Lecture 2 : Ideal and interacting harmonically trapped Bose gases: BEC ?

i) Ideal Bose gas in 3D harmonic trap

$$N_{nc} = \sum_{\vec{n}} \frac{1}{e^{\beta(\hbar\vec{\omega}\cdot\vec{n} - \mu)} - 1}$$

with
$$\begin{cases} \vec{n} = (n_x, n_y, n_z) \in [0,\infty]^3 \\ \vec{\omega} = (\omega_x, \omega_y, \omega_z) \\ \text{reabsorb 0-point energy into } \mu \rightarrow \mu + \frac{1}{2}(\omega_x + \omega_y + \omega_z) \end{cases}$$

$$\simeq \int_0^\infty dn_x\, dn_y\, dn_z \frac{1}{e^{\beta(\hbar\vec{\omega}\cdot\vec{n} - \mu)} - 1} =$$

$$= \int_0^\infty d^3\vec{n}' \frac{1}{e^{\beta\hbar\bar{\omega}(n'_x + n'_y + n'_z)} - 1}$$

$$\vec{n}' = \left(\frac{\omega_x}{\bar{\omega}} n_x, \ldots \frac{\omega_z}{\bar{\omega}} n_z\right)$$

$$\bar{\omega} = \sqrt[3]{\omega_x \omega_y \omega_z}$$

$$= \int_0^\infty \frac{n_T^2}{2} dn_T \frac{1}{e^{\beta\hbar\bar{\omega} n_T} - 1} =$$

$$n_T = n'_x + n'_y + n'_z$$

$$= \left(\frac{k_B T}{\hbar\bar{\omega}}\right)^3 \cdot g_3(1) \quad < \infty$$

$\Rightarrow$ BEC possible in 3D Harmonic Trap

$$k_B T_c = \left(\frac{N}{g_3(1)}\right)^{1/3} \hbar\bar{\omega}$$

$g_3(1) = 1{,}202$

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

Note different exponent w/r homogeneous gas.

Replacement $\sum \longrightarrow \int$ is valid if $k_B T \gg \hbar\omega$.

Thermodynamic limit:

- homogeneous system : $N, V \to \infty$ with $\frac{N}{V}$ = constant
- trapped system : $N \to \infty$, $\omega \to 0$
  keeping $N^{1/3}\omega$ = constant

$\hookrightarrow$ gives constant T_c

$\longrightarrow$ for given T gives a constant N_{BEC}/N

A quite complicate calculation shows that BEC transition corresponds to central density getting to critical value $n(r)\lambda_T^3 = g_{3/2}(1)$
[see Castin lecture notes]

ii) Semiclassical theory

$$n(r,p) = \frac{1}{\exp\left[\beta(\varepsilon(r,p)-\mu)\right]-1} \quad , \quad \varepsilon(r,p) = V(r) + \frac{p^2}{2m}$$

Above T_c : $n(r) = \int d^3p \; n(r,p) = \frac{1}{\lambda_T^3} g_{3/2}\left(e^{-\beta(V(r)-\mu)}\right)$

Below T_c : $n(r) = \frac{1}{\lambda_T^3} g_{3/2}\left(e^{-\beta V(r)}\right) + N_{BEC}\,\delta^3(r)$ $\rightarrow$ can not account for BEC zero-point motion

with N_{BEC} defined so that $\int n(r)\, d^3r = N$

$$n(p) = \frac{1}{(\lambda_T \cdot m\bar{\omega})^3}\, g_{3/2}\left(e^{-\beta p^2/2m}\right)$$

Thermal, non-BEC component:

* anisotropic spatial distribution $\sim g_{3/2}(e^{-\beta V(r)})$, broader along weakly confining axis.

* isotropic momentum distribution.

* wings $\left(m\omega^2 r^2/2, \frac{p^2}{2m} >> k_B T\right) \Longrightarrow \begin{cases} n(r) \simeq \frac{1}{\lambda^3} e^{-\beta m\omega^2 r^2/2} \\ n(p) \simeq e^{-\beta p^2/2m} \end{cases}$

(apart from # coeff. $\left(\frac{\zeta(4)}{\zeta(3)} \simeq 1\right)$: $\Delta r_T \simeq \left(\frac{k_B T}{m\omega^2}\right)^{1/2}$ $\quad \Delta p_T = \left(m k_B T\right)^{1/2}$

BEC component:

* $\phi_0(r) = \left(\frac{m\bar{\omega}}{\pi\hbar}\right)^{3/4} \exp\left[-\frac{m}{2\hbar}\left(\omega_x x^2 + \omega_y y^2 + \omega_z z^2\right)\right]$

anisotropic spatial distribution $\quad a_i = \left(\frac{\hbar}{m\omega_i}\right)^{1/2}$

* $\phi_0(p) = \left(\frac{1}{\hbar\pi m\bar{\omega}}\right)^{3/4} \exp\left[-\frac{1}{m\hbar}\left(\frac{p_x^2}{\omega_x} + \frac{p_y^2}{\omega_y} + \frac{p_z^2}{\omega_z}\right)\right]$

anisotropic momentum distribution $\quad \Delta p_i \sim \sqrt{m\hbar\omega_i}$

opposite to the one of spatial distribution

(Heisenberg principle $\Delta x \Delta p \sim \hbar$)

iii) Semiclassical theory of 2D, harmonically trapped gas

critical number $\quad N_{nc} = \int d^2r \, d^2p \, \frac{1}{e^{\beta \varepsilon(r,p)} - 1}$

[i.e. setting $\mu = 0$]

$$= \int d^2r \, \frac{1}{\lambda_T^2} \, g_1\left(e^{-\beta V(r)}\right) = \left(\frac{k_B T}{\hbar \bar{\omega}}\right)^2 g_2(1)$$

in agreement with complete calculation via $\sum \to \int$.

but the density profile is singular at $r = 0$.

$$g_1(z) = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell} \xrightarrow{z \to 1} \infty$$

the simple argument $\quad n(r=0)\,\lambda_T^3 = g_{3/2}(1) \quad$ that was used in 3D does not hold.

BEC requires in fact an infinite density.

iv) Semiclassical + mean-field theory of interacting gas

MF approx $\begin{cases} \text{local interactions, coupling constant } g \\ V(r) = V_{ext}(r) + 2g\, n(r). \end{cases}$

what is the effect of interactions on BEC transition?

* 3D harmonic trap

$$n(r) = \frac{1}{\lambda_T^3}\, g_{3/2}\left(e^{\beta\mu}\, e^{-\beta V(r)}\right)$$

has to be solved self consistently with $V(r) = V_{ext} + 2g\, n(r)$.

NOTE: uniform gas $\longrightarrow n(r) = n$, so simple shift of $\mu \to \mu + 2gn$.

$$N_{nc} = \int d^3r\, n(r, \mu = 2g\, n(0)) \simeq \int d^3r \left[n^0(r) + \frac{\partial n^0}{\partial \mu}\left(2g\, n^0(0) - 2g\, n^0(r)\right)\right]$$

Assumption (for now being 100% valid ...):

external region dominates where $g_{3/2}(z) \simeq z$.

$$\Rightarrow \frac{\partial n^0}{\partial \mu} \simeq \beta n^0$$

in this region, $n^0(r) \ll n^0(0)$, neglect $n^0(r)^2$ terms.

$$N_{nc} \simeq N^0_{nc} + \int d^3r\; 2g\beta\, n^0(r)\, n^0(0) = N^0_{nc} + 2g\beta\, n^0(0) \cdot N^0_{nc} =$$

$$\frac{\Delta N_{mc}}{N^{\circ}_{mc}} \simeq \frac{2g\, n^{\circ}(0)}{k_B T_c^{\circ}} = \frac{2g}{\lambda_T^3\, k_B T}\, \zeta(3/2) =$$

$$= \frac{2\, \frac{4\pi\hbar^2 a}{m}}{\left(\frac{2\pi\hbar^2}{m k_B T}\right)^{3/2} k_B T_c^{\circ}}\, \zeta(3/2) = \frac{4\,\zeta(3/2)\; a}{\left(\frac{2\pi\hbar^2}{m\,\hbar\omega\,(N/\zeta(3))^{1/3}}\right)^{1/2}} =$$

[a = scattering length of atom collisions]

$$\frac{\Delta N_{mc}}{N^{\circ}_{mc}} \simeq \frac{4\,\zeta(3/2)}{\sqrt{2\pi}\,(\zeta(3))^{1/6}}\, N^{1/6}\, \frac{a}{a_{ho}} \qquad \left[a_{ho} = \sqrt{\frac{\hbar}{m\omega}} \right]$$

$$N_{mc} = N^{\circ}_{mc}(T) + \Delta N_{mc}(T) \simeq N^{\circ}_{mc}(T^{\circ} + \Delta T) + \Delta N_{mc}(T^{\circ}) + \dots$$

$$\simeq N^{\circ}_{mc}(T^{\circ}) + \frac{\partial N^{\circ}_{mc}}{\partial T}\cdot \Delta T + \Delta N_{mc}$$

$$\Delta T = -\,\Delta N_{mc} \Big/ \left(\partial N^{\circ}_{mc}/\partial T\right) = -\,\frac{\Delta N_{mc}}{\frac{3}{T_c^{\circ}}\, N^{\circ}_{mc}}$$

$$\Longrightarrow \frac{\Delta T}{T_c^{\circ}} \simeq -\,\frac{1}{3}\,\frac{\Delta N_{mc}}{N^{\circ}_{mc}} = -\,\frac{4\,\zeta(3/2)}{3\sqrt{2\pi}\,(\zeta(3))^{1/6}}\,\frac{a}{a_{ho}}\, N^{1/6}$$

$$\simeq -1{,}35\, \frac{a}{a_{ho}}\, N^{1/6}$$

which is not far from Giorgini's result!

* 2D harmonic trap

non interacting gas $\longrightarrow$ infinite density at centre if BEC

perturbative theory in gn not possible

$$n(r) = \frac{1}{\lambda_T^2}\, g_1\!\left(e^{-\beta\left(V_{ext}(r) + 2g\,n(r) - \mu\right)}\right)$$

with $g_1(z) = -\log(1-z)$

$V_{ext}(r) = \frac{1}{2} m \omega^2 r^2$

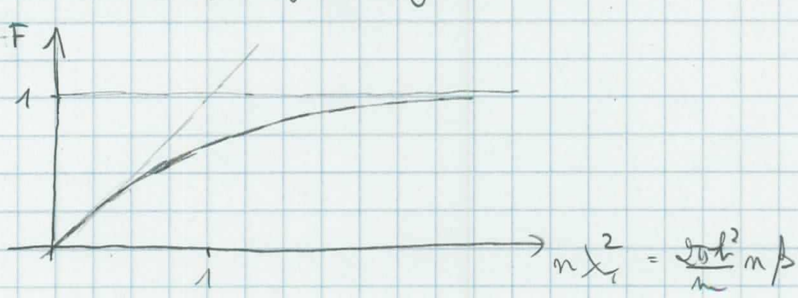
$$e^{-n(r)\lambda_T^2} = 1 - e^{-\beta\left(V_{ext}(r) + 2g\,n(r) - \mu\right)}$$

$$\lambda_T^2 = \frac{2\pi\hbar^2}{m k_B T} = \frac{2\pi\hbar^2\beta}{m}$$

$$\overbrace{e^{2\beta g\,n(r)}\left(1 - e^{-\frac{2\pi\hbar^2}{m}\beta n}\right)}^{F} = e^{\beta\left(\mu - V_{ext}(r)\right)}$$

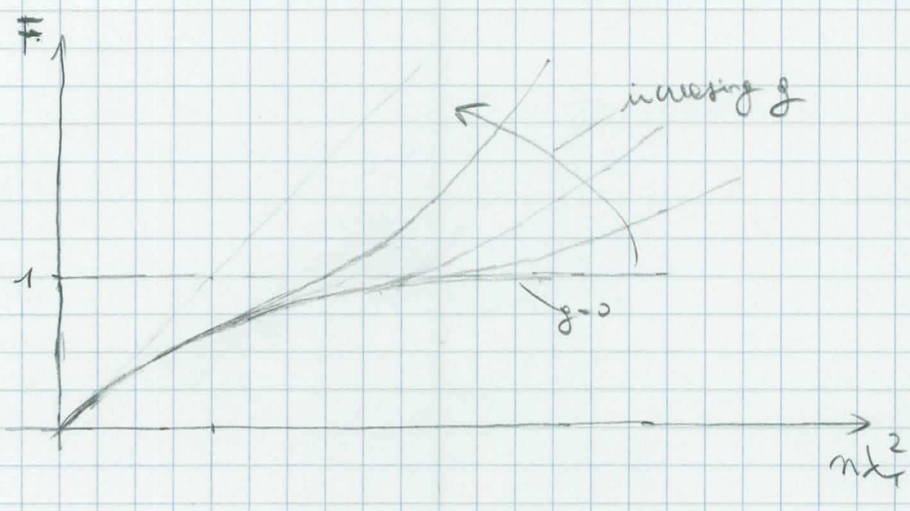
NOTE: MF theory valid only for small $g \ll \frac{2\pi\hbar^2}{m}$

i) non-interacting gas $g=0$



- $\mu - V_{ext}(r) \leq 0$, i.e. $\mu \leq \min(V_{ext})$
- logarithmic $\Rightarrow$ integrable singularity at $n \to \infty$. $\int d^2r\, n(r) < \infty$.

ii) interacting gas $g > 0$



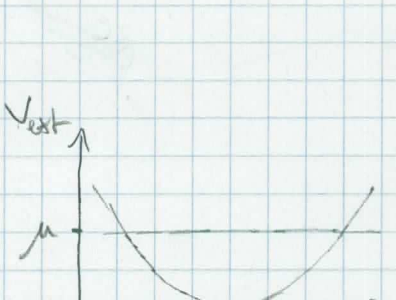
• degenerate limit $\frac{2\pi\hbar^2\beta n}{m} = n\lambda_T^2 \gg 1$

$\Longrightarrow$ $2g\,n(r) + V_{ext}(r) = \mu$ in the bulk
(Thomas - Fermi profile)

$n(r) \sim \frac{1}{\lambda_T^2} e^{\beta(\mu - V_{ext}(r))}$ in tails where $n\lambda_T^2 \ll 1$

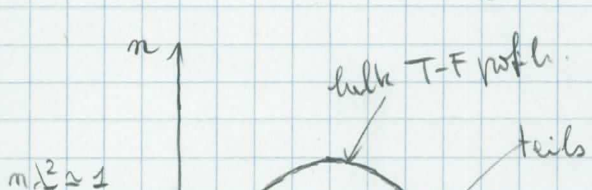
i.e. $\beta(\mu - V_{ext}(r)) \gg 1$

$\hookrightarrow$ BIMODAL SHAPE



• Low - temperature : neglect tails

$$N_{TF} = \int_{\mu > V_{ext}(r)} d^2r \, \frac{1}{2g}\left(\mu - V_{ext}(r)\right) =$$



$$= \int_0^{r_{max}} \frac{\pi}{2g}(2r\,dr)\left(\mu - \frac{1}{2}m\omega^2 r^2\right) =$$

$$= \int_0^{R_{max}} \frac{\pi}{2g}\, dR \left(\mu - \frac{1}{2}m\omega^2 R\right) = \frac{\pi}{2g}\frac{2}{m\omega^2}\int_0^{\mu} d\bar{R}\,(\mu - \bar{R}) = \frac{\pi}{gm\omega^2}\left(\mu^2 - \frac{\mu^2}{2}\right) = \frac{\pi\mu^2}{m\omega^2 g}$$

$$N_{TF} = \frac{\pi\mu^2}{2m\omega^2 g} \xrightarrow{\mu \to \infty} \infty .$$

NO BEC phenomenon!

density always finite at all points.

In conclusion:

- ideal gas in 2D harmonic trap
  → BEC phenomenon
  → infinite density at $r=0$ if BEC

- interactions smoothen singularity in $n(r)$
  → BEC disappears.

Anyway: other transition to superfluid state if
$$n\lambda_T^2 = \log\left(\frac{A\hbar^2}{mg}\right) \quad \text{with } A \simeq 380$$

Berezinskii - Kosterlitz - Thouless Transition

NOTE: BKT transition is beyond MF
bimodal density profile assumes $2gn = \mu - V_{ext}$
but factor 2 is OK only for non degenerate gas.
corrections are possibly needed

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