Lecture 1 : Ideal Bose gas

i) Grand - canonical ensemble

$$\Xi = \mathrm{Tr}\left[e^{-\beta(H-\mu N)}\right]$$ Grand - partition function

$$= \prod_i \sum_n e^{-\beta(\varepsilon_i-\mu)n} = \prod_i \frac{1}{1-e^{-\beta(\varepsilon_i-\mu)}}$$

$\prod_i$ → over modes of Bose field / eigenstates of single particle h.

$$\langle N\rangle = k_B T \frac{\partial}{\partial\mu}\log\Xi = -k_B T\frac{\partial}{\partial\mu}\sum_i \log\left(1-e^{-\beta(\varepsilon_i-\mu)}\right) =$$

$$= -\cancel{k_B T}\sum_i \frac{-\beta\, e^{-\beta(\varepsilon_i-\mu)}}{1-e^{-\beta(\varepsilon_i-\mu)}} = \underline{\sum_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1}}$$

Bose occupation laws n_i

$$\Delta N^2 \doteq \langle N^2\rangle - \langle N\rangle^2 = k_B T \frac{\partial\langle N\rangle}{\partial\mu}$$ "compressibility"

$$= k_B T\frac{\partial}{\partial\mu}\sum_i \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1} = k_B T\sum_i \frac{-\beta\, e^{\beta(\varepsilon_i-\mu)}}{-\left(e^{\beta(\varepsilon_i-\mu)}-1\right)^2} =$$

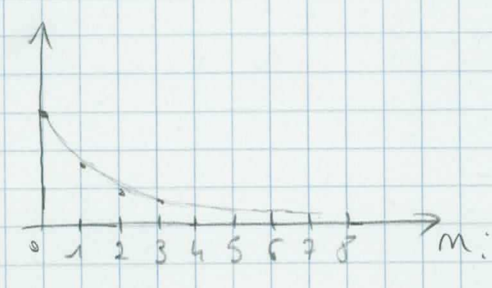
$$= \sum_i n_i(1+n_i)$$

* modes are statistically independent
* fluctuations stronger on highly populated modes

$$\Delta n_i^2 \simeq \begin{cases} n_i & \text{if} \quad n_i \ll 1 \\ n_i^2 & \text{if} \quad n_i \gg 1 \end{cases}$$

$$p(n_i) \sim e^{-\beta(\varepsilon_i - \mu) n_i}$$

"thermal laser"



$\hookrightarrow$ $n_i = 0$ is most probable state.

A general theorem:

Operator $\hat{O}$ such that $[\hat{O}, \hat{H}] = \emptyset$

$$\langle \Delta \hat{O}^2 \rangle = \langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2$$

Response function χ_{OO} : $H' = H - \varepsilon \hat{O}$, $\langle O \rangle_\varepsilon - \langle O \rangle_{\varepsilon=0} = \chi_{OO} \cdot \varepsilon$

Set : $\delta\hat{O} = \hat{O} - \langle \hat{O} \rangle_{\varepsilon=0}$

$$H' = H - \varepsilon \delta\hat{O} + \cancel{\varepsilon \langle \hat{O} \rangle_{\varepsilon=0}}$$

additive constant $\rightarrow$ neglected.

$$\langle \delta\hat{O} \rangle = \frac{\mathrm{Tr}\left[\exp\left[-\beta(\hat{H} - \varepsilon\delta\hat{O})\right] \cdot \delta\hat{O}\right]}{\mathrm{Tr}\left[\exp\left[-\beta(\hat{H} - \varepsilon\delta\hat{O})\right]\right]} =$$

averages to $\emptyset$

$$= \frac{\mathrm{Tr}\left[e^{-\beta\hat{H}} e^{\beta\varepsilon\delta\hat{O}} \cdot \delta\hat{O}\right]}{\mathrm{Tr}\left[e^{-\beta H} e^{\beta\varepsilon\delta O}\right]} \simeq \frac{\mathrm{Tr}\left[e^{-\beta H}(\cancel{1} + \beta\varepsilon\delta\hat{O})\delta\hat{O} + \dots\right]}{\mathrm{Tr}\left[e^{-\beta H}(1 + \beta\varepsilon\cancel{\delta\hat{O}}) + \dots\right]}$$

averages to $\emptyset$

$$= \beta\varepsilon \langle \delta\hat{O}^2 \rangle .$$

$$\chi_{oo} = \frac{1}{k_B T} \langle \delta\hat{O}^2 \rangle = \frac{1}{k_B T}\left(\langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2 \right)$$

ii) BEC phenomenon (in homogeneous gas)

$$N = \sum_{n_x n_y n_z} \frac{1}{e^{\beta(\varepsilon_{n_x n_y n_z} - \mu)} - 1} \qquad (n_{x,y,z} \in [-\infty, \infty]),$$

$$\varepsilon_{n_x n_y n_z} = \frac{(2\pi)^2 \hbar^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$$\simeq \int \frac{\overbrace{L_x L_y L_z}^{V}}{(2\pi)^3} dk_x\, dk_y\, dk_z \frac{1}{e^{\beta(\frac{\hbar^2 k^2}{2m} - \mu)} - 1} + \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1}$$

thermodynamic limit $L_{x,y,z} \to \infty$

So : $$n = \frac{1}{\lambda_T^3} g_{d/2}\left(e^{-\beta(\varepsilon_0 - \mu)}\right) + \frac{1}{V} \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1}$$

where : $$\lambda_T = \sqrt{\frac{2\pi \hbar^2}{m k_B T}}, \quad g_r(z) = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell^r} = \frac{1}{\Gamma(r)} \int_0^\infty dx\, x^{r-1} \frac{1}{z^{-1} e^x - 1}$$

for $r > 1$, $g_r(z)$ has finite upper bound $g_r(1)$
monotonically growing function of z.

For $d = 3$, $$n_{nc}^{max} = \frac{1}{\lambda_T^3} \overbrace{g_{3/2}(1)}^{2.612} = c^{te} \cdot T^{3/2} < \infty$$

If $n > n_{nc}^{max}$, other particles have to go into $k = 0$ mode

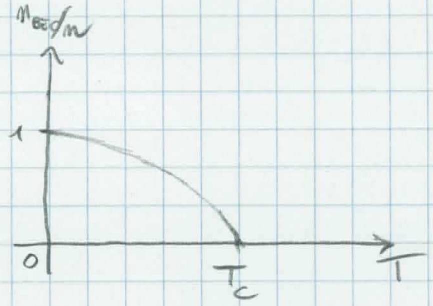
$$V\left(n - n_{nc}^{max}\right) = \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1} \simeq \frac{k_B T}{\varepsilon_0 - \mu}$$

i.e. $\mu \to \varepsilon_0^-$ as $V \to \infty$, $(\varepsilon_0 - \mu) = O(1/V)$.

Condensate fraction :

$$n = n_{nc}^{max} + n_{BEC}$$

$$\frac{n_{BEC}}{n} = 1 - \frac{n_{nc}^{max}}{n} = 1 - \left(\frac{T}{T_c}\right)^{3/2}$$



As a function of d

$$n_{nc}^{max} = \lim_{\mu \to \varepsilon_0^-} \frac{1}{\lambda_T^3} g_{d/2}\left(e^{\beta(\mu - \varepsilon_0)}\right) = \begin{cases} < \infty & \text{for } d > 2 \\ \infty & \text{for } d \leq 2 \end{cases}$$

$\longrightarrow$ BEC possible only in $d = 3$ or higher.

iii) Correlation functions

$g^{(1)} = \langle \psi^+(x)\, \psi(y) \rangle$ = 1-body density matrix

$$= \sum_i \phi_i^*(x)\, \phi_i(y) \quad n_i =$$

$$= \sum_k \frac{e^{ik(y-x)}}{V} \cdot N(k) = \frac{N_0}{V} + \frac{1}{V}\int \frac{V}{(2\pi)^3} d^3k \; e^{ik(y-x)} \cdot \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1}$$

fully coherent BEC

non-condensed waves.

$$g_{nc}(\underline{r}) = \int \frac{1}{(2\pi)^3} d^3\underline{k}\; e^{i\underline{k}\underline{r}} \frac{1}{e^{\beta(\varepsilon_k-\mu)}-1}$$

a) $|\beta\mu| \gg 1 \longrightarrow$ non-degenerate gas (all modes $N(\underline{k}) \ll 1$).

$$g_{nc}(r) \simeq \int \frac{V\, d^3k}{(2\pi)^3} e^{-\beta\mu} \, e^{-\frac{\beta\hbar^2}{2m}k^2} \, e^{i\underline{k}\cdot\underline{r}}.$$

gaussian weight

$$g_{nc}(r) \simeq n \cdot e^{-\pi r^2/\lambda_T^2}$$ (gaussian, charact length $\simeq \lambda_T$)

b) $|\beta\mu| \lesssim 1 \longrightarrow$ degenerate gas but not BEC.

$$g_{nc}(\underline{r}) \overset{\text{low-}k\text{ expansion}}{\simeq} \int \frac{V\, d^3k}{(2\pi)^3} \frac{k_B T}{\frac{\hbar^2 k^2}{2m} + |\mu|} e^{i\underline{k}\cdot\underline{r}} =$$

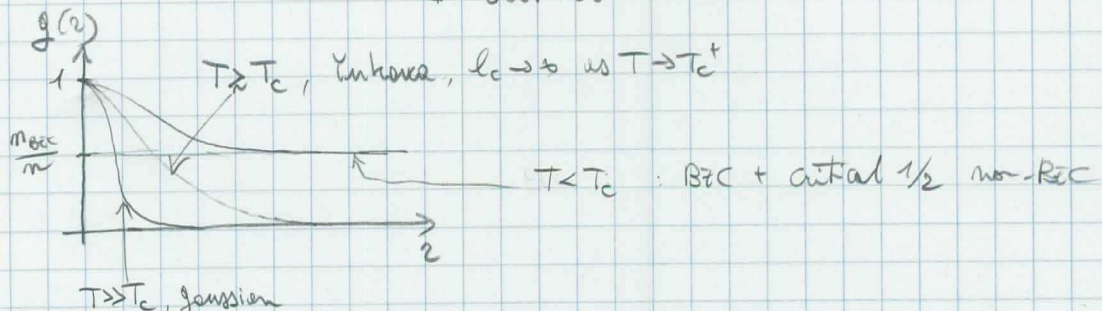
$$\overset{r\to\infty}{\simeq} c^{te} \frac{e^{-r/\ell_c}}{r} \quad \text{with } \ell_c = \frac{\lambda_T}{\sqrt{4\pi\left(1-e^{\beta\mu}\right)}} \simeq \frac{\lambda_T}{\sqrt{4\pi|\beta\mu|}}$$

* Yukawa-like shape, $\ell_c \gg \lambda_T$
* $\ell_c \to \infty$ as critical point approached $|\beta\mu| \to 0$.

c) BEC $\mu = 0$:

$$g_{nc}(r) \simeq \int \frac{V\, d^3k}{(2\pi)^3} \frac{k_B T}{\frac{\hbar^2}{2m} k^2} e^{i k \cdot r} \overset{r\to\infty}{\simeq} \frac{1}{(2\pi)^3 \lambda_T^2 \cdot r}$$

* critical behavior



iv) <u>Spontaneous symmetry breaking and η-ensemble</u>

BEC = appearance of long-range order in $g^{(1)}(r)$.

$$H - \mu N - \int d^3r \left(\eta(r) \cdot \hat{\psi}^\dagger(r) + \eta^*(r)\, \hat{\psi}(r) \right)$$

η-field couples to matter field ψ

uniform in space $\eta(r) = \eta \Rightarrow H - \mu N - V(\eta \psi_0^\dagger + \eta^* \psi_0)$

couples only to BEC $\left[\psi_0 = \frac{1}{\sqrt{V}} \cdot a_0 \right]$

Canonical transformation $b_0 = a_0 - \frac{\sqrt{V}}{\varepsilon_0 - \mu} \eta$, $[b_0, b_0^\dagger] = 1$

$$H' = H - \mu N - V(\eta \psi_0^\dagger + \eta^* \psi_0) = \sum_{n \neq 0} (\varepsilon_n - \mu)\, a_n^\dagger a_n + (\varepsilon_0 - \mu)\, b_0^\dagger b_0 + - \frac{V}{\varepsilon_0 - \mu} |\eta|^2$$

$$\Xi = \mathrm{Tr}\left[e^{-\beta H'}\right]$$

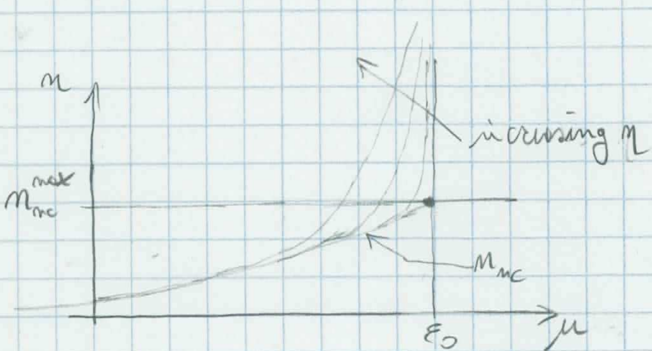
$$N = k_B T \frac{\partial}{\partial \mu} \log \Xi = \frac{V}{\mu^2}|\eta|^2 + N_{\eta=0}(T,\mu)$$

$$n = \frac{|\eta|^2}{\mu^2} + n_{nc}(T,\mu) + \frac{1}{V}\frac{1}{e^{-\beta\mu}-1}$$

<u>for any $|\eta|>0$</u> : $\frac{|\eta|^2}{\mu^2} + n_{nc}(T,\mu) \longrightarrow \infty$ as $\mu \to 0^-$

No need for setting $\mu = 0$

3^{rd} term not contributing ($V \to \infty$ first)



$$\langle \psi \rangle = \frac{\eta}{|\mu|}$$

$$n = |\langle \psi \rangle|^2 + n_{nc}$$

<u>Limit $\eta \to 0$</u> :

a) $n < n_{nc}^{max}$: $\mu \to \bar{\mu}$ such that $n_{nc}(\bar{\mu}, T) = n$

$|\langle \psi \rangle| \to 0$

b) $n > n_{nc}^{max}$: $\mu \to 0^-$ as $\mu \simeq |\eta|$

so that $\langle \psi \rangle \to$ finite constant

such that $|\langle \psi \rangle|^2 = n - n_{nc}$.

* Phase of ψ determined by phase of η.

* Crucial point : <u>order of limits</u>, first $V \to \infty$, then $\eta \to 0$

(see discussion in Huang's book)

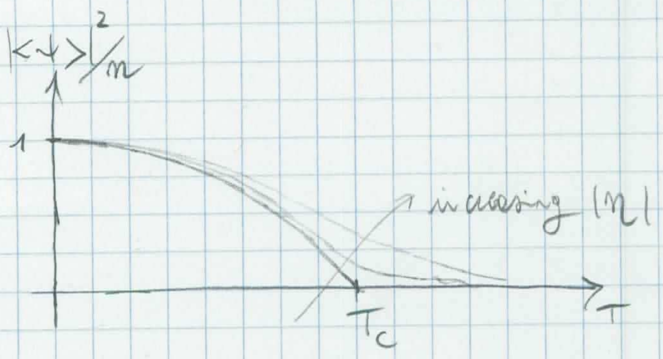


Diagram very similar to MF theory of ferromagnets.

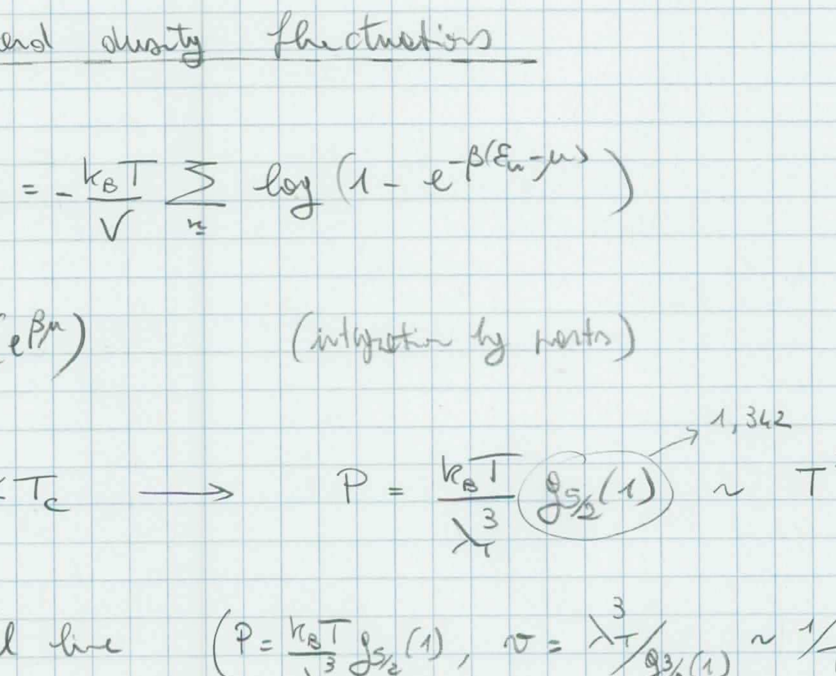
v) Equation of state and density fluctuations

$$P = \frac{k_B T}{V} \log \Xi = -\frac{k_B T}{V} \sum_n \log\left(1 - e^{-\beta(\varepsilon_n - \mu)}\right)$$

$$= \frac{k_B T}{\lambda_T^3}\, g_{5/2}(e^{\beta\mu}) \qquad \text{(integration by parts)}$$

* $T < T_c \longrightarrow P = \frac{k_B T}{\lambda_T^3} \underbrace{g_{5/2}(1)}_{1{,}342} \sim T^{5/2}$

* critical line $\left(P = \frac{k_B T}{\lambda_T^3} g_{5/2}(1),\ v = \lambda_T^3 / g_{3/2}(1) \sim 1/T^{3/2}\right)$



* for $T < T_c$: $\frac{\partial P}{\partial v} = 0 \longrightarrow$ pathological behaviour
infinite compressibility

At given P $\longrightarrow$ what fluctuations $\Delta V^2 = k_B T \frac{\partial V}{\partial \mu} \longrightarrow \infty$.

Related to diverging number fluctuations of condensate mode

$$\Delta N_0^2 \sim N_0 (N_0 + 1).$$

NOTE : with different boundary conditions also BEC can contribute to μ
(see CCT lecture 97-98, III-12)

Number fluctuations of non-condensed modes:

$$\Delta N_{nc}^2 = \sum_{n \neq 0} n_n (1 + n_n) \sim \frac{m^2 (k_B T)^2}{\hbar^4} V^{4/3} \quad \text{for } T < T_c.$$

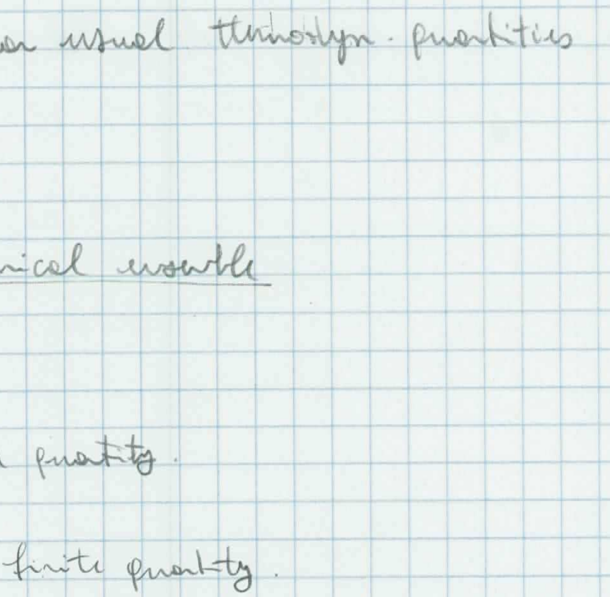
relative fluctuations $\frac{\Delta N_{nc}^2}{N_T^2} \sim V^{-2/3} \longrightarrow 0$ in thermodyn limit

but slower than usual thermodyn. quantities $\sim 1/V$

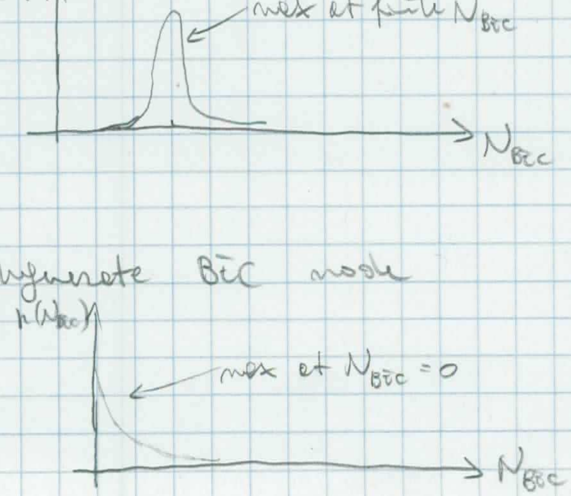
Pathology is solved in canonical ensemble

$$N_{BEC} = \underbrace{N_T}_{\text{fixed quantity}} - N_{nc}$$

$$\left.\begin{array}{l} * \ \Delta N_{BEC}^2 = \text{finite quantity.} \\ * \ \left(\frac{\Delta N_{BEC}}{N_T}\right)^2 \longrightarrow 0 \ \text{in thermodynamic limit.} \end{array}\right\} T < T_c$$



While for $T > T_c$: non-degenerate BEC mode



Another, related pathology of the ideal Bose gas

So far: periodic boundary conditions

$$\phi_{BEC}(x) = 1/\sqrt{V}$$

Dirichlet boundary conditions : $\phi_{BEC}(x) = \sqrt{\frac{8}{V}} \sin\left(\frac{\pi x}{L_x}\right) \cdot \sin\left(\frac{\pi y}{L_y}\right) \sin\left(\frac{\pi z}{L_z}\right)$

→ completely different density profile at low T.
→ related to infinite compressibility.

All pathologies disappear when interactions (even weak ones) are included in the theory.

* C. Cohen-Tannoudji's lectures at Collège de France, year 97-98 and 99-00
  http://www.phys.ens.fr/cours/college-de-france

* Pitaevskii and Stringari, "BEC", Clarendon Press, Oxford, 2003
* Huang, "Statistical Mechanics", Wiley, 1963

* Ziff, Uhlenbeck, Kac, Phys Rep 32, 169 (1977) "The ideal B-E gas, revisited"
* Gunton, Buckingham, Phys Rev 166, 152 (1968) "Condensation of the ideal Bose gas as a cooperative transition"

* IC and Y. Castin, J. Phys. B 34, 4059 (2001). In particular Fig. 5.