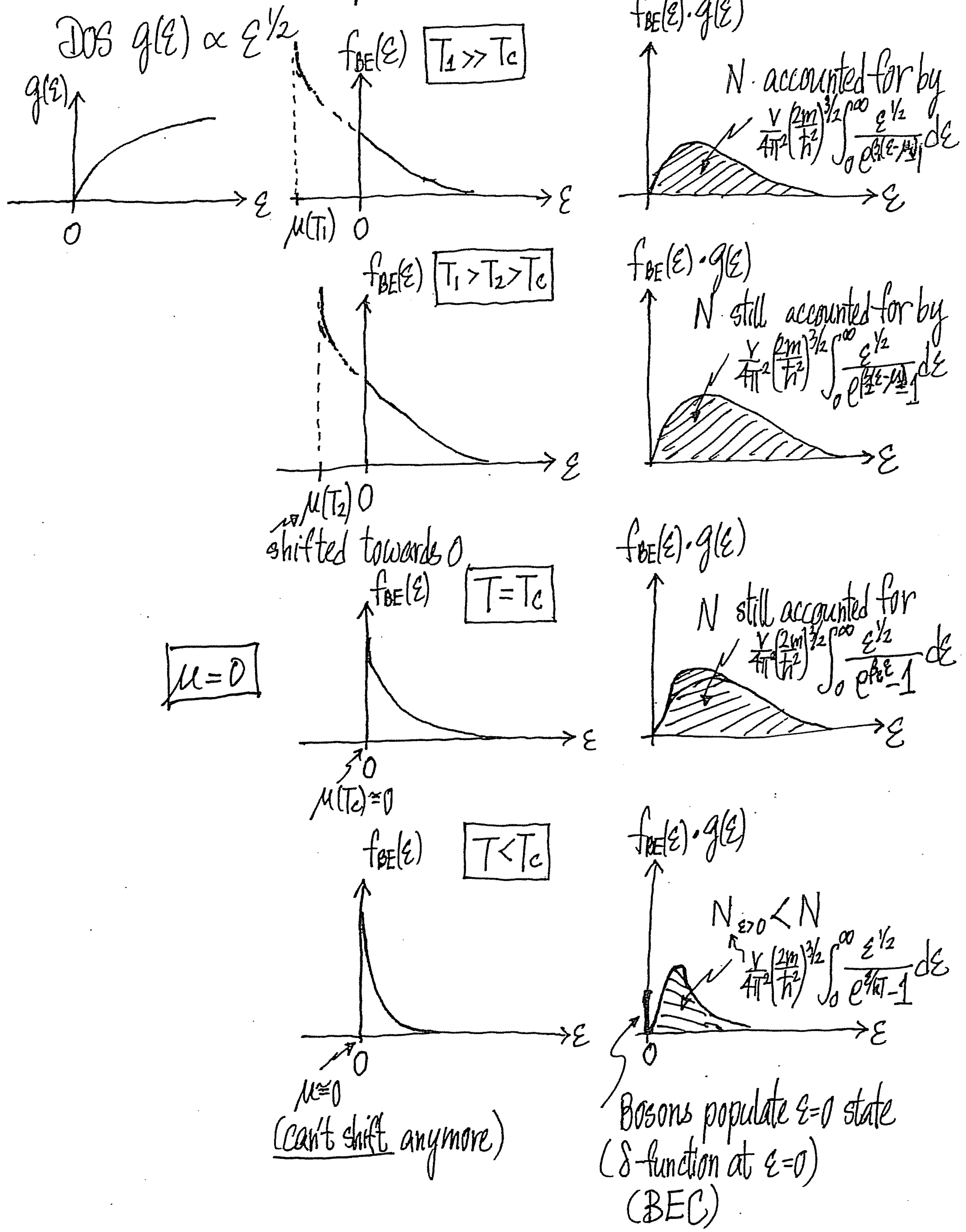
$$N = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}\,d\varepsilon}{e^{-\frac{\mu}{kT}}e^{\frac{\varepsilon}{kT}}-1} \quad (1) \text{ works}$$

Given $\frac{N}{V}$, an equation to adjust μ as T changes



$$\frac{N}{V} = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}\,d\varepsilon}{e^{-\frac{\mu}{kT}}e^{\frac{\varepsilon}{kT}}-1}$$

A Pictorial way of realizing something should happen at some low-temperature T_c



A quick way to determine T_c

- As T decreases, μ becomes less negative
- T_c is the temperature that μ touches zero and the integral still accounts for N

$\therefore$ $\underbrace{T=T_c,\ \mu=0\ \&\ N = \text{integral}}$

$$T=T_c: \boxed{N = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\varepsilon^{1/2}\, d\varepsilon}{e^{\varepsilon/kT_c}-1} \quad \text{determines } T_c}$$

Def.: $x = \frac{\varepsilon}{kT_c}$

$$N = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(kT_c)^{3/2} \overbrace{\int_0^\infty \frac{x^{1/2}\,dx}{e^x-1}}^{\frac{\sqrt{\pi}}{2}\cdot(2.612)}$$

$$= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(kT_c)^{3/2}\,\frac{\sqrt{\pi}}{2}\cdot(2.612) \qquad (*)$$

- $T_c = \frac{h^2}{2\pi k}\frac{1}{m}\left(\frac{1}{2.612}\frac{N}{V}\right)^{2/3} = \frac{2\pi\hbar^2}{k}\frac{1}{m}\left(\frac{1}{2.612}\frac{N}{V}\right)^{2/3}$

Note: $T_c \sim \frac{1}{m}$

$T_c \sim \left(\frac{N}{V}\right)^{2/3} \sim n^{2/3}$

Remark: For 3D Fermi Gas, $T_F = E_F/k = \frac{\hbar^2}{k2m}\left(3\pi^2\frac{N}{V}\right)^{2/3}$ actually has a very similar form! It is not surprising as $T<T_F$ and $T<T_c$ both signify that quantum nature of particles should be accounted for.

$\therefore$ If we want T_c to be not so small, then try to use bosons of smaller mass and gas of higher density

↳ trouble: but gas would become a liquid as T decreases (when there is a bit of interaction)!

Q: Will there be BEC in 2D/1D ideal Bose gas?

Go back to (*): Recall $\lambda_{th}(T) = \frac{h}{\sqrt{2\pi m kT}}$

(*) can be written as:

$$\underbrace{\boxed{\lambda_{th}^3(T_c) = \left(\frac{V}{N}\right)\cdot(2.612)}}_{} \quad \text{determines } T_c$$

this is exactly what we expect

$$\underbrace{\lambda_{th}(T_c)}_{\text{thermal de Broglie wavelength at } T_c} \approx \underbrace{\left(\frac{V}{N}\right)^{1/3}}_{\text{particle separation}}$$

[BEC is a quantum phenomenon]

D. Number of particles in Condensate for $T<T_c$

$T<T_c$

$$N = N_0(T) + \underbrace{\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}\,d\varepsilon}{e^{\varepsilon/kT}-1}}_{\text{since } T<T_c,\ \text{integral} < N}\,, \quad T<T_c$$

$$= N_0(T) + \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(kT)^{3/2}\underbrace{\int_0^\infty \frac{x^{1/2}\,dx}{e^x-1}}_{\text{same number } \frac{\sqrt{\pi}}{2}\cdot(2.612)}$$

$$= N_0(T) + \underbrace{\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(kT_c)^{3/2}\int_0^\infty \frac{x^{1/2}\,dx}{e^x-1}}_{N}\cdot\left(\frac{T}{T_c}\right)^{3/2}$$

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

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

bosons in $\varepsilon=0$ state

$\boxed{\text{scales with } N}$

fraction of particles in condensate
("macroscopic occupation of single-particle ground state")

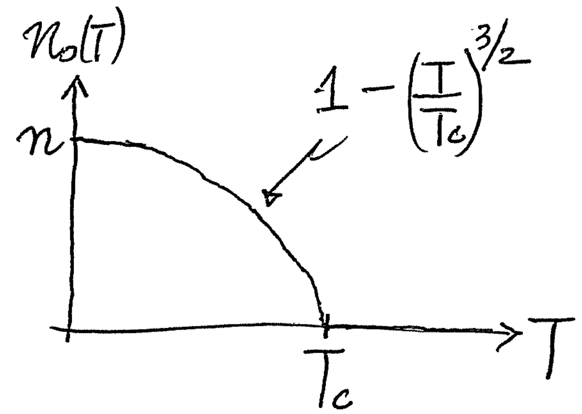
this happens for $T<T_c$

[For $T>T_c$, even though $N_0 \neq 0$, it does not scale with N and thus is negligible.]

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

or

$$n_0(T) = n\left(1-\left(\frac{T}{T_c}\right)^{3/2}\right)$$



- The phenomenon of BEC was predicted by Einstein in 1925, after reading Bose 1924 manuscript.
- The first realization of BEC was made in 1995 (see Anderson, Ensher, Matthews, Wieman, Cornell, Science 269, 198 (1995)) (see Davis, Mewes, Andrews, van Druten, Durfee, Kurn, Ketterle, Phys. Rev. Lett. 75, 3969 (1995))
- Wieman, Cornell, Ketterle were awarded the 2001 Nobel Physics Prize.