Bose–Einstein Condensation in laser cooled gases

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

- all have a single s-electron in outer-most shell. Important for trapping of laser cooling
- use isotopes such that total intrinsic spin of all electrons and nucleons add up to an integer \( \hbar \)
  \( \Rightarrow \) atoms are bosons

- all have a net magnetic moment - used to confine dilute gas of atoms in a "magnetic trap"

- 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

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

1995 - 10^3 atoms with \( T \approx 100 \text{ nK} \)
1999 - 10^8 atoms with \( T < 1 \text{ nK} \) gas size many microns

How was BEC in these systems observed?

Energy levels of ideal (non-interacting)

bosons in harmonic trap

\[
E(n_x, n_y, n_z) = (n_x + n_y + n_z + \frac{3}{2}) \hbar \omega_0
\]

\( n_x, n_y, n_z \) integer

Ground state condensate wavefunction

\[
\psi_0(r) \sim e^{-r^2/2a^2} \quad \text{with} \quad a = \left( \frac{\hbar}{m \omega_0} \right)^{3/2}
\]

\( a \approx 1 \mu \text{m} \) for current traps
\[ \Rightarrow \text{Condensate has spatial extent } n \alpha \]

The spatial extent of the \( n \)th excited energy level is roughly

\[ m \omega_0^2 \langle r^2 \rangle \approx E(n) \approx n \hbar \omega_0 \]

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

For \( k_B T \gg \hbar \omega_0 \), the atoms are excited up to level \( n \approx \frac{k_B T}{\hbar \omega_0} \)

\[ \Rightarrow \text{spatial extent of the normal component of the gas is} \]

\[ R \approx \left( \frac{n \hbar}{m \omega_0} \right)^{\frac{1}{2}} \approx \left( \frac{\hbar k_B T}{\hbar m \omega_0^2} \right)^{\frac{1}{2}} = \left( \frac{k_B T}{m \omega_0^2} \right)^{\frac{1}{2}} \]

\[ R \approx a \left( \frac{k_B T}{m \omega_0^2} \right)^{\frac{1}{2}} \Rightarrow a \]

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 \( R \approx a \left( \frac{k_B T}{m \omega_0^2} \right)^{\frac{1}{2}} \gg a \).

But when one cools to \( T < T_c \), one now has a finite fraction of the atoms condensed in the ground state, 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

\[ N = \sum_{n_x, n_y, n_z} \left[ \frac{1}{2} \frac{1}{\epsilon(n_x, n_y, n_z) / k_b T - 1} \right] \leq \text{Bose occupation function} \]

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 \( \Rightarrow \frac{1}{\epsilon} e^{-\epsilon / k_b T} \geq 1 \Rightarrow \frac{1}{\epsilon} \leq e^{-\epsilon / k_b T} \)

\( \Rightarrow \mu \leq \epsilon_0 \)

For the Bose condensed state, \( \mu \) assumes its upper limit, i.e. \( \mu = \epsilon_0 \) possible \( \frac{1}{\epsilon} = e^{-\epsilon / k_b T} \)

this gives the greatest density in the excited states

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

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

\[ \Rightarrow \text{number in ground state} \quad \text{number in excited states} \]

\[ n_x = n_y = n_z = 0 \quad \Delta n_x = \Delta n_y = \Delta n_z = 1 \]

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

\[ = N_0 + \left( \frac{k_b T}{\hbar \omega_0} \right)^3 \int (3) \]

\[ \S(3) = 1 + \frac{1}{23} + \frac{1}{39} + \frac{1}{43} + ... \]

At \( T_c \), \( N_0 = 0 \Rightarrow k_b T_c = \hbar \omega_0 \left( \frac{N}{\S(3)} \right)^{1/3} \)

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

The power of \( T/T_c \) term is different from ideal free gas due to presence of magnetic field.
Classical spin models

\[ H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \] simple model of interacting magnetic

classical spins \( \vec{S}_i \) of unit magnitude \( |\vec{S}| = 1 \) 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
in spins are in lower energy state when they are aligned.

\[ \vec{S}_i \text{ interacts with spins on sites} \]

\[ \vec{S}_i \text{ labeled by } i. \]

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

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

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

\( \vec{S} = S_z = \pm 1 \) restricted to lie in one direct
\( n = 1 \) called the \textit{Ising model}

less obvious \( \left\{ \begin{array}{ll}
\frac{n = 0}{n = \infty} \text{ called the polymer model} \\
\end{array} \right. \)
\textit{called the spherical model}
We will focus on the Ising model (1925)

\[ S = \pm 1 \]

Ensembles

1. **fixed magnetization**

\[ M = \sum s_i \]

\[ M \text{ is total magnetization} \]

**partition function**

\[ Z(T, M) = \sum e^{-\beta H[s_i]} \]

\[ \text{sum over all spin configurations} \]

\[ \text{obeying the constraint } \sum s_i = M = N^+ - N^- \]

\[ \text{similar to canonical ensemble with } \sum s_i = N \text{ total \# particles} \]

**Helmholtz free energy**

\[ F(T, M) = -k_B T \ln Z(T, M) \]

2. **fixed magnetic field**

\[ \text{to remove constraint of fixed } M \text{ we can Legendre transform to a conjugate variable } h, \text{ the magnetic field. We will see that } h \text{ is just the magnetic field} \]

**Gibbs free energy**

\[ G(T, h) = F(T, M) - h M \]

where

\[ \frac{\partial F}{\partial M} = h \quad \rightarrow \quad \frac{\partial G}{\partial h} = -M \]

\[ dF = -SdT + h dM \quad \text{and} \quad dG = -SdT - M dh \]

\[ \text{entropy} \quad \text{entropy} \]
To get partition function for $G$, take Laplace transform of $Z$:

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

$$= \sum_M e^{\beta H M} \sum_{\varepsilon i_j s_i} e^{-\varepsilon H[\varepsilon i_j s_i]}$$

Use $M = \sum s_i$

looks like interaction of magnetic field $H$

$$Z(T, \beta) = \sum_{\varepsilon i_j s_i} e^{-\beta [H[\varepsilon i_j s_i] - \varepsilon \sum s_i]}$$

with total magnetization $M = \sum s_i$

(looks like constrained sum over all spin configs $\varepsilon i_j s_i$)

(same to grand canonical ensemble with $\sum n_i = N$ unconstrained)

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

Check:

$$\frac{\partial G}{\partial k} = -k_B T \frac{\partial Z}{\partial k} = -k_B T \sum_{\varepsilon i_j s_i} \frac{\partial}{\partial k} (e^{-\beta [H - \varepsilon \sum s_i]})$$

$$= -k_B T \frac{\partial}{\partial k} \left( \sum_{\varepsilon i_j s_i} e^{-\beta [H - \varepsilon \sum s_i]} (\beta \sum s_i) \right)$$

$$= - \sum_{\varepsilon i_j s_i} e^{-\beta [H - \varepsilon \sum s_i]} (\beta \sum s_i)$$

$$= \sum_{\varepsilon i_j s_i} e^{-\beta [H - \varepsilon \sum s_i]} \langle \varepsilon s_i \rangle$$

$$= -\langle \sum \varepsilon s_i \rangle = -M$$

so $\frac{\partial G}{\partial k} = -M$ as required.
we can work in fixed magnetization or fixed magnetic field ensemble according to our convenience. Usually it is easiest to work with fixed magnetic field. In this case we usually write

\[ H = -J \sum_{<i,j>} S_i S_j - h \sum_i S_i \]

including the magnetic field part in the definition of \( H \).

\[ Z = \sum_{\{S_i\}} e^{-\beta H} \]

\( \beta = \frac{1}{k_B T} \) includes \( k \) term

define magnetization density

\[ m = \frac{M}{N} = \frac{1}{N} \langle \sum_i S_i \rangle \quad \text{N = total number spins} \]

Heinrich free energy density: In limit \( N \to \infty \), \( F(T, M) = NF(T, m) \)

\[ \frac{F}{N} = f(T, m) \quad \text{depends on magnetization density} \]

\[ df = -dM + h \, dm \]

\( A = \frac{S}{N} \quad \text{entropy per spin} \)

Gibbs free energy density: In limit \( N \to \infty \), \( G(T, \mu) = Ng(T, \mu) \)

\[ \frac{G}{N} = g(T, \mu) \]

\[ dg = -dM - m \, d\mu \]

\[ \left( \frac{\partial f}{\partial m} \right)_T = h \quad \therefore \quad \left( \frac{\partial g}{\partial \mu} \right)_T = -m \]