Bose–Einstein Condensation in laser cooled gases

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

- all have a single s-electron in outermost shell, important for trapping by laser cooling
- use isotopes such that total intrinsic spin of all electrons and nucleons add up to an integer \( F \)
  \( \Rightarrow \) atoms are bosons
- all have a net magnetic moment - used to confine dilute gas of atoms in a "magnetic trap" \( F = \nabla V(r) \cdot B \)
  - 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

\[ V(r) = \frac{1}{2} m \omega^2 r^2 \]

\( \omega_0 \approx 2 \pi \times 100 \text{ Hz} \)

1995 - \( 10^3 \) atoms with \( T_c \approx 100 \text{ nK} \)

1999 - \( 10^8 \) atoms with \( T_c \approx \mu \text{ K} \) gas size \( \approx \text{many microns} \)

How was BEC in these systems observed?

energy levels of ideal (non-interacting)

bosons in harmonic trap

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

\( n_x, n_y, n_z \) integers

grand state condensate wavefunction

\[ \psi_0(r) \sim e^{-r^2/2 \alpha^2} \text{ with } \alpha = \left( \frac{\hbar}{m \omega_0} \right)^{1/2} \]

\( \alpha \approx 1 \mu \text{m} \) for current traps
\[ \Rightarrow \text{Condensate has spatial extent } \propto n^2 \]

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

\[ m w_0^2 \langle r^2 \rangle \sim E(n) \approx n \hbar w_0 \]

\[ \Rightarrow \langle r^2 \rangle \sim \frac{n \hbar}{m w_0} \quad \text{or} \quad \sqrt{\langle r^2 \rangle} = \left( \frac{n \hbar}{m w_0} \right)^{1/2} \]

For \( k_B T \gg \hbar w_0 \), the atoms are excited up to level \( n \sim \frac{k_B T}{\hbar w_0} \)

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

\[ R \sim \left( \frac{n \hbar}{m w_0} \right)^{1/2} \sim \left( \frac{\hbar k_B T}{\hbar m w_0^2} \right)^{1/2} = \left( \frac{k_B T}{m w_0^2} \right)^{1/2} \]

\[ R \sim a \left( \frac{k_B T}{\hbar w_0^2} \right)^{1/2} \Rightarrow a \]

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 \( R \sim a \left( \frac{k_B T}{\hbar w_0} \right)^{1/2} \gg a \).

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

\[ N = \sum_{n_x, n_y, n_z} \left[ \frac{1}{Z - 1} \right] \rightarrow \text{Bose occupation function} \]

Let \( \varepsilon_0 = \varepsilon(0,0,0) = \frac{3}{2} \hbar \omega_0 \) the ground state energy that the Bose occupation function can not be negative \( \Rightarrow \frac{1}{Z} e^{\varepsilon_0/k_B T} > 1 \) \( \Rightarrow Z < e^{\varepsilon_0/k_B T} \) \( \Rightarrow \mu < \varepsilon_0 \)

For the Bose condensed state, \( z \) assumes its upper limit \( \Rightarrow \mu = \varepsilon_0 \) \( \Rightarrow \) possible \( \Rightarrow \frac{1}{Z} = e^{\varepsilon_0/k_B T} \) which gives the greatest density in the excited states.

\[ \Rightarrow \text{for } T \ll T_c, \quad N = \sum_{n_x, n_y, n_z} \left[ \frac{1}{e^{(\varepsilon_0 + n_x \hbar \omega_0/k_B T) - 1}} \right] \]

\[ \Rightarrow N = N_0 + \int_0^\infty \int_0^\infty \int_0^\infty \frac{1}{e^{(\varepsilon_0 + n_x \hbar \omega_0/k_B T) - 1}} \]

number in

\[ \text{ground state} \]
\[ n_x = n_y = n_z = 0 \]

\[ \Rightarrow N = N_0 + \int \frac{k_B T^3}{\hbar^3 \omega_0} \int 0^\infty \int 0^\infty \int n_x n_y n_z \left[ \frac{1}{e^{(x+y+z) \hbar \omega_0/k_B T} - 1} \right] \int (3) \]

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

\[ \int (3) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[ \frac{1}{e^{x+y+z} - 1} \right] \]

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

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

power of \( T/T_c \) term is different from ideal free gas due to presence of magnetic field.
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 \( |\vec{s}| = 1 \) 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.

\[ \vec{s}_i \text{ interacts with spins on sites labeled by } \oplus. \]

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 Heisenberg model.

- \( \vec{s} = (s_x, s_y) \) restricted to lie in a plane \( n = 2 \) called the XY model.

- \( s = s_z = \pm 1 \) restricted to lie in one direction \( n = 1 \) called the Ising model.

less obvious possibilities \( \{ \begin{array}{c} n = 0 \text{ \text{ called the polymer model}} \\ n = \infty \text{ \text{ called the spherical model}} \end{array} \)
We will focus on the Ising model (1925)

\[ S = \pm 1 \]

**Ensembles**

1. **Fixed magnetization**
   
   \[ M = \sum_s s \]

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

   sum over all spin configurations

   obeying the constraint
   
   \[ \sum_s s = M = N^+ - N^- \]

   (similar to canonical ensemble with \( \sum_s n_s = N \) total particles)

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

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

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

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

\[
Z(T, \mathbf{h}) = \sum_{\mathbf{M}} e^{\beta \mathbf{h} \cdot \mathbf{M}} Z(T, \mathbf{M})
\]

\[
= \sum_{\mathbf{M}} e^{\beta \mathbf{h} \cdot \mathbf{M}} \sum_{\mathbf{s} \in \mathcal{S}} e^{-\beta H[\mathbf{s} \cdot \mathbf{c}]} \quad \text{use } \mathbf{M} = \sum_{i} \mathbf{s}_{i}
\]

\[
Z(T, \mathbf{h}) = \sum_{\mathbf{s} \in \mathcal{S}} e^{-\beta \left[ H[\mathbf{s} \cdot \mathbf{c}] - \mathbf{h} \cdot \sum_{i} \mathbf{s}_{i} \right]} \quad \text{looks like interaction of magnetic field } \mathbf{h} \text{ with total magnetization } \sum_{i} \mathbf{s}_{i} = \mathbf{M}
\]

This unconstrained sum over all spin configs \( \mathcal{S} \) (similar to grand canonical ensemble with \( \sum_{i} n_{i} = N \) unconstrained).

\[
G(T, \mathbf{h}) = -k_{B} T \ln Z(T, \mathbf{h})
\]

Check:

\[
\frac{\partial G}{\partial \mathbf{h}} = -k_{B} T \frac{\partial Z}{Z} \frac{\partial Z}{\partial \mathbf{h}} = -k_{B} T \sum_{\mathbf{s} \in \mathcal{S}} \frac{\partial}{\partial \mathbf{h}} \left( e^{-\beta \left[ H - \mathbf{h} \cdot \sum_{i} \mathbf{s}_{i} \right]} \right)
\]

\[
= -k_{B} T \sum_{\mathbf{s} \in \mathcal{S}} e^{-\beta \left[ H - \mathbf{h} \cdot \sum_{i} \mathbf{s}_{i} \right]} \left( \beta \sum_{i} \mathbf{s}_{i} \right)
\]

\[
= -\sum_{\mathbf{s} \in \mathcal{S}} e^{-\beta \left[ H - \mathbf{h} \cdot \sum_{i} \mathbf{s}_{i} \right]} \left( \sum_{i} \mathbf{s}_{i} \right)
\]

\[
= - \left( \sum_{\mathbf{s} \in \mathcal{S}} e^{-\beta \left[ H - \mathbf{h} \cdot \sum_{i} \mathbf{s}_{i} \right]} \right) \sum_{\mathbf{s} \in \mathcal{S}} e^{-\beta \left[ H - \mathbf{h} \cdot \sum_{i} \mathbf{s}_{i} \right]} \sum_{\mathbf{s} \in \mathcal{S}} \left( \sum_{i} \mathbf{s}_{i} \right)
\]

\[
= -\langle \sum_{i} \mathbf{s}_{i} \rangle = -M
\]

so \( \frac{\partial G}{\partial \mathbf{h}} = -M \) as required.