Lec. 17 Ideal Bose gas

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} - 1} = \frac{1}{z^{-1} e^{\beta\varepsilon} - 1}$$

$$N = \sum_{\varepsilon} f(\varepsilon) = \sum_{\varepsilon} \frac{1}{z^{-1} e^{\beta\varepsilon} - 1}$$

$$\Omega = -pV = +k_B T \sum_{\varepsilon} \ln\left(1 - z e^{-\beta\varepsilon}\right)$$

3D system of (spinless) bosons

$$\sum_{\varepsilon} \rightarrow \int d\varepsilon \, g(\varepsilon)$$

$$N(\varepsilon) = \frac{V}{(2\pi)^3} \frac{4\pi}{3} k^3(\varepsilon) = \frac{V}{6\pi^2} \left(\frac{2m\varepsilon}{\hbar^2}\right)^{3/2}$$

$$g(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2} = a\, \varepsilon^{1/2} V$$

$$\frac{N}{V} \simeq a \int_0^{\infty} \frac{\varepsilon^{1/2} \, d\varepsilon}{z^{-1} e^{\beta\varepsilon} - 1} + \frac{1}{V} \frac{z}{1-z}$$

particles in $\varepsilon = 0$ orbital

Let $x = \beta\varepsilon$

$$\frac{N}{V} = a\left(k_B T\right)^{3/2} \int_0^\infty \frac{x^{1/2}\, dx}{z^{-1} e^{x} - 1} + \underbrace{\frac{1}{V}\frac{z}{1-z}}_{\frac{N_0}{V}}$$

$$\frac{N - N_0}{V} = \frac{2\pi \left(2m k_B T\right)^{3/2}}{h^3} \int_0^\infty \frac{x^{1/2}\, dx}{z^{-1} e^{x} - 1} = \frac{1}{\lambda^3} g_{3/2}(z)$$

$$\lambda = \frac{h}{\sqrt{2\pi m k_B T}} \qquad g_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}\, dx}{z^{-1} e^{x} - 1}$$

$$\frac{P}{k_B T} = -\frac{2\pi \left(2m k_B T\right)^{3/2}}{h^3} \int_0^\infty x^{1/2} \ln\left(1 - z e^{-x}\right) dx = \frac{1}{\lambda^3} g_{5/2}(z)$$

$$E = -\frac{\partial}{\partial \beta} \ln \mathcal{Z} = k_B T^2 \frac{\partial}{\partial T}\left(\frac{PV}{k_B T}\right) = \frac{3}{2} k_B T \frac{V g_{5/2}(z)}{\lambda^3}$$

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

1) <u>Bose-Einstein condensation</u>

$z = e^{\beta\mu} < 1$ If $\lim_{z\to 1} \frac{N - N_0}{V} < \frac{N}{V}$, then there must be a macroscopic # of particles in g.s. orbital.

$$\frac{N_e}{V} = \frac{N - N_0}{V} = \frac{(2\pi m k_B T)^{3/2}}{h^3} g_{3/2}(z)$$

$$\lim_{z \to 1} g_{3/2}(z) = g_{3/2}(1)$$

In general,

$$g_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}\, dx}{z^{-1} e^x - 1} = z + \frac{z^2}{2^\nu} + \frac{z^3}{3^\nu} + \cdots$$

$$g_\nu(1) = 1 + \frac{1}{2^\nu} + \frac{1}{3^\nu} + \cdots$$

$$= \sum_{\ell=1}^{\infty} \frac{1}{\ell^\nu} = \zeta(\nu)$$ Riemann zeta function

$$\zeta(3/2) = 2.61238$$

$$\frac{N_e}{V} \le \frac{(2\pi m k_B T)^{3/2}}{h^3} \zeta(3/2)$$

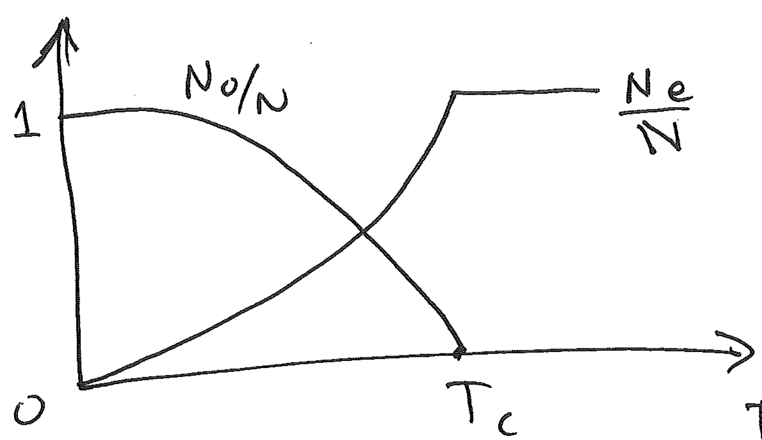
Critical temperature

$$\frac{N}{V} = \frac{(2\pi m k_B T_c)^{3/2}}{h^3} \zeta(3/2)$$

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

For $T < T_c$,

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



Chemical potential

$$N_0 = \frac{z}{1-z} \qquad z = \frac{N_0}{N_0+1} = \frac{1}{1+\frac{1}{N_0}} \approx 1 - \frac{1}{N_0}$$

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

$$\mu \simeq k_B T \ln\left(1 - \frac{1}{N_0}\right) \simeq -\frac{k_B T}{N_0}$$

$$\mu \simeq -\frac{k_B T}{N\left(1-\left(T/T_c\right)^{3/2}\right)}$$

pressure

Below T_c, $z \approx 1$

$$p = \frac{k_B T}{\lambda^3}\zeta\left(\tfrac{5}{2}\right), \quad \zeta\left(\tfrac{5}{2}\right) = 1.34149$$

$$p(T_c) = \left(\frac{2\pi m}{h^2}\right)^{3/2}(k_B T_c)^{5/2}\zeta\left(\tfrac{5}{2}\right)$$

$$= \frac{\zeta\left(\frac{5}{2}\right)}{\zeta\left(3/2\right)}\frac{N}{V}k_B T_c \simeq 0.5134\,\frac{N k_B T_c}{V}$$

Specific heat

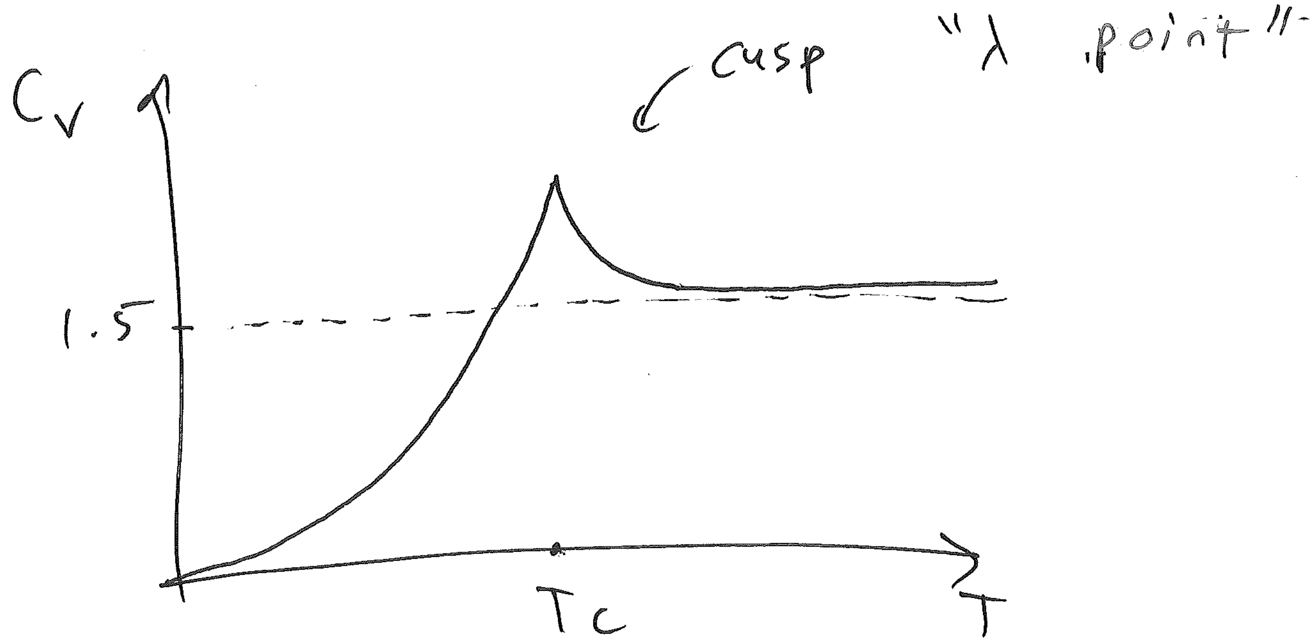
$$C_V = \left.\frac{\partial E}{\partial T}\right|_{V,N} = \frac{3}{2}\frac{\partial}{\partial T}(pV)\Big|_{V,N}$$

For $T < T_c$,

$$\frac{C_V}{N k_B} = \frac{3}{2} \frac{V}{N} \zeta\left(\tfrac{5}{2}\right) \frac{d}{dT}\left(\frac{T}{\lambda^3}\right) = \frac{15}{4} \zeta\left(\tfrac{5}{2}\right) \frac{V}{N\lambda^3}$$

$$\frac{C_V(T_c)}{N k_B} = \frac{15}{4} \frac{\zeta\left(\tfrac{5}{2}\right)}{\zeta\left(\tfrac{3}{2}\right)} = 1.925 > 1.5$$

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



Cf. transition in He^4 @ 2.19 K

(theory of ideal Bose gas predicts $T_c = 3.13$ K)

2) 2D spinless bosons

$$N(\varepsilon) = \frac{A}{(2\pi)^2} \pi k^2 = \frac{mA\varepsilon}{2\pi\hbar^2}$$

$$g(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{mA}{2\pi\hbar^2} = \text{const.}$$

$$\frac{N-N_0}{A} = \frac{m}{2\pi\hbar^2} \int_0^\infty \frac{d\varepsilon}{z^{-1}e^{\beta\varepsilon} - 1}$$ let $x = \beta\varepsilon$

$$\frac{N-N_0}{A} = \frac{mk_BT}{2\pi\hbar^2} \int_0^\infty \frac{dx}{z^{-1}e^{x} - 1} = \frac{mk_BT}{2\pi\hbar^2} \int_0^\infty \frac{ze^{-x}\,dx}{1 - ze^{-x}}$$

$$= \frac{mk_BT}{2\pi\hbar^2} \ln\left(1 - ze^{-x}\right)\Big|_0^\infty = -\frac{mk_BT}{2\pi\hbar^2} \ln(1-z)$$

$$\frac{N-N_0}{A} \longrightarrow \infty \quad \text{as} \quad z \to 1$$

<u>No BEC in 2D!</u>

Also not in 1D, where $g(\varepsilon) \propto \varepsilon^{-1/2}$.

The absence of BEC in $d < 3$ is

a consequence of the <u>Mermin-Wagner theorem</u>, according to which a continuous symmetry cannot be broken at $T > 0$ in 2D (but can be broken at $T = 0$ in 2D). A continuous symmetry cannot be broken even at $T = 0$ in 1D.

The continuous symmetry in question is the $U(1)$ symmetry corresponding to the phase of the ground state orbital:

$$\psi_0(\vec{r}) \longrightarrow e^{i\theta}\psi_0(\vec{r}).$$

In the BEC, the macroscopic occupation of the g.s. orbital renders $\psi_0(\vec{r})$ observable, so the phase symmetry is broken.

3) BEC in a harmonic potential

Consider a system of N spinless bosons in a harmonic confinement potential:

$$V(\vec{r}) = \frac{1}{2} m \left(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2 \right)$$

Single-particle eigenstates:

$$\varepsilon(n_1, n_2, n_3) = \hbar \omega_1 (n_1 + \tfrac{1}{2}) + \hbar \omega_2 (n_2 + \tfrac{1}{2}) + \hbar \omega_3 (n_3 + \tfrac{1}{2})$$

$$n_i = 0, 1, 2, \ldots, \infty$$

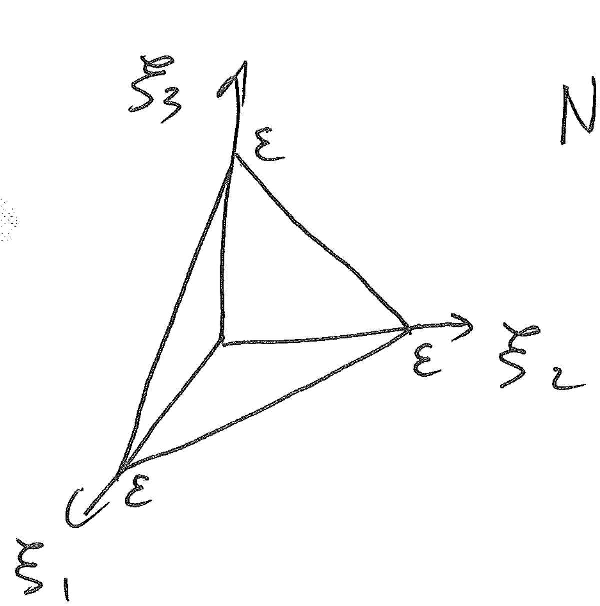
Let $\varepsilon = \varepsilon(n_1, n_2, n_3) - \frac{\hbar}{2}(\omega_1 + \omega_2 + \omega_3)$

$$N(\varepsilon) \cong \int_0^\infty dn_1 \int_0^\infty dn_2 \int_0^\infty dn_3 \; \theta(\varepsilon - \hbar\omega_1 n_1 - \hbar\omega_2 n_2 - \hbar\omega_3 n_3)$$

Let $\xi_i = \hbar \omega_i n_i$

$$N(\varepsilon) \simeq \frac{1}{(\hbar\omega_0)^3} \int_0^\infty d\xi_1 \int_0^\infty d\xi_2 \int_0^\infty d\xi_3 \; \theta(\varepsilon - \xi_1 - \xi_2 - \xi_3),$$

where $\omega_0^3 = \omega_1 \omega_2 \omega_3$.



$$N(\varepsilon) = \frac{1}{6}\frac{\varepsilon^3}{(\hbar\omega_0)^3}$$

$$g(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{1}{2}\frac{\varepsilon^2}{(\hbar\omega_0)^3}$$

$$N - N_0 = \int_0^\infty \frac{g(\varepsilon)\,d\varepsilon}{z^{-1}e^{\beta\varepsilon} - 1} = \frac{1}{2}\frac{1}{(\hbar\omega_0)^3}\int_0^\infty \frac{\varepsilon^2\,d\varepsilon}{z^{-1}e^{\beta\varepsilon} - 1}$$

$$= \frac{1}{2}\left(\frac{k_B T}{\hbar\omega_0}\right)^3 \int_0^\infty \frac{x^2\,dx}{z^{-1}e^{x} - 1}$$

$$= \left(\frac{k_B T}{\hbar\omega_0}\right)^3 g_3(z)$$

critical temperature

$$N = \left(\frac{k_B T_c}{\hbar\omega_0}\right)^3 g_3(1) = \left(\frac{k_B T_c}{\hbar\omega_0}\right)^3 \zeta(3)$$

$$k_B T_c = \hbar\omega_0\left(\frac{N}{\zeta(3)}\right)^{1/3}$$

For $T < T_c$,

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

BEC in a dilute gas of ultracold atoms was observed for the first time in 1995 for ^{87}Rb and ^{23}Na.