Ideal Bose Gas

- This section fills in more mathematics in the $T < T_c$ physics in an ideal Bose Gas
- Read the essential part first
- Here the discussion is based on $\xi \, (\equiv e^{\beta\mu})$ and $g_n(\xi) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{x^{n-1}}{\xi^{-1} e^x - 1} dx$

For $T < T_c$, $\xi \to 1$

Background Math Results†

$$\int_0^\infty \frac{x^{n-1}}{\xi^{-1} e^x - 1} dx = g_n(\xi) \cdot \underbrace{\Gamma(n)}_{\text{Gamma Function}}$$

$$g_n(\xi) \equiv \sum_{k=1}^{\infty} \frac{\xi^k}{k^n} \quad \text{(Polylogarithm function)}$$

In particular, $\displaystyle\int_0^\infty \frac{x^{1/2}\, dx}{\xi^{-1} e^x - 1} = g_{3/2}(\xi) \cdot \Gamma\left(\tfrac{3}{2}\right) = \frac{\sqrt{\pi}}{2} g_{3/2}(\xi)$

$$\int_0^\infty \frac{x^{3/2}\, dx}{\xi^{-1} e^x - 1} = g_{5/2}(\xi) \cdot \Gamma\left(\tfrac{5}{2}\right) = \frac{3\sqrt{\pi}}{4} g_{5/2}(\xi)$$

$$\int_0^\infty \frac{x^{n-1}}{e^x - 1} dx = g_n(1) \cdot \Gamma(n) = \zeta(n) \cdot \Gamma(n)$$

where $\displaystyle\zeta(n) \equiv \sum_{k=1}^{\infty} \frac{1}{k^n}$ (Riemann zeta function)

In particular, $\zeta\left(\tfrac{3}{2}\right) \approx 2.612$

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† This is analogous to $f_n(\xi) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{x^{n-1}}{\xi^{-1} e^x + 1} dx$ in Fermi Gas, where $f_n(\xi) = \displaystyle\sum_{k=1}^{\infty} \frac{(-1)^{k+1} \xi^k}{k^n}$.

General Equation

From Equation for N:[†]

$$N = \underbrace{\frac{\xi}{1-\xi}}_{N_0} + \underbrace{\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}}{\xi^{-1}e^{\beta\varepsilon}-1}\,d\varepsilon}_{N_{\varepsilon>0}} \qquad (1)$$

N_0 ↖ particles in lowest single-particle state.

$N_{\varepsilon>0}$ ↖ particles in all other single-particle states

($\underbrace{G_s = 1 \text{ assumed}}$) spin = 0 particles

$$= \frac{\xi}{1-\xi} + \frac{V}{\lambda_{th}^3}\, g_{3/2}(\xi) \qquad (1')$$

[Valid for all T]

- Formally, serves to fix ξ (or μ) for a temp. T

It can be rewritten as

$$\frac{N}{V} = \underbrace{\frac{1}{V}\frac{\xi}{1-\xi}}_{\frac{N_0}{V}} + \underbrace{\frac{1}{\lambda_{th}^3}\, g_{3/2}(\xi)}_{\frac{N_{\varepsilon>0}}{V}} \qquad (1'')$$

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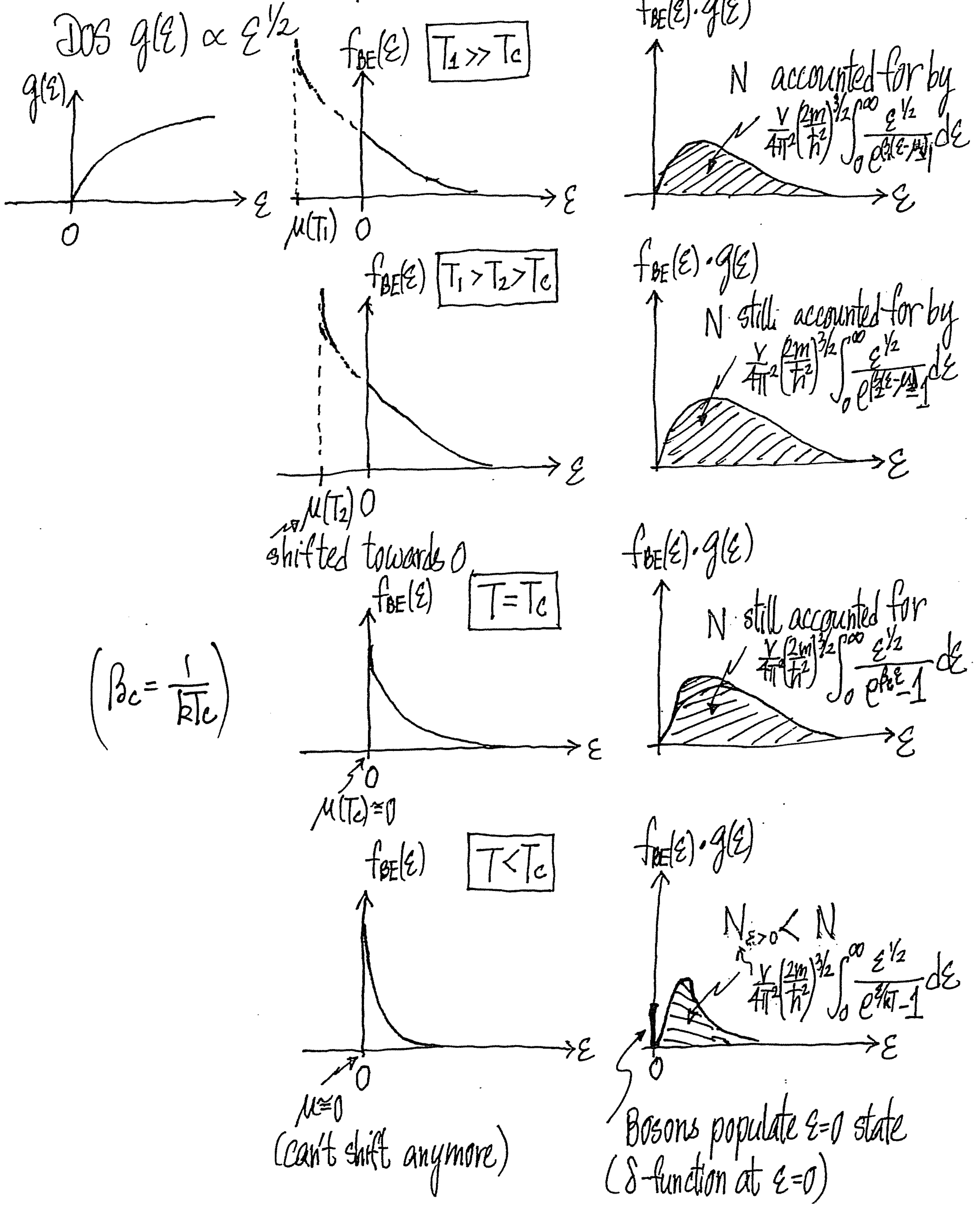
† The N_0 term comes from $\dfrac{1}{e^{\beta(0-\mu)}-1} = \dfrac{1}{\xi^{-1}-1} = \dfrac{\xi}{1-\xi}$

↖ The $\varepsilon=0$ term in the N-equation

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



A quick way to get T_c: the condensation temperature

Key Idea

General Equation

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

- Valid for all T

For $T > T_c$

- N_0 term is negligible!
  - Meaning: Even $N_0 \neq 0$, the number N_0 does not scale with N for $T > T_c$.
    [This is also the case in fermionic systems.]

$\therefore$ for $T > T_c$

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

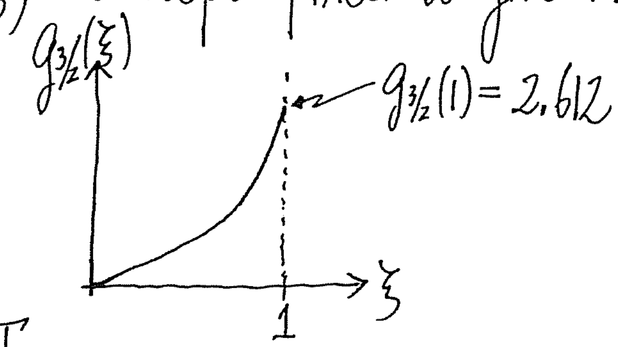
OR

$$\boxed{N = \frac{V}{\lambda_{th}^3}\, g_{3/2}(\xi), \quad T > T_c} \quad (3) \qquad \lambda_{th} \equiv \frac{h}{\sqrt{2\pi m k T}}$$

Eq. (3) serves to fix $\xi(T)$ or $\mu(T)$

As T decreases towards T_c

- $\frac{1}{\lambda_{th}^3} \sim T^{3/2}$
- Factor $\frac{V}{\lambda_{th}^3}$ decreases
- μ shifts from a negative value to a less negative value (or ξ shifts towards 1), so that $g_{3/2}(\xi)$ increases and the product $\frac{V}{\lambda_{th}^3} g_{3/2}(\xi)$ is kept fixed to give N



- At some temperature T_c,
  $\mu \to 0$ (or $\xi \to 1$)
  this is the last temperature that the product
  $$\frac{V}{\lambda_{th}^3(T_c)}\, g_{3/2}(1) \text{ can give } N$$

OR

$$N = \frac{V}{\lambda_{th}^3(T_c)} \cdot \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2}\,dx}{e^x - 1}$$

Thus, T_c for 3D non-relativistic bosons is given by

$$N = \frac{V}{\lambda_{th}^3(T_c)} g_{3/2}(1) \quad (4)$$

$$= \frac{V}{\lambda_{th}^3(T_c)} \cdot (2.612)$$

Note: $g_{3/2}(1) = \sum_{k=1}^{\infty} \frac{1}{k^{3/2}} = \zeta(\frac{3}{2}) = 2.612$

$$\lambda_{th}^3 = \frac{h^3}{(2\pi m k T_c)^{3/2}}$$

$$\therefore \boxed{T_c = \frac{h^2}{2\pi m k}\left(\frac{N}{V}\cdot\frac{1}{2.612}\right)^{2/3} = \frac{2\pi\hbar^2}{mk}\left(\frac{N}{V}\cdot\frac{1}{2.612}\right)^{2/3}} \quad (5)$$

- $T_c \sim \frac{1}{m}$
- $T_c \sim \left(\frac{N}{V}\right)^{2/3} = n^{2/3}$

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

↳ but gas would become liquid!

Q: Will there be Bose-Einstein condensation in 2D ideal Bose gas? 1D ideal Bose gas?

Summary on arguments in obtaining T_c

$$\frac{N}{V} = \frac{1}{V}\frac{\zeta}{1-\zeta} + \frac{1}{\lambda_{th}^3} g_{3/2}(\zeta)$$

- 3D Ideal Bose Gas
- General

- If we approach T_c from above, ζ is not close to 1 and $\frac{1}{V}\frac{\zeta}{1-\zeta}$ is negligible (V large).

Thus,

$$\frac{N}{V} = \underbrace{\left[\frac{1}{\lambda_{th}^3}\right]}_{\frac{1}{\lambda_{th}^3} \sim T^{3/2}} \cdot \underbrace{g_{3/2}(\zeta)}$$

$\frac{1}{\lambda_{th}^3} \sim T^{3/2}$ drops with T as T decreases

For T drops below T_c, product cannot make up $\frac{N}{V}$

to maintain $\frac{N}{V}$ on LHS, ζ increases towards 1 and $g_{3/2}(\zeta)$ increases.

- But $\zeta \to 1$ as T decreases and $g_{3/2}(1) = \zeta(\frac{3}{2}) = 2.614$ is a number

Thus, T_c is given by:

$$\frac{N}{V} = \frac{1}{\lambda_{th}^3(T_c)} \cdot g_{3/2}(1)$$

$$\Rightarrow T_c = \frac{h^2}{2\pi m k}\left(\frac{N}{V}\cdot\frac{1}{g_{3/2}(1)}\right)^{2/3} \quad ※$$

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

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

[Note: $\mu \to 0$ at T_c,
$T<T_c$, μ cannot shift anymore!]

$$= N_0 + \underbrace{\frac{V}{\lambda_{th}^3(T)}\, g_{3/2}(1)}$$

$$= N_0 + N_{\varepsilon>0}$$

Consider $N_{\varepsilon>0} = \dfrac{V}{\lambda_{th}^3(T)}\, \overbrace{g_{3/2}(1)}^{\text{constant}} \propto T^{3/2}$

Recall: $\lambda_{th} = \dfrac{h}{\sqrt{2\pi m k T}}$

$$= \underbrace{\frac{V}{\lambda_{th}^3(T_c)}\, g_{3/2}(1)}\cdot \frac{\lambda_{th}^3(T_c)}{\lambda_{th}^3(T)}$$

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

all particles! $\quad < 1 \; (T<T_c)$

$\therefore N_{\varepsilon>0} < N$ for $T<T_c$

- Where do the particles $(N - N_{\varepsilon>0})$ go?
  They occupy the lowest single-particle states!

$$N = N_0 + N_{\varepsilon>0}$$

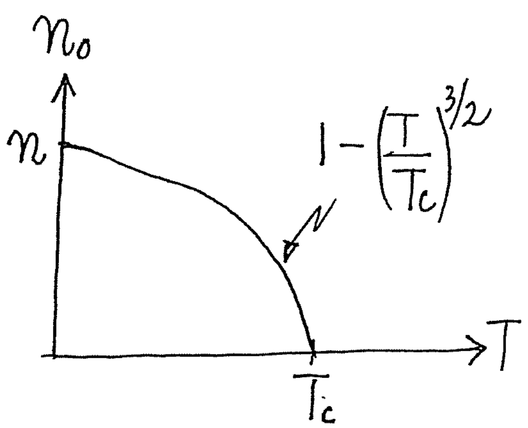
$$= N_0 + N\left(\frac{T}{T_c}\right)^{3/2}$$

$$\Rightarrow \boxed{N_0 = N\left(1-\left(\frac{T}{T_c}\right)^{3/2}\right)} \qquad (6)$$

OR $$\boxed{\frac{N_0}{V} = \frac{N}{V}\left(1-\left(\frac{T}{T_c}\right)^{3/2}\right)} \qquad (6')$$

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

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



Note: From Eq. (6), we have

$$N_0 \propto N$$

This is the point! For $T<T_c$, when we scale up the system (increase N), the number of particles in the condensate N_0 also increases!
[This should be contrasted with the Fermi Gas case and the $T>T_c$ case.]

E. $E(T)$ and C_V for $T<T_c$

In general,

$$pV = -\Omega = -kT \sum_{s.p.\, i} \ln(1 - \xi e^{-\beta\varepsilon_i})$$

If we single out the lowest single-particle state, for a 3D Ideal Bose Gas, we have

$$pV = \underbrace{kT \frac{V}{\lambda_{th}^3} g_{5/2}(\xi)}_{\text{all other states}} \underbrace{- kT \ln(1-\xi)}_{\varepsilon_i = 0 \text{ state}}$$

$$\Rightarrow \frac{p}{kT} = \overbrace{\frac{1}{\lambda_{th}^3} g_{5/2}(\xi)}^{\text{all other states}} \underbrace{\overbrace{- \frac{1}{V} \ln(1-\xi)}^{\varepsilon_i=0 \text{ state}}}_{\text{this term is unimportant for all } T} \quad \text{General} \quad (7)$$

- $T>T_c$, ξ is not close to 1, negligible in thermodynamic limit.
- $T<T_c$, $\xi \to 1$ as $\xi = 1 - \frac{a}{V}$, thus $\frac{1}{V}\ln(1-\xi) \sim \frac{1}{V}\ln\frac{a}{V} \to 0$ as $V \to \infty$.

Thus, for $T<T_c$,

$$\frac{p}{kT} = \frac{1}{\lambda_{th}^3} g_{5/2}(1) \quad \text{governs the behaviour} \quad (8)$$

Recall: $pV = \frac{2}{3}E$

Thus, $E = \frac{3}{2}pV = \frac{3}{2} \overbrace{kT \frac{V}{\lambda_{th}^3} g_{5/2}(1)}^{\text{only bosons in } \varepsilon>0 \text{ states contribute to } E} = \frac{3}{2} kT \frac{V}{\lambda_{th}^3} \cdot (1.341)$.

$$E = \frac{3}{2} kT \frac{V}{\lambda_{th}^3(T)} \cdot \overbrace{(1.341)}^{g_{5/2}(1)} \quad \text{for } T<T_c$$

$$\propto T \cdot T^{3/2} \propto T^{5/2}$$

$$E = \frac{3}{2} g_{5/2}(1) \cdot kT \cdot \frac{V}{\lambda_{th}^3(T)}$$

Recall: $N_{\varepsilon>0} = \frac{V}{\lambda_{th}^3(T)} g_{3/2}(1)$

$$\therefore E = \underbrace{\frac{3}{2} \frac{g_{5/2}(1)}{g_{3/2}(1)}} \cdot N_{\varepsilon>0} kT$$

$$= 0.770 \underbrace{N_{\varepsilon>0}} kT$$

these particles contribute to E

$$\Rightarrow \frac{E}{N_{\varepsilon>0}(T)} = 0.770 kT$$ gives contribution to E per particle in $\varepsilon>0$ states

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$$E = \frac{3}{2} kT \frac{V}{\lambda_{th}^3(T)} g_{5/2}(1) \qquad (T<T_c)$$

$$= \frac{3}{2} kT \left[\frac{V}{\lambda_{th}^3(T_c)} g_{3/2}(1)\right] \cdot \left(\frac{\lambda_{th}^3(T_c)}{\lambda_{th}^3(T)}\right) \cdot \frac{g_{5/2}(1)}{g_{3/2}(1)}$$

$$= \frac{3}{2} kT\, N \cdot \left(\frac{T}{T_c}\right)^{3/2} \frac{g_{5/2}(1)}{g_{3/2}(1)} \propto T^{5/2}$$

$$= 0.770 \underbrace{N \cdot \left(\frac{T}{T_c}\right)^{3/2}}_{N_{\varepsilon>0}} kT \qquad (9)$$

$$C_V = \text{Heat capacity} = \left(\frac{\partial E}{\partial T}\right)_V = \frac{5}{2}\cdot\frac{3}{2}\frac{Vk}{\lambda_{th}^3(T)}\cdot\underbrace{(1.341)}_{\zeta\left(\frac{5}{2}\right) = g_{5/2}(1)}$$

$$= \frac{5}{2}\cdot 0.770\, k\left(\frac{T}{T_c}\right)^{3/2} N$$

$$= 1.925k\,\underbrace{N\left(\frac{T}{T_c}\right)^{3/2}}\qquad (10)$$

$$= 1.925k\cdot N_{\varepsilon>0}\qquad (T<T_c)$$

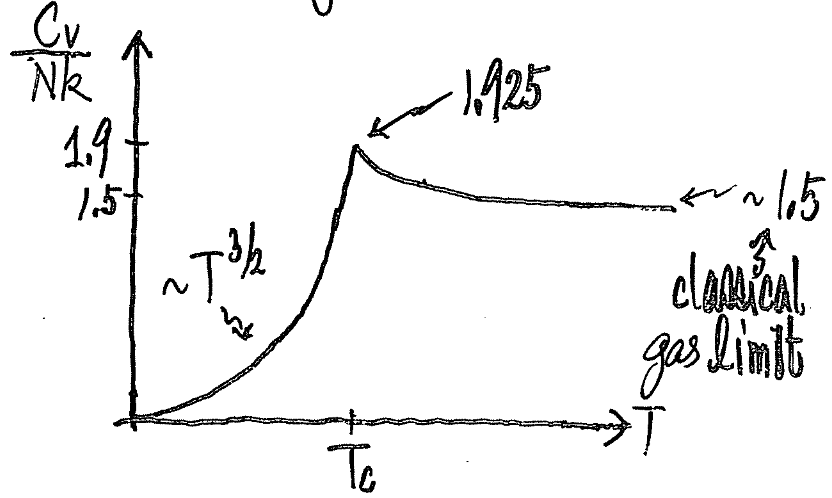
Behaviour: As $T\to 0$, $C_V\to 0$

For $T<T_c$, $C_V \sim T^{3/2}$

At $T=T_c$, $C_V \cong 1.9\,k\cdot N$

this is larger than $\frac{3}{2}kN$ as expected in the high temp. ($T\gg T_c$) limit (equipartition theorem)

Thus, we expect (without doing detailed calculations for all T):



{ C_V has a cusp at T_c, but it is continuous

This is a result of detail calculation.

F. Other $T<T_c$ Properties

From Eq.(8), we have

$$\frac{pV}{kT} = \frac{V}{\lambda_{th}^3}g_{5/2}(1) \quad \text{for 3D Ideal Bose Gas}$$

$$\Omega = -pV = -kT\frac{V}{\lambda_{th}^3}g_{5/2}(1)$$

{ Note: $\frac{1}{\lambda_{th}^3} \sim T^{3/2}$

$$S = -\frac{\partial\Omega}{\partial T} = \frac{5}{2}k\frac{V}{\lambda_{th}^3}g_{5/2}(1)$$

Recall: $E = \frac{3}{2}pV = \frac{3}{2}kT\frac{V}{\lambda_{th}^3}g_{5/2}(1)$ [Condensate does not contribute to E]

$$S = \frac{5}{3}\frac{E}{T} \qquad (E \text{ given by Eq. (9)})$$

F = Helmholtz Free energy $= E - TS = -\frac{2}{3}E$

$$p = \frac{kT}{\lambda_{th}^3}g_{5/2}(1) \sim T^{5/2} \text{ and } \underbrace{\text{independent of } V}_{\text{a result due to non-interacting bosons}}$$

Contrast with Fermi Gas [degenerate pressure even at T=0]

$\therefore$ $K =$ compressibility $\sim \frac{\partial V}{\partial P} \sim \frac{1}{\left(\frac{\partial P}{\partial V}\right)} \to \infty$ for <u>Ideal Bose Gas</u>
$(T<T_c)$

At constant T, if we change the volume, the pressure remains fixed.

- This unrealistic feature disappears when the bosons <u>interact</u> with each other.

- "Two-fluid" model — We see that for $T<T_c$, the whole gas behaves as if it consists of two different gases: one from those in the condensate ($\epsilon=0$ state) (these bosons do <u>NOT</u> contribute to E, C_V, S, F, p, and so quite "super") and one from those bosons in the $\epsilon>0$ states.