PHYS 425 - w7l2

Systems of Non-interacting Bosons at Low Temps.

Recall wavefcn for monatomic particle in 3-D box (cube w/ sides length L)

$$\phi_i(x,y,z) = A \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right)$$

normalization const.

$n_x = 1, 2, 3, \ldots$

$n_y = 1, 2, 3, \ldots$

$n_z = 1, 2, 3, \ldots$

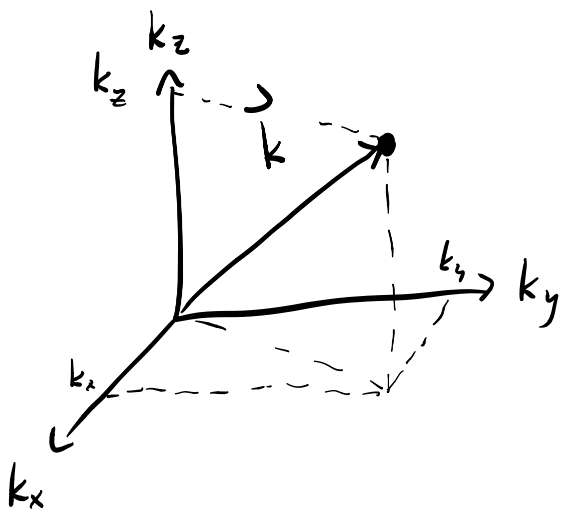
$$= A \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

$$k = \frac{n\pi}{L}$$

$$\hat{H} = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

$$\hat{\mathcal{H}} \phi_i = \frac{\hbar^2 k^2}{2m} \phi_i \qquad k^2 = k_x^2 + k_y^2 + k_z^2$$

$$\therefore \quad \varepsilon_i = \frac{\hbar^2 k^2}{2m} \Rightarrow \varepsilon = \varepsilon(k)$$



Look at properties of non-interacting gas of Bosons.

Bose-Einstein dist'n

$$\Rightarrow \bar{N}_{BE}(k) = \frac{1}{e^{(\varepsilon(k)-\mu)/k_B T} - 1}$$

avg. no. of Bosons in state k w/ energy $\varepsilon(k)$.

Gnd state corresponds to $n_x = n_y = n_z = 1$

$$\therefore \varepsilon' = \frac{\hbar^2}{2m}\left[\left(\frac{\pi}{L}\right)^2 + \left(\frac{\pi}{L}\right)^2 + \left(\frac{\pi}{L}\right)^2\right]$$

gnd state energy

$$= \frac{3\hbar^2\pi^2}{2mL^2}$$

Value of gnd state energy not physically important, only differences in energy matter.

Shift $\varepsilon(k)$ by $-\varepsilon'$

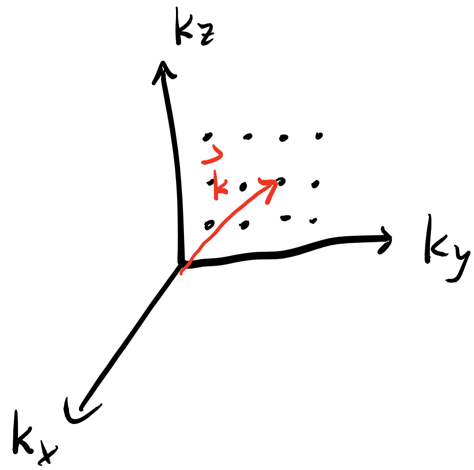
$$\varepsilon(k) = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right) - \varepsilon'$$

$$= \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2 - 3\right)$$

Now gnd state energy is $\varepsilon_0 = 0$.

Total no. of Bosons in the system is

$$N = \sum_{\substack{\text{all quantum}\\ \text{states}}} \bar{N}_{BE}$$



$$\boxed{N = \sum_{\vec{k}} \frac{1}{e^{(\varepsilon(k)-\mu)/k_BT}-1}}$$

sum over all $\vec{k}$ vectors.

$$\therefore N = \frac{1}{e^{(\varepsilon_0-\mu)/k_BT}-1} + \frac{1}{e^{(\varepsilon_1-\mu)/k_BT}-1} + \frac{1}{e^{(\varepsilon_2-\mu)/k_BT}-1} + \ldots$$

since $\varepsilon_0 = 0$

$$= \underbrace{\frac{1}{e^{-\mu/k_BT}-1}}_{\bar{N}_0} + \underbrace{\frac{1}{e^{(\varepsilon_1-\mu)/k_BT}-1}}_{\bar{N}_1} + \underbrace{\frac{1}{e^{(\varepsilon_2-\mu)/k_BT}-1}}_{\bar{N}_2} + \ldots$$

$\bar{N}_0$ avg. no. of particles in gnd state

Examine $\bar{N}_0 = \dfrac{1}{e^{-\mu/k_BT} - 1}$

If $\mu > 0$, then $e^{-\mu/k_BT} < 1$

& $\dfrac{1}{e^{-\mu/k_BT} - 1} < 0$

$\bar{N}_0 < 0$ is unphysical (can't have neg. no. of particles in a state).

$\Rightarrow$ Require $\mu < 0$.

What happens to $\bar{N}_0, \bar{N}_1, \bar{N}_2, \ldots$ as $T \to 0$? To answer this question, we need to know the temp. dependence of μ so that we can evaluate $\dfrac{\mu}{k_BT}$ in the exponential.

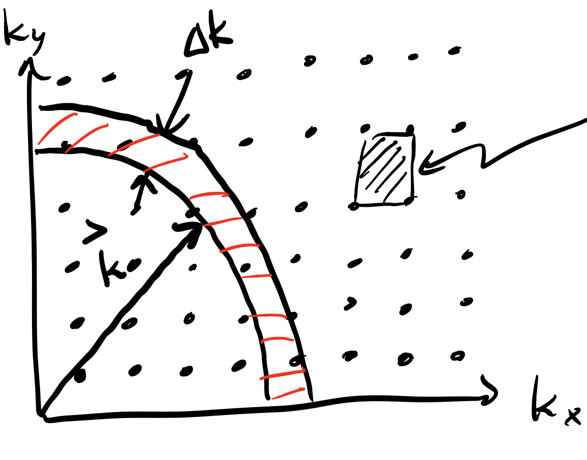
First, we will turn sum over $\vec{k}$ in our expression for N into a sum over mag. of $\vec{k} \Rightarrow k$. Then we will transform the sum into an integral over k.

Consider $\sum_{\vec{k}} \underbrace{f(k)}$

any fcn of the mag. of k.

eg. $\varepsilon(k)$, $\bar{N}_{BE}(k)$

Eg. look in 2-D



each k-state occupies an area in k-space equal to $\left(\frac{\pi}{L}\right)^2$

ring of const k has area of $\dfrac{2\pi k \Delta k}{4}$

no. of states in ring is: $\dfrac{\frac{2\pi k \Delta k}{4}}{\left(\frac{\pi}{L}\right)^2} = \dfrac{L^2 k \Delta k}{2\pi}$

2-D	3-D
$A_k = \left(\frac{\pi}{L}\right)^2$	$V_k = \left(\frac{\pi}{L}\right)^3$
$A_{ring} = \dfrac{\pi k \Delta k}{2}$	$V_{shell} = \dfrac{4\pi k^2 \Delta k}{8} = \dfrac{\pi k^2 \Delta k}{2}$
$g_{ring} = \dfrac{L^2 k \Delta k}{2\pi}$	$g_{shell} = \dfrac{L^3 k^2 \Delta k}{2\pi^2}$

$$\underset{\text{sum over vector } \vec{k}}{\sum_{\vec{k}} f(k)} \xrightarrow{\text{equiv to}} \underset{\text{sum over mag. of } \vec{k}\text{-vectors}}{\sum_{k}} f(k) \underbrace{\frac{V k^2 \Delta k}{2\pi^2}}_{\text{no. of states in shell of radius } k \text{ thickness } \Delta k} \qquad V \equiv L^3$$

$$N = \sum_{\vec{k}} \bar{N}_{BE}(k) = \frac{V}{2\pi^2} \sum_{k} \frac{k^2 \Delta k}{e^{(\varepsilon(k)-\mu)/k_B T} - 1}$$

in limit Δk small $\quad \lim_{\Delta k \to 0} \sum_k f'(k) \Delta k = \int f'(k) dk$

$$N = \frac{V}{2\pi^2} \int_{k=0}^{\infty} \frac{k^2 dk}{e^{(\varepsilon(k)-\mu)/k_B T} - 1} \qquad \varepsilon(k) = \frac{\hbar^2 k^2}{2m}$$

$$N = \frac{V}{2\pi^2} \int_0^{\infty} \frac{k^2 dk}{e^{\hbar^2 k^2/2mk_B T} e^{-\mu/k_B T} - 1}$$

make sub. $\quad x^2 = \frac{\hbar^2 k^2}{2mk_B T}$

$$k = \sqrt{\frac{2mk_B T}{\hbar^2}}\, x \qquad dk = \sqrt{\frac{2mk_B T}{\hbar^2}}\, dx$$

$$N = \frac{V}{2\pi^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{x^2\,dx}{e^{x^2}e^{-\eta}-1} \quad \text{where } \eta \equiv \frac{\mu}{k_BT}$$

$$\therefore \quad 2\pi^2 \underbrace{\frac{N}{V}}_{n \text{ no. density of Bosons}}\left(\frac{\hbar^2}{2mk_BT}\right)^{3/2} = \int_0^\infty \frac{x^2\,dx}{e^{x^2-\eta}-1}$$

$$\boxed{2\pi^2 n\left(\frac{\hbar^2}{2mk_BT}\right)^{3/2} = \int_0^\infty \frac{x^2\,dx}{e^{x^2-\eta}-1}}$$

use this expression to determine temperature dependence of $\eta = \frac{\mu}{k_BT}$

For example, for liquid ^{4}He $\quad n = 2.2\times10^{28}\,m^{-3}$, $m = 6.68\times10^{-27}\,kg$

$$\therefore \left(\frac{3.42\,K}{T}\right)^{3/2} = \int_0^\infty \frac{x^2\,dx}{e^{x^2-\eta}-1}$$

1. Pick a temp T → evaluate LHS
2. adjust η until RHS = LHS (integral evaluated numerically)
3. now know η at that temp. Can calc. $\mu = k_B T \eta$
4. Repeat for a new temp.

T	LHS	η	μ
T_1	$\left(\frac{3.42\,K}{T_1}\right)^{3/2}$	η_1	$\mu_1 = k_B T \eta_1$
T_2	$\left(\frac{3.42\,K}{T_2}\right)^{3/2}$	η_2	$\mu_2 = k_B T \eta_2$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

This analysis shows that $\eta = \frac{\mu}{k_B T} \to 0$

as $T \to 0$

$$\bar{N}_0 = \frac{1}{e^{-\mu/k_B T} - 1} \gg 1 \text{ when } T \to 0$$

On the other hand $\bar{N}_x$ $(x = 1, 2, 3, \ldots)$

$$\bar{N}_x = \frac{1}{e^{\varepsilon_x / k_B T} \underbrace{e^{-\mu/k_B T}}_{1} - 1} \to \frac{1}{e^{\varepsilon_x / k_B T} - 1}$$

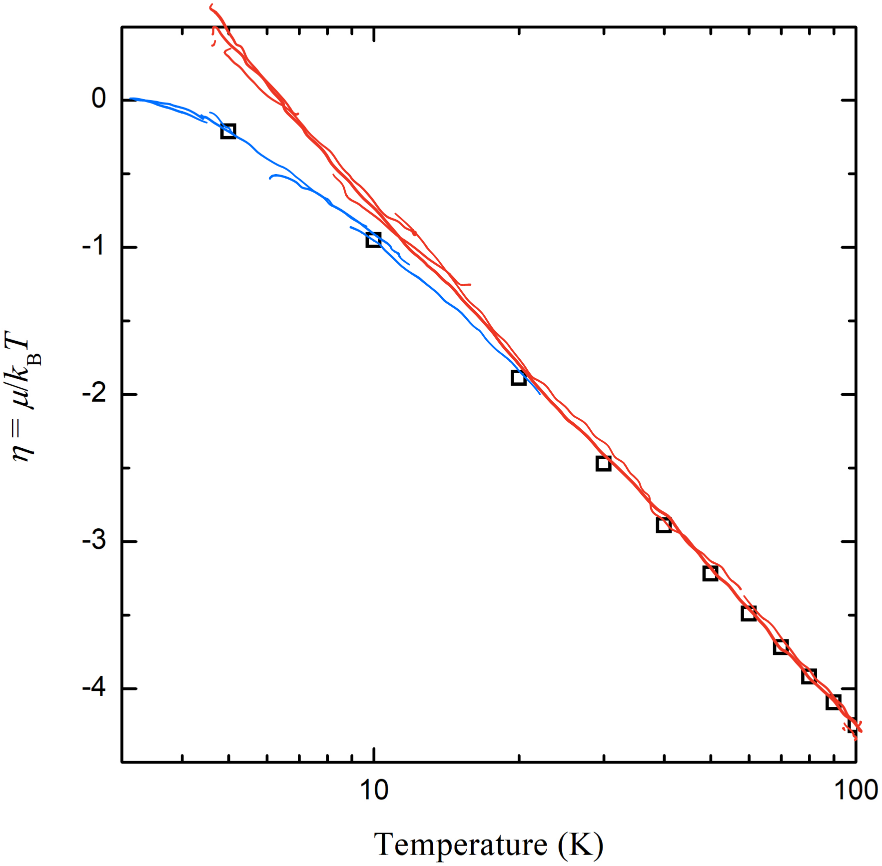
as $T \to 0$.

ε_x is positive (above grnd state energy)

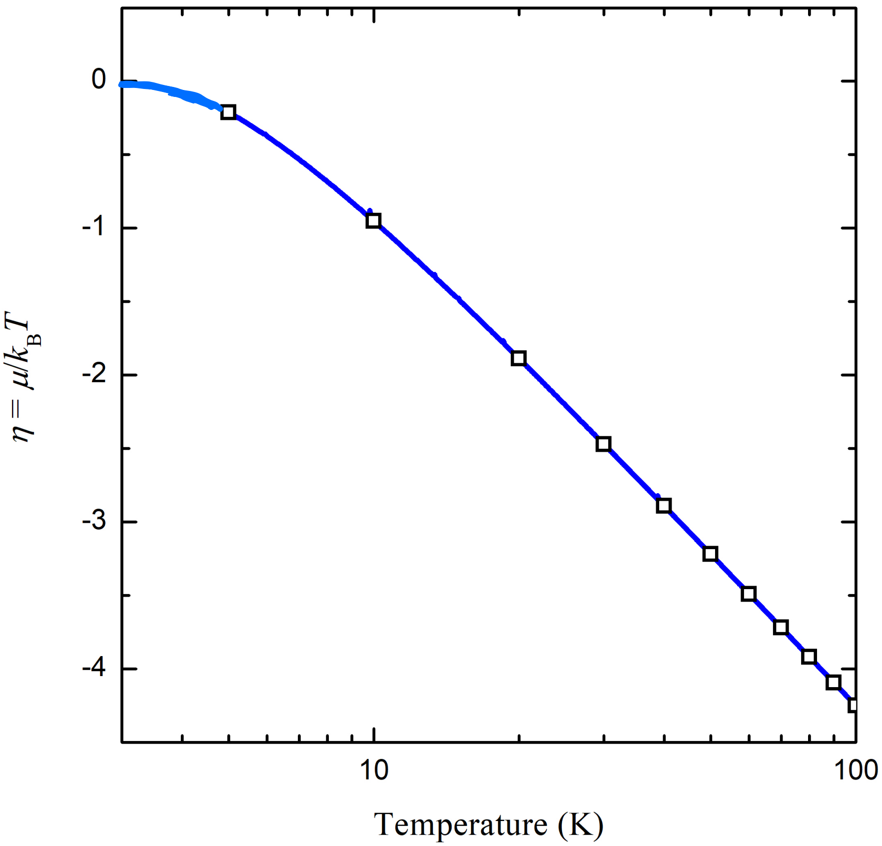
$\therefore e^{\varepsilon_x / k_B T} \gg 0$ as $T \to 0$

$$\therefore \bar{N}_x = \frac{1}{e^{\varepsilon_x / k_B T} - 1} \approx \frac{1}{e^{\varepsilon_x / k_B T}} \to 0$$

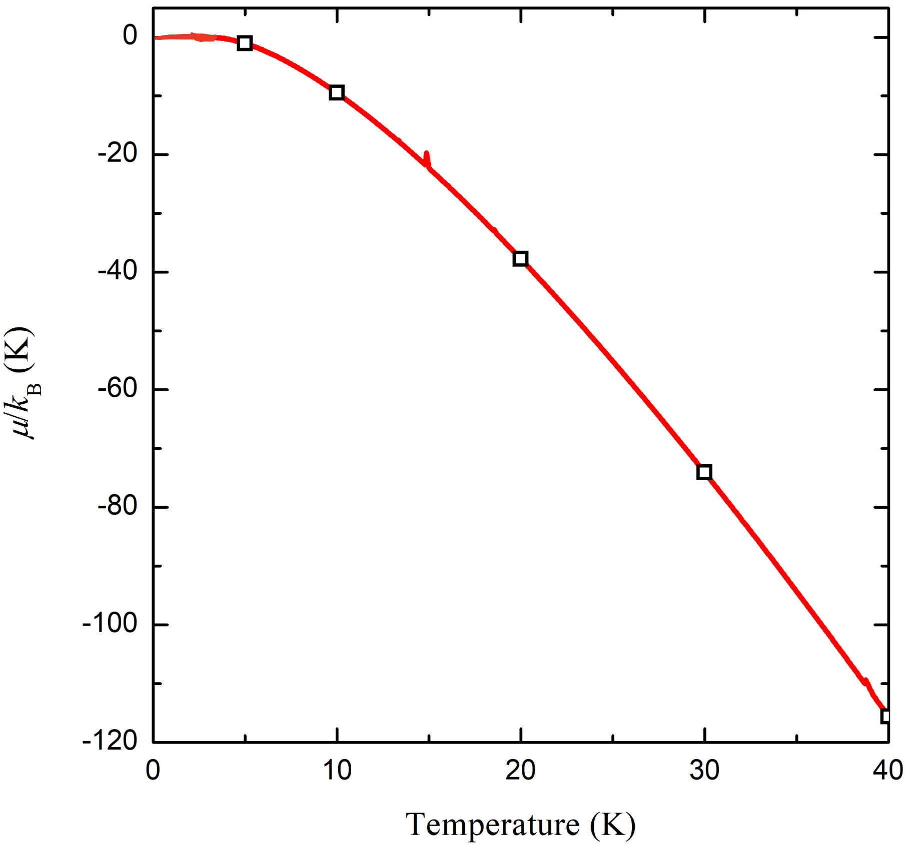
Next time $\Rightarrow$ Bose-Einstein condensation.



0
-1
-2
-3
-4
10
100
Temperature (K)
$\eta = \mu/k_B T$



0
-1
-2
-3
-4
10
100
$\eta = \mu/k_B T$
Temperature (K)


0
-20
-40
-60
-80
-100
-120
0
10
20
30
40
Temperature (K)
μ/k_B (K)