

## Bose-Einstein Condensation in laser cooled gases

Gases of alkali atoms Li, Na, K, Rb, Cs

- all have a single s-electron in outermost shell.  
- important for efficiency of laser cooling
- use isotopes such that total intrinsic spin of all electrons and nucleons add up to an integer  $T_0$   
 $\Rightarrow$  atoms are bosons
- all have a net magnetic moment - used to confine dilute gas of atoms in a "magnetic trap"  $\vec{F} = \nabla(\vec{\mu} \cdot \vec{B})$
- use "laser cooling" to get very low temperatures in low density gases, to try and see BEC

magnetic trap  $\rightarrow$  effective harmonic potential for atoms

$$V(r) = \frac{1}{2} m \omega_0^2 r^2 \quad \omega_0 \approx \pi \times 100 \text{ Hz}$$

1995 -  $10^3$  atoms with  $T_0 \sim 100 \text{ nK}$

1999 -  $10^8$  atoms with  $T_0 \sim \mu\text{K}$  gas size  $\sim$  many microns

How was BEC in these systems observed?

energy levels of ideal (non-interacting) bosons in harmonic trap

$$E(n_x, n_y, n_z) = (n_x + n_y + n_z + 3/2) \hbar \omega_0$$

$n_x, n_y, n_z$  integers

ground state condensate wavefunction

$$\psi_0(r) \sim e^{-r^2/2a^2} \quad \text{with} \quad a = \left(\frac{\hbar}{m\omega_0}\right)^{1/2}$$

$a \sim 1 \mu\text{m}$  for current traps

$\Rightarrow$  Condensate has spatial extent  $\sim a$

The spatial extent of the  $n^{\text{th}}$  excited energy level is roughly

$$m\omega_0^2 \langle r^2 \rangle \sim E(n) \approx n\hbar\omega_0$$

$$\Rightarrow \langle r^2 \rangle \sim \frac{n\hbar}{m\omega_0} \quad \text{or} \quad \sqrt{\langle r^2 \rangle} = \left(\frac{n\hbar}{m\omega_0}\right)^{1/2}$$

For  $k_B T \gg \hbar\omega_0$ , the atoms are excited up to level  $n \sim \frac{k_B T}{\hbar\omega_0}$

$\Rightarrow$  spatial extent of the normal component of the gas is

$$R \sim \left(\frac{n\hbar}{m\omega_0}\right)^{1/2} \sim \left(\frac{\hbar k_B T}{\hbar m\omega_0^2}\right)^{1/2} = \left(\frac{k_B T}{m\omega_0^2}\right)^{1/2}$$

$$R \sim a \left(\frac{k_B T}{\hbar\omega_0}\right)^{1/2} \Rightarrow a$$

If  $T_c$  is the BEC transition temperature, then for  $T > T_c$  one sees a more or less uniform cloud of atoms with radius  $R \sim a \left(k_B T / \hbar\omega_0\right)^{1/2} \gg a$ . But when one cools to  $T < T_c$ , one now has a finite fraction of the atoms condensed in the ground state,  $\rightarrow$  superimposed on the atomic cloud of radius  $R$  one sees the growth of a sharp peak in density at the center of cloud - this peak has a radius  $a \ll R$ .

To find the Bose-Einstein condensation temperature

The number of particles in the system is

$$N = \sum_{n_x, n_y, n_z} \left[ \frac{1}{z^{-1} e^{\epsilon(n_x, n_y, n_z)/k_B T} - 1} \right] \leftarrow \text{Bose occupation function}$$

Let  $\epsilon_0 = \epsilon(0, 0, 0) = \frac{3}{2} \hbar \omega_0$  the ground state energy

that the Bose occupation function can not be negative  $\Rightarrow z^{-1} e^{\epsilon_0/k_B T} \geq 1 \Rightarrow z \leq e^{\epsilon_0/k_B T}$   
 $\Rightarrow \mu \leq \epsilon_0$

For the Bose condensed state,  $z$  assumes its upper limit, i.e.  $\mu = \epsilon_0$  or  $z = e^{\epsilon_0/k_B T}$   
 - this gives the greatest possible density in the excited states.

$$\Rightarrow \text{for } T \leq T_c, N = \sum_{n_x, n_y, n_z} \left[ \frac{1}{e^{(n_x + n_y + n_z) \hbar \omega_0 / k_B T} - 1} \right]$$

$$\Rightarrow N = N_0 + \int_0^\infty dn_x \int_0^\infty dn_y \int_0^\infty dn_z \left[ \frac{1}{e^{(n_x + n_y + n_z) \hbar \omega_0 / k_B T} - 1} \right]$$

$\uparrow$   
 number in ground state  
 $n_x = n_y = n_z = 0$

$\uparrow$   
 number in excited states.  
 Make integral approx from sum using  $\Delta n_x = \Delta n_y = \Delta n_z = 1$

$$N = N_0 + \left( \frac{k_B T}{\hbar \omega_0} \right)^3 \int_0^\infty dx \int_0^\infty dy \int_0^\infty dz \left[ \frac{1}{e^{(x+y+z)} - 1} \right]$$

$$= N_0 + \left( \frac{k_B T}{\hbar \omega_0} \right)^3 \zeta(3) \quad \zeta(3) = 1 + \frac{1}{2^3} + \frac{1}{3^3} + \frac{1}{4^3} + \dots$$

At  $T_c$ ,  $N_0 = 0 \Rightarrow k_B T_c = \hbar \omega_0 \left( \frac{N}{\zeta(3)} \right)^{1/3}$   
 for  $T < T_c$ ,  $N_0(T) = N \left( 1 - (T/T_c)^3 \right)$

power of  $T/T_c$  term is different from ideal free gas due to presence of magnetic potential

The existence of Bose Einstein condensation is particular to the dimensionality of the system. To see this, consider a general  $d$ -dimensional system. Then

$$\frac{1}{V} \sum_k n(\epsilon(k)) \rightarrow \propto \int dk k^{d-1} \frac{1}{z^{-1} e^{\beta \hbar^2 k^2 / 2m} - 1}$$

is largest when  $z \rightarrow 1$ , so consider this case

$$\propto \int dk k^{d-1} \frac{1}{e^{\beta \hbar^2 k^2 / 2m} - 1}$$

$$\text{let } y = \frac{\beta \hbar^2 k^2}{2m}$$

$$k = \sqrt{\frac{2m y}{\beta \hbar^2}}$$

$$\propto \left(\frac{2m}{\beta \hbar^2}\right)^{d/2} \int_0^\infty dy \frac{y^{d/2-1}}{e^y - 1}$$

$$dk = \sqrt{\frac{2m y}{\beta \hbar^2}} \frac{dy}{2y}$$

again the most singular part of the integral is as  $y \rightarrow 0$

$$\text{for } y^* \ll 1, \quad \int_0^{y^*} dy \frac{y^{d/2-1}}{e^y - 1} \approx \int_0^{y^*} dy \frac{y^{d/2-1}}{y} = \int_0^{y^*} dy y^{d/2-2}$$

The integral will converge at its lower limit  $y \rightarrow 0$

only for  $\frac{d}{2} - 2 > -1$  or  $d > 2$

For  $d \leq 2$ , the integral will diverge. Therefore it will always be possible to find a  $z$  such that

$$n = \frac{N}{V} = \frac{1}{(2\pi)^d} \int d^d k \frac{1}{z^{-1} e^{\beta \hbar^2 k^2 / 2m} - 1}$$

$\Rightarrow$  No Bose Einstein Condensation in two dimensions or below!

## Classical spin models

$$U = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

simple model of interacting magnetic moments

classical spins  $\vec{S}_i$  of unit magnitude  $|\vec{S}_i| = 1$  on sites  $i$  of a periodic  $d$ -dimensional lattice.

$\vec{S}_i$  interacts only with its neighbors  $\vec{S}_j$

$\langle ij \rangle$  indicates nearest neighbor bonds of the lattice.

If coupling  $J > 0$ , then ferromagnetic interaction i.e. spins are in lower energy state when they are aligned.



$\vec{S}_i$  interacts with spins on sites labeled by  $\odot$ .

Behavior of model depends significantly on dimensionality of lattice  $d$ , and number of components of the spin  $\vec{S}$   $n$ .

Examples:  $\vec{S} = (S_x, S_y, S_z)$  points in 3-dimensional space  
 $\underline{n=3}$  called the Heisenberg model

$\vec{S} = (S_x, S_y)$  restricted to lie in a plane  
 $\underline{n=2}$  called the XY model

$S = S_z = \pm 1$  restricted to lie in one direction  
 $\underline{n=1}$  called the Ising model

less obvious possibilities  $\left\{ \begin{array}{l} \underline{n=0} \text{ called the } \underline{\text{polymer model}} \\ \underline{n=\infty} \text{ called the } \underline{\text{spherical model}} \end{array} \right.$

We will focus on the Ising model (1925)

$$S = \pm 1$$

## Ensembles

① fixed magnetization  $M = \sum_i S_i$   $M$  is total magnetization

partition function  $\tilde{Z}(T, M) = \sum_{\{S_i\}} e^{-\beta \mathcal{H}[S_i]}$   
s.t.  $\sum_i S_i = M$

sum over all spin configurations

obeying the constraint  $\sum_i S_i = M = N^+ - N^-$

$\uparrow$  # up spins  $\uparrow$  # down spins

(similar to canonical ensemble with  $\sum_i n_i = N$  total # particles)

Helmholtz free energy  $F(T, M) = -k_B T \ln \tilde{Z}(T, M)$

② fixed magnetic field

to remove constraint of fixed  $M$  we can Legendre transform to a conjugate variable  $h$ , ~~the magnetic field~~. We will see that  $h$  is just the magnetic field

Gibbs free energy  $G(T, h) = F(T, M) - hM$

where ~~the~~  $\left(\frac{\partial F}{\partial M}\right)_T = h \quad \Rightarrow \quad \left(\frac{\partial G}{\partial h}\right)_T = -M$

$$dF = -SdT + h dM \quad \text{and} \quad dG = -SdT - Mdh$$

$\uparrow$  entropy  $\uparrow$  entropy

To get partition function for  $G$ , take Laplace transform of  $\tilde{Z}$

$$Z(T, h) = \sum_M e^{\beta h M} \tilde{Z}(T, M)$$

$$= \sum_M e^{\beta h M} \sum_{\{s_i\}} e^{-\beta H[s_i]} \quad \text{use } M = \sum_i s_i$$

$s.t. \sum_i s_i = M$

$$Z(T, h) = \sum_{\{s_i\}} e^{-\beta [H[s_i] - h \sum_i s_i]}$$

← looks like interaction of magnetic field  $h$  with total magnetization  $M = \sum_i s_i$

↳ unconstrained sum over all spin configs  $\{s_i\}$   
(similar to grand canonical ensemble with  $\sum_i n_i = N$  unconstrained)

$$G(T, h) = -k_B T \ln Z(T, h)$$

check:

$$\frac{\partial G}{\partial h} = -k_B T \frac{\partial Z}{Z \partial h} = -k_B T \sum_{\{s_i\}} \frac{\partial}{\partial h} \left( e^{-\beta [H - h \sum_i s_i]} \right)$$

$$= -k_B T \sum_{\{s_i\}} e^{-\beta [H - h \sum_i s_i]} \left( \beta \sum_i s_i \right)$$

$$= - \frac{\sum_{\{s_i\}} e^{-\beta [H - h \sum_i s_i]} \left( \sum_i s_i \right)}{\sum_{\{s_i\}} e^{-\beta [H - h \sum_i s_i]}}$$

$$= - \langle \sum_i s_i \rangle = -M$$

so  $\frac{\partial G}{\partial h} = -M$  as required