Bose-Einstein Condensation in Ultra Cold Atoms

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Bibliorgaphy

- *Bose-Einstein Condensation and Superfluidity*
  by Lev Pitaevskii and Sandro Stringari (Oxford, 2016)

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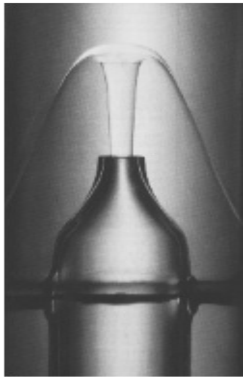
Brief History

1924 - 1925

S.N. Bose and A. Einstein study quantum statistics of photons and atoms and predict a macroscopic population of ground state of an ideal gas of bosons below certain temperature – Bose-Einstein Condensation (BEC)

1938

Discovery of superfluidity of liquid ^{4}He (Allen and Misener, Kapitza). F. London proposes a link with BEC.
See also works (1940) by L. Tisza (died in 2009 aged 101)



1941

Two-fluid theory by L. Landau explaining superfluid properties of helium by presence of a normal and superfluid components of the density. The later was associated with the condensate (not by Landau himself).

Brief History

1947

N. Bogoliubov proposes a theory of elementary excitations of weakly interacting Bose gases which provides a microscopical foundation of Landau phenomenological theory

1951

Concept of the Off-Diagonal Long Range Order and its relation to BEC proposed by Landau and Lifshits, Penrose and Onsager

1949-1956

Prediction of penetration of normal component into superfluid in the form of quantised vortices by Onsager, Feynman. Experimental discovery of vortices in helium by Hall and Vinen

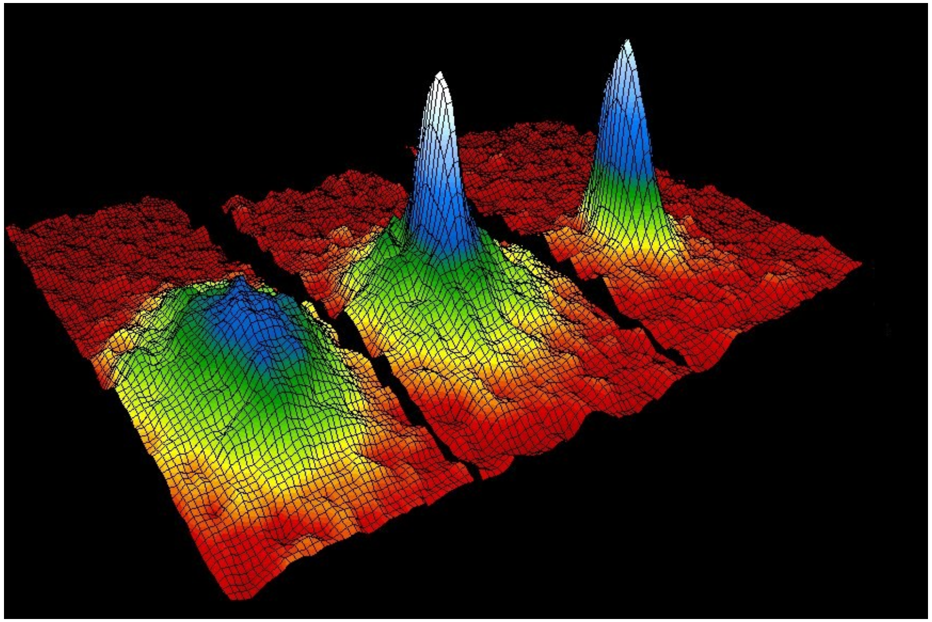
BEC in Ultra Cold Atoms

1970-1995

Experiments with cold atoms (spin-polarised H, alkali): laser cooling and trapping

1995

First observation of BEC with ultracold atoms at JILA (^{87}Rb) and MIT (^{23}Na)



1995-today

BEC observed with 7Li, spin-polarised H, metastable ^{4}He, ^{41}K, ^{52}Cr, …
around the world, see http://www.uibk.ac.at/exphys/ultracold/atomtraps.html

Quantum mechanics of 1,2,...,N particles

One particle is described by wave function $\Psi(\mathbf{x})$ depending on the position $\mathbf{x}$

Free particle

$$\hat{H}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi$$

$$\Psi = \frac{1}{\sqrt{L^3}}e^{i\mathbf{k}\cdot\mathbf{x}} \qquad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \varepsilon_{\mathbf{k}}$$

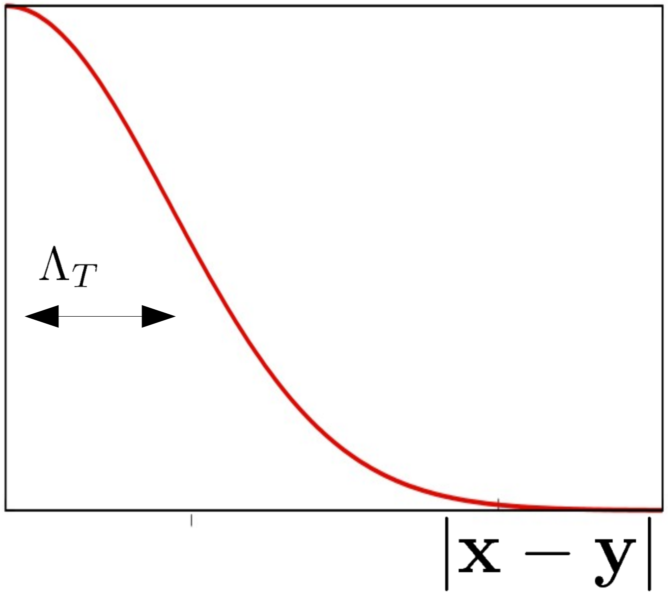
Periodic boundary conditions: $$\mathbf{k} = \frac{2\pi}{L}(n_x, n_y, n_z) \qquad n \in \mathbb{Z}$$

Finite temperature – density matrix

$$\rho_T(\mathbf{x},\mathbf{y}) = \frac{1}{Z}\langle \mathbf{x}| e^{-\hat{H}/T} |\mathbf{y}\rangle =$$

$$= \left(\frac{\Lambda_T}{L}\right)^3 \sum_{\mathbf{k}} e^{-\varepsilon_{\mathbf{k}}/T} \Psi_{\mathbf{k}}(x)\Psi^*_{\mathbf{k}}(y)$$

$$= \frac{1}{L^3}\exp\left(-\frac{\pi|\mathbf{x}-\mathbf{y}|^2}{\Lambda_T^2}\right)$$ *



De Broglie Thermal Length $\Lambda_T = \left(\frac{2\pi\hbar^2}{mT}\right)^{1/2}$

2 identical particles

No interactions

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \Psi_1(\mathbf{x}_1)\Psi_2(\mathbf{x}_2)$$

$$\hat{H}\Psi = (\hat{H}_1 + \hat{H}_2)\Psi = (E_1 + E_2)\Psi$$

Symmetry under particle permutation $\Psi(\mathbf{x}_1, \mathbf{x}_2) \longrightarrow \Psi(\mathbf{x}_2, \mathbf{x}_1)$

Bosons (even)

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = +\Psi(\mathbf{x}_2, \mathbf{x}_1)$$

Fermions (odd)

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = -\Psi(\mathbf{x}_2, \mathbf{x}_1)$$

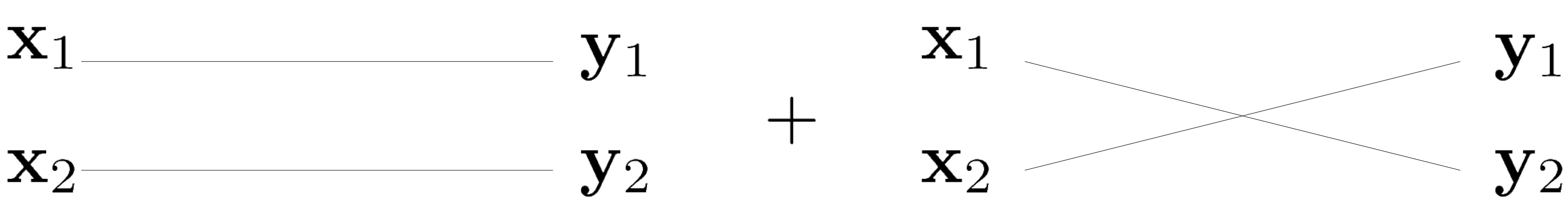
Density matrix for 2 bosons

Symmetrise:

$$\Psi_{\mathbf{k}_1,\mathbf{k}_2}(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{\sqrt{2}}\left[\Psi_{\mathbf{k}_1}(\mathbf{x}_1)\Psi_{\mathbf{k}_2}(\mathbf{x}_2) + \Psi_{\mathbf{k}_1}(\mathbf{x}_2)\Psi_{\mathbf{k}_2}(\mathbf{x}_1)\right]$$

$$\rho_T^{(2)}(\mathbf{x}_1,\mathbf{x}_2;\mathbf{y}_1,\mathbf{y}_2) = \frac{1}{Z}\sum_\alpha e^{-E_\alpha/T}\Psi_\alpha^*(\mathbf{x}_1,\mathbf{x}_2)\Psi_\alpha(\mathbf{y}_1,\mathbf{y}_2)$$

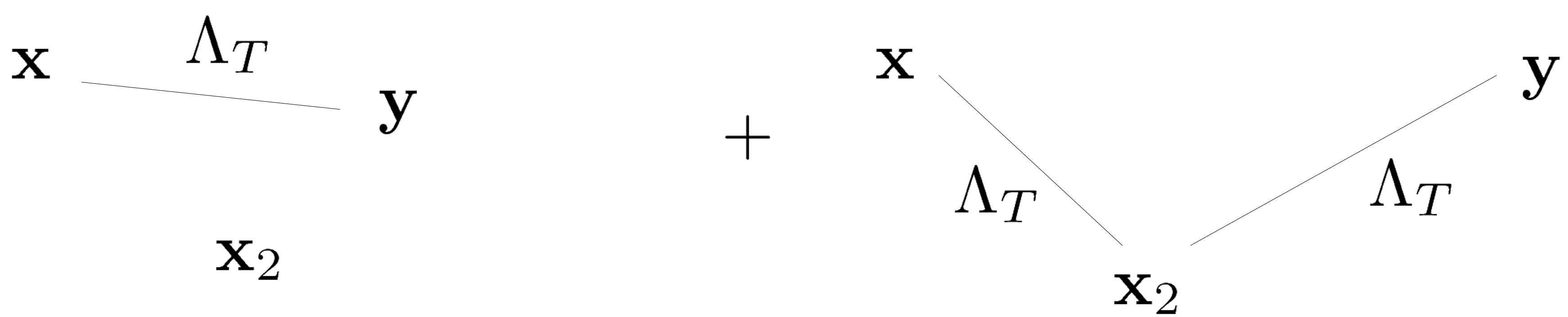
$$= \frac{1}{2}\left[\rho_T(\mathbf{x}_1,\mathbf{y}_1)\rho_T(\mathbf{x}_2,\mathbf{y}_2) + \rho_T(\mathbf{x}_1,\mathbf{y}_2)\rho_T(\mathbf{x}_2,\mathbf{y}_1)\right]$$



Effective 1 particle density matrix

$$\rho_T^{(1)}(\mathbf{x},\mathbf{y}) = \int \mathrm{d}\mathbf{x}_2\, \rho_2(\mathbf{x},\mathbf{x}_2;\mathbf{y},\mathbf{x}_2)$$

$$= \rho_T(\mathbf{x},\mathbf{y}) + \int \mathrm{d}\mathbf{x}_2 \rho_T(\mathbf{x},\mathbf{x}_2)\rho_T(\mathbf{x}_2,\mathbf{y})$$ *



has larger correlation range as a result of statistics

N particles. Spin-Statistics Theorem

Many body wavefunction of N identical particles* $\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$

is either *totally symmetric* (bosons)

$$\Psi(\mathbf{x}_{P_1}, \mathbf{x}_{P_2}, \dots, \mathbf{x}_{P_N}) = \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$$

or *totally antisymmetric* (fermions)

$$\Psi(\mathbf{x}_{P_1}, \mathbf{x}_{P_2}, \dots, \mathbf{x}_{P_N}) = (-1)^{\delta_P}\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$$

under any permutation P of particles

$\delta_P =$ number of swaps required to bring $P_1, P_2, P_3, \dots, P_N$ back to $1, 2, 3, \dots, N$

example $\delta_{(3,1,2)} = 2$

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* can be interacting

One body density matrix - definition

N bosons in many body state (interacting or not) $\Psi_\alpha(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$

$$\rho_\alpha^{(1)}(\mathbf{x}, \mathbf{y}) = \langle \alpha | \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}(\mathbf{y}) | \alpha \rangle =$$

$$= N \int \mathrm{d}\mathbf{x}_2 \ldots \mathrm{d}\mathbf{x}_N \Psi_\alpha^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N) \Psi_\alpha(\mathbf{y}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

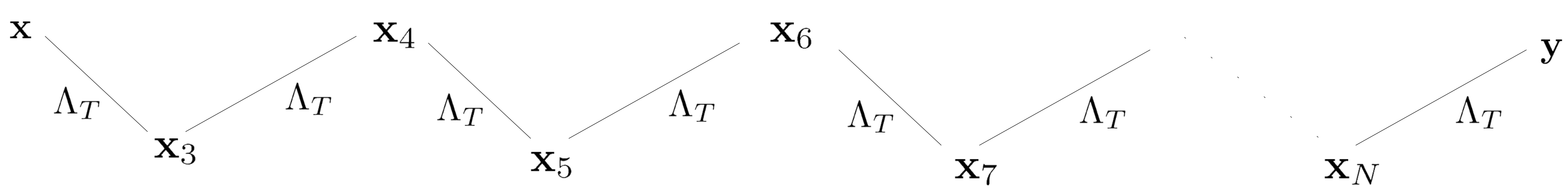
At thermal equilibrium

$$\rho_T^{(1)}(\mathbf{x}, \mathbf{y}) = \frac{1}{Z_N} \sum_\alpha e^{-E_\alpha/T} \rho_\alpha^{(1)}(\mathbf{x}, \mathbf{y})$$

Off Diagonal Long Range Order

Thermodynamic limit: $N, L \longrightarrow \infty$ constant density $n = N/L^3$

Another length scale appears: mean interparticle spacing $d = n^{-1/3}$



When temperature is lowered Λ_T increases and becomes larger than d

Correlation range increases and one can expect a ODLRO at $T < T_c$ *i.e.*

$$\rho_T^{(1)}(\mathbf{x}, \mathbf{y}) \longrightarrow n_0 \qquad\qquad |\mathbf{x} - \mathbf{y}| \longrightarrow \infty$$

Momentum distribution

For translationally invariant system density matrix depends only on the distance

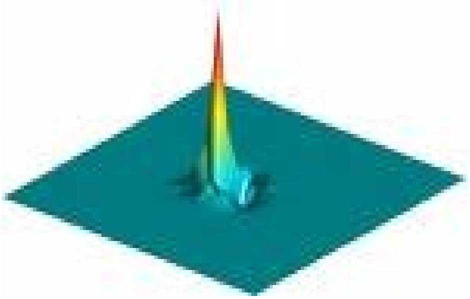
$\rho_T^{(1)}(\mathbf{x},\mathbf{y}) = \rho_T^{(1)}(\mathbf{x}-\mathbf{y})$ and can be diagonalised by Fourrier transform:

$$\rho_T^{(1)}(\mathbf{x}) = \frac{1}{L^3}\int \mathrm{d}\mathbf{p}\, n(\mathbf{p})\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}$$

$n(\mathbf{p})$ is called momentum distribution or occupation number of the state $\mathbf{p}$

OLDRO implies a peak in the momentum distribution

$$n(\mathbf{p}) = N_0\delta(\mathbf{p}) + \tilde{n}(\mathbf{p})$$



Long Range Order and Condensate fraction

$$\rho_T^{(1)}(\mathbf{x}) = \frac{1}{L^3}\int \mathrm{d}\mathbf{p}\, n(\mathbf{p})\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}$$

$$n_0/n = N_0/N \leq 1$$

Example of density matrix behaviour in helium
(Ceperley and Pollack, 1987)

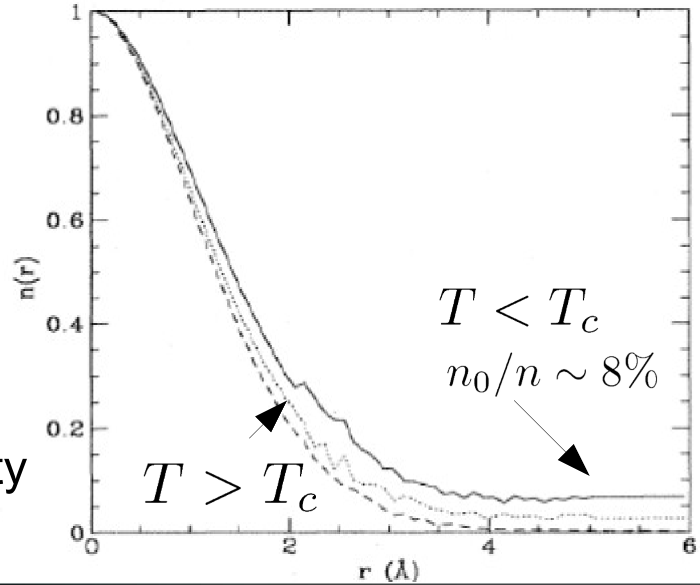
Above T_c $n(\mathbf{p})$ is smooth

$$\rho_T^{(1)}(\mathbf{x}) \to 0$$

$$|\mathbf{x}| \to \infty$$

Below T_c

$$\rho_T^{(1)}(\mathbf{x}) \sim \frac{N_0}{L^3} = n_0$$ - condensate density



Condensation in Ideal Gas

Grand canonical ensemble: chemical potential μ and temperature T,

$$\beta = 1/k_B T$$

Occupation of the state $\mathbf{p}$ is the **Bose-Einstein distribution**

$$n(\mathbf{p}) = \frac{1}{e^{\beta(\varepsilon_{\mathbf{p}}-\mu)} - 1} \qquad (\mu < 0)$$

Total number of particles

$$N(T,\mu) = \sum_{\mathbf{p}} n(\mathbf{p}) = L^3 \int \frac{\mathrm{d}\mathbf{p}}{(2\pi\hbar)^3} \frac{1}{e^{\beta(\varepsilon_{\mathbf{p}}-\mu)} - 1}$$

Density of states

$$\rho(\varepsilon) = \sum_{\mathbf{p}} \delta(\varepsilon - \varepsilon_{\mathbf{p}}) = L^3 \int \frac{\mathrm{d}\mathbf{p}}{(2\pi\hbar)^3} \delta(\varepsilon - p^2/2m)$$

$$= L^3 \int \frac{p^2 dp}{2\pi^2\hbar^3} \delta(p - \sqrt{2m\varepsilon}) \sqrt{\frac{m}{2\varepsilon}} = L^3 \left(\frac{m}{2}\right)^{3/2} \frac{\sqrt{\varepsilon}}{\pi^2\hbar^3}$$

In $d = 1, 2, 3$ dimensions

$$\rho(\varepsilon) = L^d \frac{\Omega_d}{(2\pi\hbar)^d} m p^{d-2}(\varepsilon) \sim \varepsilon^{\frac{d}{2}-1}$$

Maximum Number of Particles

Total number of particles $$N(T,\mu) = \int \frac{\rho(\varepsilon)d\varepsilon}{e^{\beta(\varepsilon-\mu)} - 1}$$

is an increasing function of $\mu \quad (\mu \leq 0)$

Consider $$N_{\max} = \int \frac{\rho(\varepsilon)d\varepsilon}{e^{\beta\varepsilon} - 1}, \qquad \rho(\varepsilon) \sim \sqrt{\varepsilon}$$

the integral converges for small energies

$$\boxed{\frac{N_{\max}}{L^3} = n_{\max} = \frac{g_{3/2}(1)}{\Lambda_T^3}}$$

$$g_p(z) = \frac{1}{\Gamma(p)} \int_0^\infty \frac{x^{p-1}dx}{z^{-1}e^x - 1} = \sum_{l=1}^{\infty} \frac{z^l}{l^p} \qquad g_{3/2}(1) = \frac{2}{\sqrt{\pi}} \int \frac{x^{1/2}}{e^x - 1} \simeq 2.612$$

What is wrong?

Q. What if the number of particles is larger than $N_{\max} \sim T^{3/2}$?

A. In calculating N we have replaced a discrete sum over states by an integral

This completely ignores the occupation of the lowest state

$$N_0(T,\mu) = \frac{1}{e^{-\beta\mu} - 1}$$

since $\rho(\varepsilon = 0) = 0$

In fact it diverges as $\mu \longrightarrow 0^-$ and the state $\mathbf{p} = 0$ gets macroscopically occupied $N_0 \sim N$

Bose-Einstein Condensation

Below critical temperature calculated from the condition

$$n\Lambda_T^3 = g_{3/2}(1) \qquad \text{or} \qquad \Lambda_T \sim d$$

particles condense in the lowest energy state

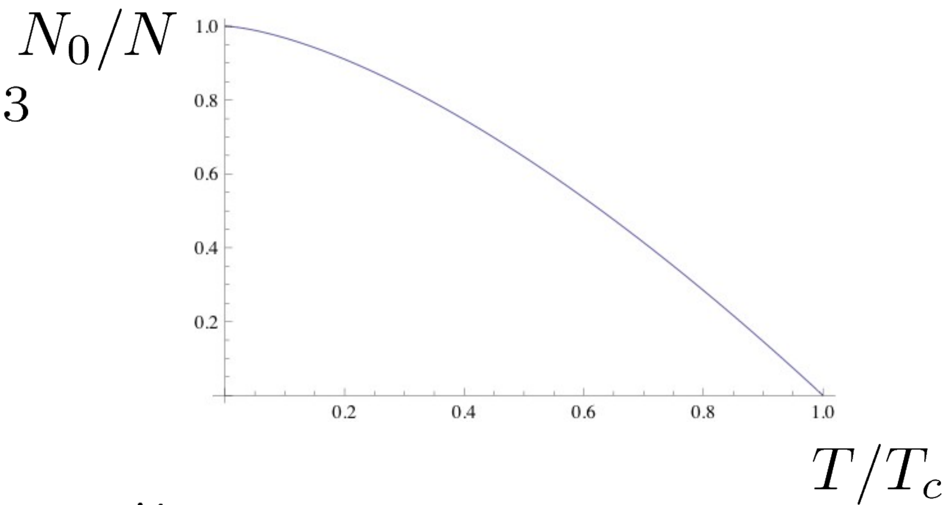
$$N_T = \frac{\Lambda_{T_c}^3}{\Lambda_T^3} N = \left(\frac{T}{T_c}\right)^{3/2} N$$

$$N_0 = N - N_T = \left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right] N$$

Condensed phase

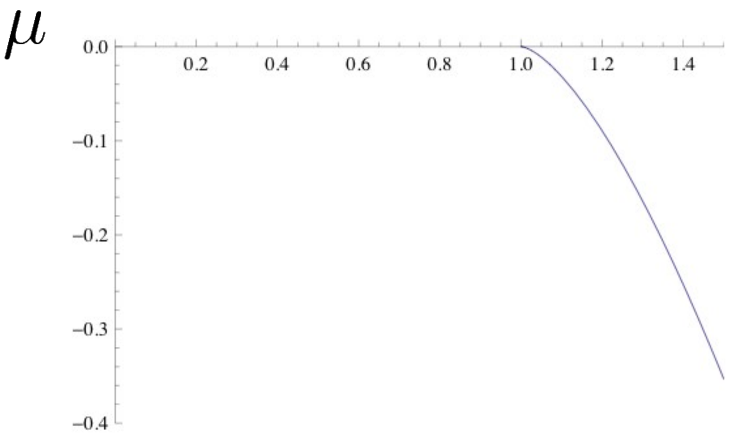
Condensation temperature $T_c \sim n^{2/3}$ must be distinguished from the *microscopic* temperature

$$T_1 = \varepsilon_1 \sim \hbar^2/2mL^2$$



Chemical potential

$$-\mu = T \ln\left(1 + \frac{1}{N_0}\right) \simeq \frac{T}{N_0}$$



is microscopically small below condensation energy

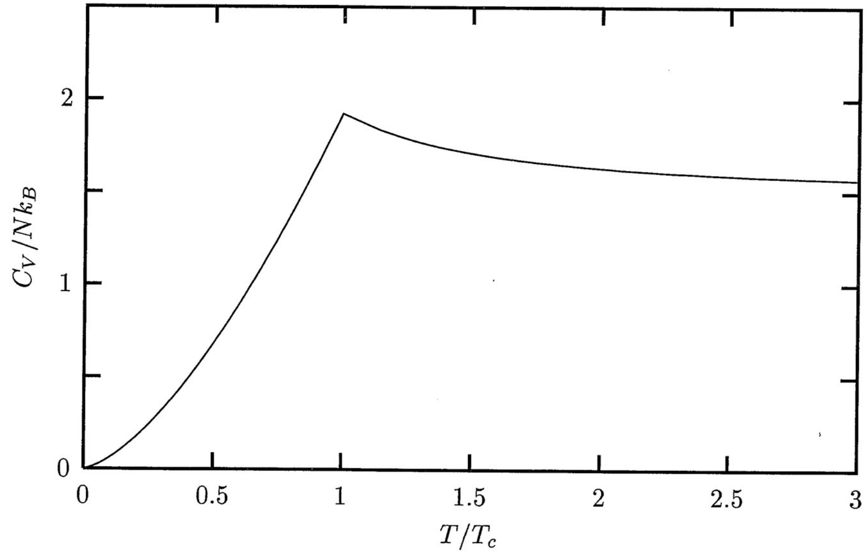
Thermodynamics

Energy

$$E = \int d\varepsilon \frac{\varepsilon \rho(\varepsilon)}{e^{\beta(\varepsilon-\mu)} - 1} = \frac{3}{2} T \frac{L^3}{\Lambda_T^3} g_{5/2}(e^{\beta\mu})$$

Specific heat $\quad C_V = \partial E / \partial T$

is continuous at the transition



Pressure

$$P = \frac{2}{3}\frac{E}{V} = \frac{T}{\Lambda_T^3} g_{5/2}(1)$$

is volume independent - infinite compressibility

Condensation and density of states

Total number of particles $N = N_T + N_0$

$$N_T \leq N_{\max}(T) = \int \frac{\rho(\varepsilon) d\varepsilon}{e^{\beta\varepsilon} - 1}$$

BEC occurs when $N_{\max}(T_c) = N$

NB. $N_{\max}$ can be infinite (integral diverges) and one can accommodate any number of particles by adjusting chemical potential

Example: uniform system in low dimension (no interactions)

$$d = 2 \qquad \rho(\varepsilon) \sim \varepsilon^0$$

$$d = 1 \qquad \rho(\varepsilon) \sim \varepsilon^{-1/2}$$

Harmonic Trap

$$V(x,y,z) = \frac{1}{2}m\omega_x^2x^2 + \frac{1}{2}m\omega_y^2y^2 + \frac{1}{2}m\omega_z^2z^2$$

Energy levels $$\varepsilon_{n_x,n_y,n_z} = E_0 + \hbar\omega_x n_x + \hbar\omega_y n_y + \hbar\omega_z n_z$$

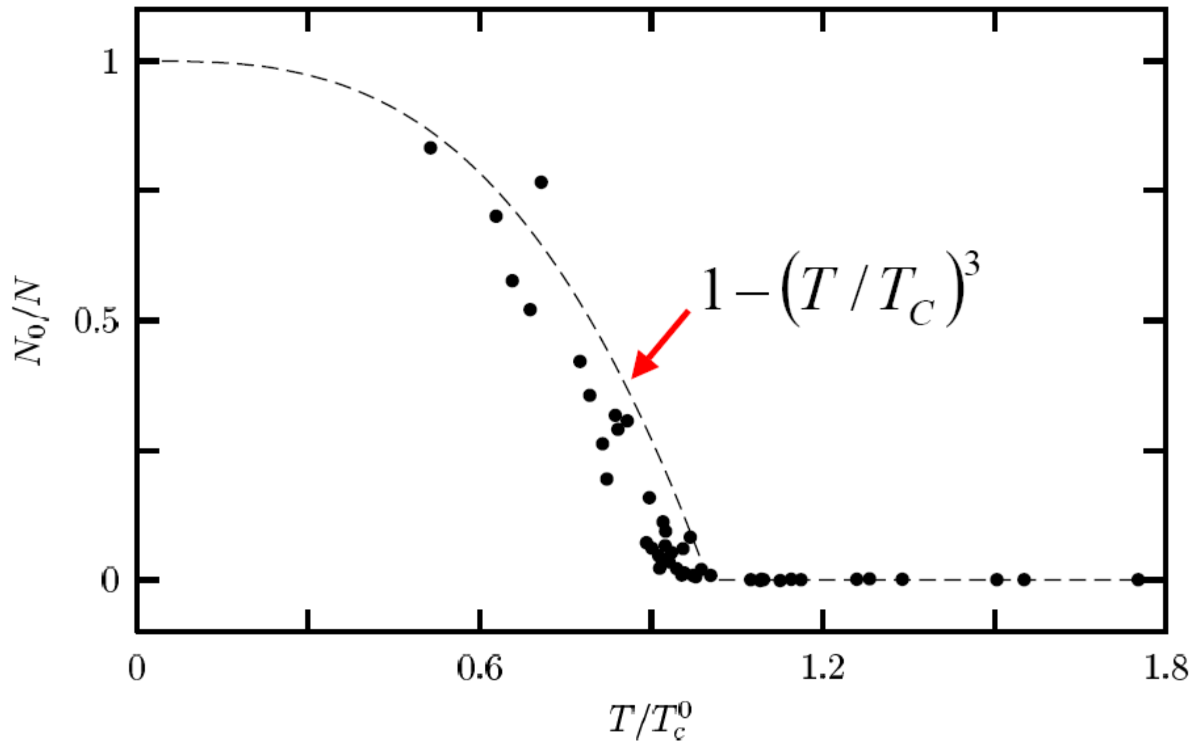
Density of states $$\rho(\varepsilon) = \frac{1}{2}\frac{\varepsilon^2}{\hbar^3\omega_{\text{ho}}^3}$$ * $$\omega_{\text{ho}} = (\omega_x\omega_y\omega_z)^{\frac{1}{3}}$$

$$N_{\max}(T) = \frac{T^3}{2\hbar^3\omega_{\text{ho}}^3}\int\frac{x^2dx}{e^x-1} = \left(\frac{T}{\hbar\omega_{\text{ho}}}\right)^3 g_3(1)$$

$$T_c \simeq 0.94\hbar\omega_{\text{ho}}N^{1/3} \gg \hbar\omega_{\text{ho}}$$

Number of condensed particles

Below T_c $$N_0 = N - N_T = N\left[1 - \left(\frac{T}{T_c}\right)^3\right]$$



Experimental evidence
(JILA 96)

of the number
of condensed particles

Condensate wave function

Density matrix can be diagonalised $\rho^{(1)}(\mathbf{x},\mathbf{y}) = \sum_\alpha n_\alpha \psi_\alpha^*(\mathbf{x})\psi_\alpha(\mathbf{y})$

n_α are occupation numbers

(for ideal gas $\psi_\alpha(\mathbf{x})$ are 1-particle wavefunctions)

$n_0 = N_0 \sim N$ $\psi_0(\mathbf{x})$ is the condensate wavefunction

Penrose, Onsager, 1956

Uniform system $\psi_0(x,y,z) = 1/L^{3/2}$

Harmonic oscillator

$$\psi_0(x,y,z) = \left(\frac{m\omega_{\mathrm{ho}}}{\pi\hbar}\right)^{3/4} \exp\left[-\frac{m}{2\hbar}(\omega_x x^2 + \omega_y y^2 + \omega_z z^2)\right]$$

Density matrix below Tc

$$\rho^{(1)}(\mathbf{x},\mathbf{y}) = N_0 \psi_0^*(\mathbf{x})\psi_0(\mathbf{y}) + \sum_{\alpha\neq 0} n_\alpha \psi_\alpha^*(\mathbf{x})\psi_\alpha(\mathbf{y})$$

Density profile $n(\mathbf{x}) = \rho^{(1)}(\mathbf{x},\mathbf{x}) = n_0(\mathbf{x}) + n_T(\mathbf{x})$

$$n_0(\mathbf{x}) = N_0|\psi_0(\mathbf{x})|^2$$

Non condensed distribution is semiclassical:

$$n_T(\mathbf{x}) \simeq \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{1}{e^{\beta\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})\right)} - 1} = \frac{1}{\Lambda_T^3} g_{3/2}(e^{-\beta V(\mathbf{x})})$$

Bimodal distribution

Condesate width

$$\langle \mathbf{x}^2 \rangle_0 \sim \frac{\hbar}{2m\omega_{\rm ho}}$$

Width of thermal cloud

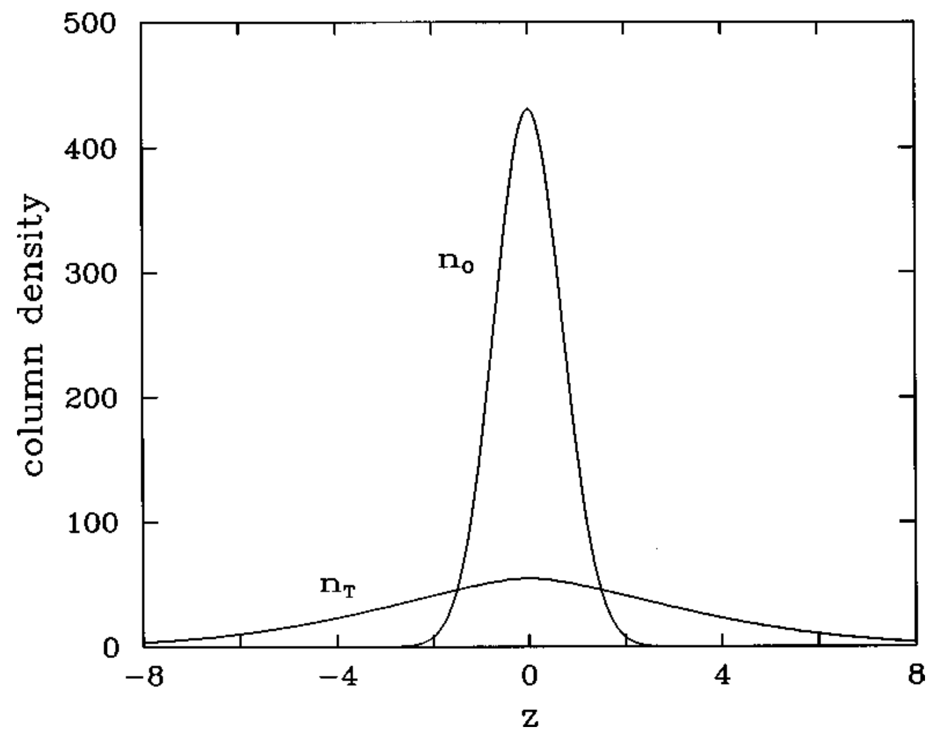
$$\langle \mathbf{x}^2 \rangle_T \sim \frac{T}{m\omega_{\rm ho}^2}$$

Ratio

$$\frac{\langle \mathbf{x}^2 \rangle_T}{\langle \mathbf{x}^2 \rangle_0} \sim \frac{T}{\hbar\omega_{\rm ho}} \gg 1$$

5000 bosons at $T = 0.9T_c$

Dalfovo et al. 1999



Summary of Lecture 1

- Quantum statistics modify thermodynamic property and may lead to long range order at low enough temperature when Λ_T is comparable with mean interparticle separation
- The long range order is in non-diagonal elements of one body density matrix and for ideal gas is connected with macroscopic occupation of ground state orbital, *i.e.* BEC
- The occurrence of condensation depends crucially on the density of states which controls number of particles for zero chemical potential: no condensation in uniform system in 2d and 1d. Very different for harmonic trap
- Ideal gas model gives a fair intuition for occurrence of BEC and is good close to T_c but is *unphysical* (infinite compressibility, shape of condensate....) at lower temperatures.