BOSE EINSTEIN CONDENSATION

1924 - Bose - developed distribution for photons treated as indistinguishable particles, yielding Planck radiation law

(Einstein helped get it published)

1925 - Einstein - extended the idea of Bose to massive integer spin particles (bosons) with the additional constraint of number conservation (i.e. included chemical potential) - found condensa[te] at $T \neq 0$, even for <u>non-interacting</u> particles

- was considered unlikely

for a box, gd. state wave fn. $\sim \cos(x)$

$n \sim \cos^2(x)$

why would non-interacting particles "clump" in the grand-canonical ensemble:

$$\frac{PV}{kT} \equiv \ln Q = -\sum_{\varepsilon} \ln\left(1 - z e^{-\beta\varepsilon}\right)$$

$$N \equiv \sum_{\varepsilon} \langle n_\varepsilon \rangle = \sum_{\varepsilon} \frac{1}{z^{-1} e^{\beta\varepsilon} - 1}$$

$$\beta = 1/kT \qquad z = e^{\mu/kT} = \text{fugacity}$$

assuming large V, the density of states can be written a[s]

$$a(\varepsilon)\,d\varepsilon = \frac{2\pi V}{h^3}(2m)^{3/2}\varepsilon^{1/2}\,d\varepsilon$$

note that this would give gd. state ($\varepsilon = 0$) no density of state weight — but q.m. we know it should exist, so we treat it separately:

turning sums into integrals

$$\frac{P}{kT} = -\frac{2\pi}{h^3}(2m)^{3/2}\int_0^\infty \varepsilon^{1/2}\ln\left(1 - z e^{-\beta\varepsilon}\right) - \frac{1}{V}\ln(1-$$

$$\frac{N}{V} = \frac{2\pi}{h^3}(2m)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}\,d\varepsilon}{z^{-1}e^{\beta\varepsilon} - 1} + \frac{1}{V}\frac{z}{1-z}$$

[illegible] 2nd [illegible]

if we are in the classical limit, $z \ll 1$

and both 2^{nd} terms are of order $1/N$

if $z \to 1$, 2^{nd} term in $\cancel{\frac{P}{kT}}$ ~~eq.~~ $\frac{N}{V}$ eq. (which is $\frac{N_0}{V}$)

may not necessarily be small

since $\frac{N_0}{V} = \left(\frac{z}{1-z}\right)\frac{1}{V} \Rightarrow N_0 = \frac{z}{1-z} \Rightarrow z = \frac{N_0}{N_0+1}$

then in $\frac{PV}{kT}$ eq. $\frac{1}{V}\ln(1-z) = \frac{1}{V}\ln(N_0+1)$

which is of order at most $N^{-1}\ln N$

and is always small and can be neglected.

using $\beta\varepsilon = p^2/2mkT \equiv x$

then: $$\frac{P}{kT} = \frac{-2\pi(2mkT)^{3/2}}{h^3}\int_0^\infty x^{1/2}\ln(1-ze^{-x})\,dx$$

$$= \frac{1}{\lambda^3}\, g_{5/2}(z)$$

where $\lambda = \frac{h}{(2\pi mkT)^{1/2}} \equiv$ Thermal deBroglie waveleng

and $$g_n(z) = \frac{1}{\Gamma(n)}\int_0^\infty \frac{x^{n-1}\,dx}{z^{-1}e^x - 1}$$

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

for small z (near classical), use expansion of g_n fns.

$$g_n(z) = \sum_{j=1}^{\infty}\frac{z^j}{j^n} = z + \frac{z^2}{2^n} + \frac{z^3}{3^n} + \cdots$$

and assume $N_0 \ll N$

inverting eqs. and eliminating z gives the eq. of state

$$\frac{PV}{NkT} = \sum_{j=1}^{\infty} a_j\left(\frac{\lambda^3}{v}\right)^{j-1} \qquad v = \frac{1}{n} \quad \text{volume/p}$$

a_j = virial coefficients

$$a_1 = 1$$

$$a_2 = -\frac{1}{4\sqrt{2}} = -0.177$$

$$a_3 = -\left(\frac{2}{9\sqrt{3}} - \frac{1}{8}\right) = -0.003$$

for the specific heat C_v

$$\frac{C_v}{Nk} = \frac{3}{2}\left\{\frac{\partial}{\partial T}\left(\frac{PV}{Nk}\right)\right\}_v$$

$$= \frac{3}{2}\sum_{j=1}^{\infty}\frac{5-3j}{2}\,a_j\left(\frac{\lambda^3}{v}\right)^{j-1}$$

$$= 3/2\left[1 + .09\left(\frac{\lambda^3}{v}\right) + .007\left(\frac{\lambda^3}{v}\right)^2 + \cdots\right]$$

as $T \to \infty$, $\lambda \to 0$ and $PV = NkT$

$C_v = \frac{3}{2}Nk$

Classical results for Bose-Einstein statistics.

now in opposite limit:

$$N - N_0 = V\frac{(2\pi mkT)^{3/2}}{h^3}\,g_{3/2}(z)$$

$g_{3/2}(z)$ increases monotonically with z, and is max at $z=1$, where

$$g_{3/2}(1) = 1 + \frac{1}{2^{3/2}} + \frac{1}{3^{3/2}} + \cdots \equiv \zeta\left(\tfrac{3}{2}\right) = 2.612$$

Riemann zeta fn.

since $N - N_0$ is no. of particles in excited states

there is a max. no. they can hold:

$$N_{e_{max}} = \frac{V(2\pi mkT)^{3/2}}{h^3}\,\zeta\left(\tfrac{3}{2}\right)$$

$\Rightarrow$ if we keep adding particles, they must go into N_0, into the ground state $\Rightarrow$ Bose-Einstein condensation

— note: unlike condensation of a vapor, this happens with no interactions

- "condensation in momentum space"

we can define a transition temperature that will depend on T, and N/V

$$T_c = \frac{h^2}{2\pi mk}\left\{\frac{N}{V\,\zeta\left(\frac{3}{2}\right)}\right\}^{2/3}$$

why does this happen?

- consider putting 3 particles into 3 bins

for M-B (distinguishable particles), a, b, c

| a | b | c |	6 permutation
| ab | c | |	6 permutations
| ac | b | |	6 "
| bc | a | |	6 "
| abc | | |	3

total of 27 possible states

states with 3 in one bin = $3/27 = 11\%$

for B-E (distinguishable)

| • | • | • |	1
| •• | • | |	6
| ••• | | |	3

total of 10 possible states

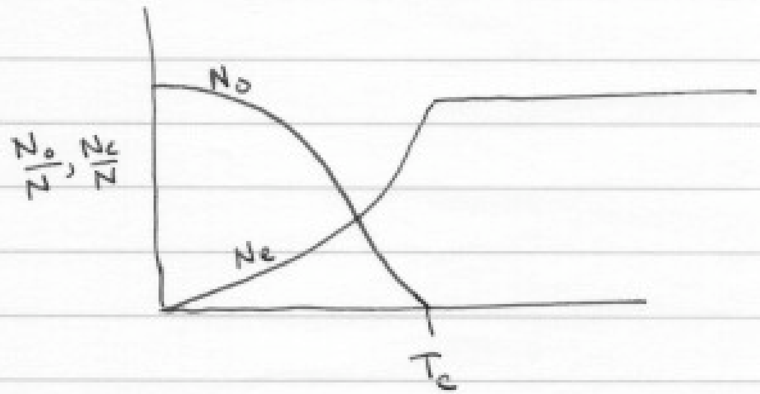
states w/ 3 occupied in 1 bin = 30%

indistinguishability greatly reduces no. of states, except for the state with all in one bin

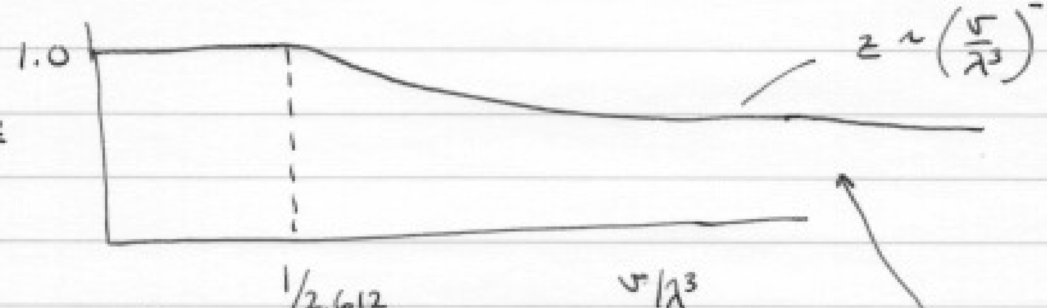
$\Rightarrow$ quantum statistics.

if we have $T < T_c$, then

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



fugacity (chemical potential also varies)



$g_{3/2}(z) \simeq z$
for $z \ll 1$

$$z = \frac{N_0}{N_0+1} \simeq 1 - \frac{1}{N_0} \simeq 1 \text{ when } N_0 \gg 1$$

the specific heat:

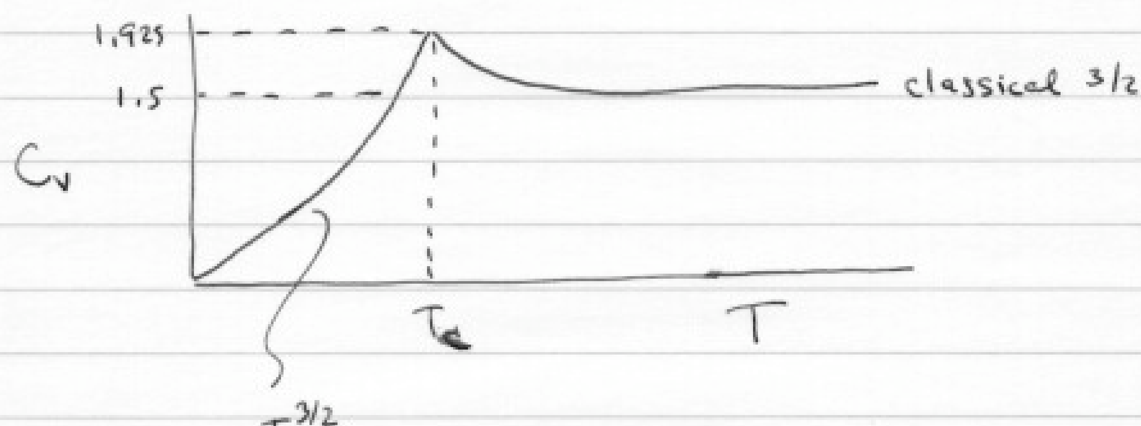
$$\frac{C_V}{Nk} = \frac{3}{2}\frac{V}{N}\zeta(5/2)\frac{d}{dT}\left(\frac{T}{\lambda^3}\right) = \frac{15}{4}\zeta(\tfrac{5}{2})\frac{v}{\lambda^3}$$

at $T = T_c$ $$\frac{C_V(T_c)}{Nk} = \frac{15}{4}\frac{\zeta(5/2)}{\zeta(3/2)} \simeq 1.925$$

note this is higher than classical value of $3/2 = 1.5$

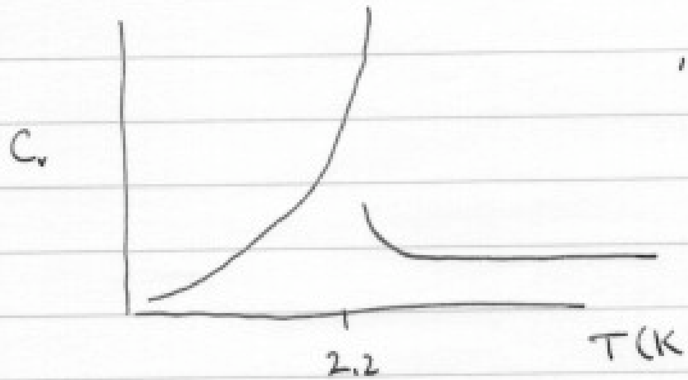
using expansion forms of $g_n(z)$ fns.

for $T > T_c$ $$\frac{C_V}{Nk} = \frac{15}{4}\frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{9}{4}\frac{g_{3/2}(z)}{g_{1/2}(z)}$$



BEC?

experimental observation in LHe (London 1938)
Keesom 1927



"Lambda transition"

$\Rightarrow$ superfluid transition $\rightarrow$ BEC?

using $\frac{N}{V}$ for LHe, expect $T_c \sim 3.13\ K$!

- maybe including interactions would give explanation for difference?

  - not so simple

Superfluidity vs. BEC

BEC – "condensation in momentum space"
atoms in the condensate occupy $p=0$ state

define BEC as macroscopic occupation
of <u>single-particle</u>* states

* – not necessarily eigenfunctions of
single-particle Hamiltonian

LHe presents a problem

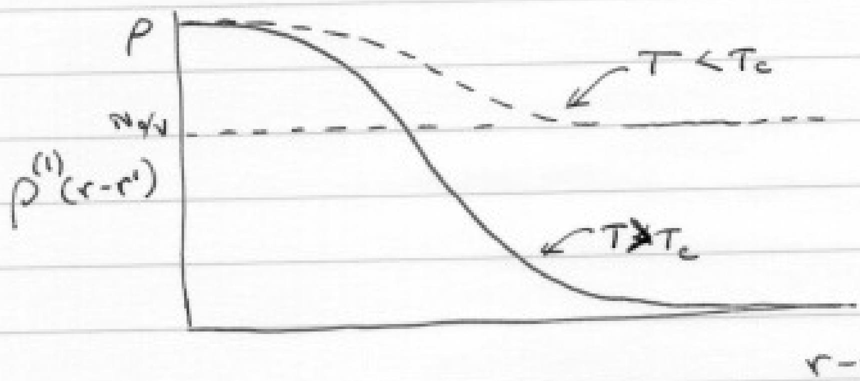
density ~ 20% of max close-packed density

- if two atoms had same single-particle wave fn., there would be large overlap, but 2 He atoms cannot occupy the same space

- Penrose & Onsager Phys. Rev. 104 (576) 1956.
  - estimate at $T=0$, LHe is 8% BEC

- confirmed by neutron scattering experiments which detect ~ 10% $p=0$ momentum peak

LHe is 100% superfluid at $T=0$?



– can write eigenvalue equation for $\rho^{(1)}$

$$\int d\vec{r}'\,\rho^{(1)}(\vec{r},\vec{r}')\,\varphi_i(\vec{r}') = n_i\,\varphi_i(\vec{r})$$

solns. give orthonormal basis of <u>single</u>-<u>particle</u> wave fns.

note: for non-interacting gas, simple solns. of H
for interacting gas, may be different, but
still <u>single particle</u>

we can write

$$\rho^{(1)}(\vec{r},\vec{r}') = \sum_i n_i\,\varphi_i^*(\vec{r})\,\varphi_i(\vec{r}')$$

n_i = single-particle occupation numbers

when $n_0 \equiv N_0$ is order N, $\Rightarrow$ BEC

$\Psi_n(\vec{r}_1, \cdots \vec{r}_N) \equiv$ N-body wave fn. for state n

one-body density matrix:

$$\rho_n^{(1)}(\vec{r}, \vec{r}\,') = N \int d\vec{r}_2 \cdots d\vec{r}_N \, \Psi_n^*(\vec{r}, \vec{r}_2 \cdots \vec{r}_N)\, \Psi_n(\vec{r}\,', \vec{r}_2 \cdots$$

can define mom. space distribution

$$\rho_n(p) = \frac{1}{2\pi \hbar^3} \int d\vec{R}\, d\vec{s}\, \rho_n^{(1)}\left(\vec{R} + \frac{\vec{s}}{2}, \vec{R} - \frac{\vec{s}}{2}\right) e^{i\vec{p}\cdot\vec{s}/\hbar}$$

for a homogenous system, volume V

$$\rho_n^{(1)}(s) = \frac{1}{V} \int d\vec{p}\; n(\vec{p})\, e^{-i\vec{p}\cdot\vec{s}/\hbar}$$

if $\rho(\vec{p})$ is smooth valued at small $\vec{p}$, then $\rho_n^{(1)}(s \to \infty) \to$

but if we have BEC (non-zero amount of atoms in $p=0$)

$$\underset{\text{condensate}}{\rho(\vec{p}) = N_0\, \delta(\vec{p})} + \underset{\text{non-condensate}}{\tilde{\rho}(\vec{p})}$$

then $\rho^{(1)}(\vec{r} - \vec{r}\,')_{\vec{r}-\vec{r}\,' \to \infty} \longrightarrow \frac{N_0}{V}$

"ODLRO = off-diagonal long range order"

can define the boson field operator

$$\hat{\Psi}(\vec{r}) = \sum_i \varphi_i \hat{a}_i$$

$\hat{a}_i$ is annihilation operator for a particle in φ_i

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \qquad [\hat{a}_i, \hat{a}_j] = 0$$

we can also write one-body density matrix in terms of $\hat{\Psi}(r)$

$$\rho^{(1)}(\vec{r}, \vec{r}\,') = \langle \hat{\Psi}^\dagger(\vec{r}) \hat{\Psi}(\vec{r}\,') \rangle$$

then $\langle \hat{a}_j^\dagger a_i \rangle = \delta_{ij} n_i$

we can write $\hat{\Psi}(\vec{r}) = \varphi_0(\vec{r}) \hat{a}_0 + \sum_{i \neq 0} \varphi_i(\vec{r}) \hat{a}_i$

treat $\varphi_0 \hat{a}_0$ as a classical field (Bogoliubov ansatz) to get

$$\hat{\Psi}(\vec{r}) = \Psi_0(r) + \delta\hat{\Psi}(\vec{r})$$

excitations (to be discussed later)

$$\Psi_0(\vec{r}) = \sqrt{N_0}\, \varphi_0$$

"wave fn. of the condensate"

- can be complex -

this classical field ansatz is equivalent to saying $\langle \Psi^* \rangle$ is non-zero – "symmetry breaking"

---

define superfluid velocity in terms of phase gradient of condensate wave fn. φ_0

$$\varphi_0 = |\varphi_0| e^{i\phi(\vec{r},t)}$$

$$\vec{v}_s(\vec{r},t) \equiv \frac{\hbar}{m} \vec{\nabla}\phi(\vec{r},t)$$

from this definition

$$\vec{\nabla} \wedge \vec{v}_s = 0 \quad \text{(irrotational flow)}$$

$$\oint \vec{v}_s \cdot d\vec{l} = n h/m$$

will lead to vortices

but note: $|\varphi_0|^2$ is not superfluid fraction.

irrotational flow, and no entropy in φ_0 (since it is a single quantum state) are basis of Ginzburg-Landau 2-fluid theory, but $\frac{N_0}{V}$ is $\neq \rho_s$!