Bose-Einstein Condensation

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04/16/2013,
Hauptseminarvortrag

What is Bose-Einstein Condensation?

Setups for BEC-Preparation

Most common way to prepare a BEC: Magneto-optical traps & evaporative cooling

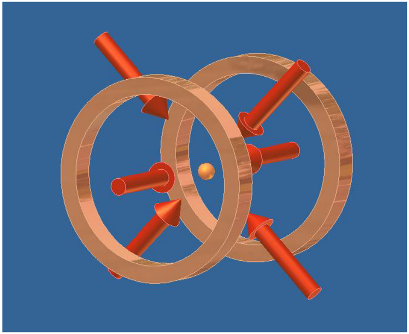

Figure: from "*Laserkühlen und Fangen von neutralen Atomen in einer magneto-optischen Falle*", *FP Physik Versuchsanleitung*

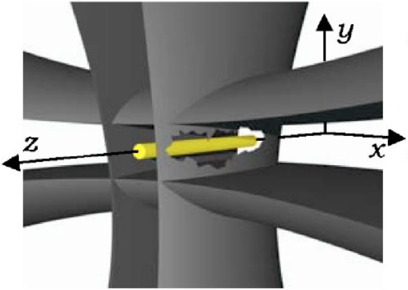

Figure: Optical trap modelling a 2D-box potential; *Meyrath et al.Physical Review A 71, 041604sRd s2005d*

Why study BEC?

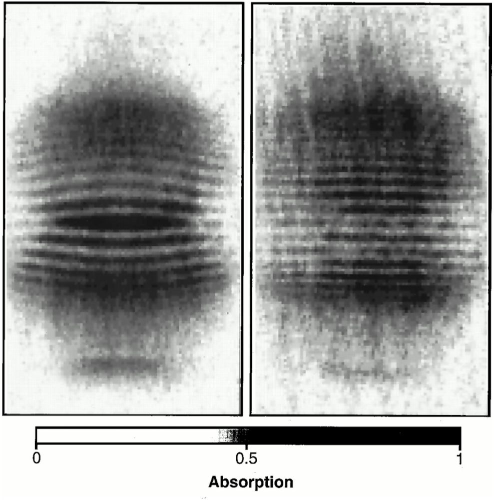

Figure: Interference of two initially separated condensates.;*Ketterle et al. Science 276, 637 (1997)*

Bose-Einstein-condensates can be used to deliver direct evidence of the wave-nature of matter and allow high-precision measurements

Outline

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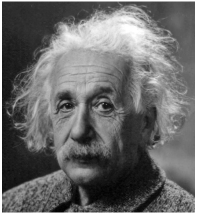
The discovery of BEC

Satyendranath Bose
(1894-1974)

1921, Time to solve the ultraviolett catastrophe. Photons are indistinguishable, so we need new statistics.



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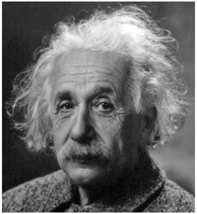

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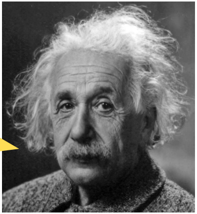

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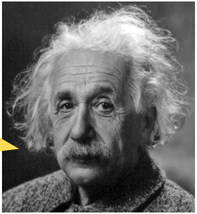

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1924: Indstinguishable atoms will condense at low T!

Remarkable developments

- 1995: First pure BECs are created at JILA (Colorado) and MIT; observation of interference effects (^{87}Rb and ^{23}Na, nK range)
- 1999: BEC preparation with magnons in an antiferromagnet at 14K
- 2006: Magnon-BEC in ferromagnets at room temperature

Outline

The grand-canonical ensemble: T, μ, V

- Setups for preparation of BECs allow the exchange of particles and energy
- The partition function ($\beta = 1/(k_\mathrm{B} T)$):

$$Z(T, \mu, V) = \sum_{i=0}^{\infty} \exp(-\beta(E_i - \mu N_i)) \tag{1}$$

Bose-Einstein distribution:

$$\bar{n}_k = \frac{1}{\exp[\beta(\varepsilon_k - \mu)] - 1} \tag{2}$$

Cold Gases in the Box

Hamiltonian of a (cold) gas:

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^{\,2}}{2m} + V(x_i) + \frac{1}{2}\sum_{i \neq j} U(x_i - x_j) \tag{3}$$

In the Box (periodic boundary conditions):

$$V(x_i) = \begin{cases} 0, & |x_i| \leq L \\ \infty & |x_i| > L \end{cases} \tag{4}$$

$$\hat{p}_i = \frac{2\pi}{L} n \tag{5}$$

First Step:

Neglect interaction; the ideal Bose-gas

Bose-Einstein Condensation of the ideal gas

Our Goals:

- Derive a critical Temperature
- Find a simple expression for the condensate fraction, N_0/N
- Draw a phase diagram of the ideal Bose-gas

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The isolation of the condensed component

Total Number of Particles:

$$\begin{aligned} N = \sum_j n_j &= \bar{n}_0 + \sum_{j\neq 0} n_j \\ &= \underbrace{N_0}_{\text{condensed component}} + \underbrace{N_T}_{\text{thermal component}} \end{aligned}$$

$$\begin{aligned} N_0 &= \frac{1}{\exp[\beta(\varepsilon_0-\mu)]-1} \overset{\varepsilon_0=0}{=} \frac{z}{1-z} \qquad / z = e^{\beta\mu} \\ &\Rightarrow \mu < \varepsilon_0 \end{aligned}$$

$$N_T = \sum_{i\neq 0} \frac{1}{\exp[\beta(\varepsilon_i-\mu)]-1} \approx \int_0^\infty \frac{dk}{(2\pi)^3} \frac{1}{\exp[\beta(\varepsilon_k-\mu)]-1}$$

The critical temperature

$$N_T \approx \frac{L^3}{\lambda^3}\frac{2}{\sqrt{\pi}}\int_0^\infty d\varepsilon \frac{\sqrt{\varepsilon}}{z^{-1}e^{\varepsilon}-1} = \frac{V}{\lambda^3} g_{\frac{3}{2}}(z) \qquad (6)$$

with $\lambda = \left(\frac{2\pi\hbar^2}{mk_B T}\right)^{\frac{1}{2}}$ [thermal wavelength]

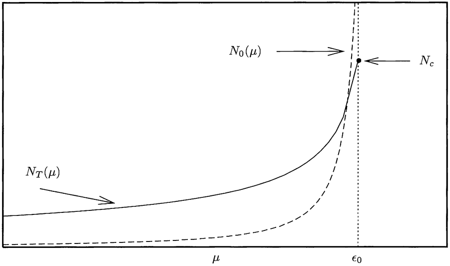


Figure: *from L.Pitaevskii, S.Stringari: Bose-Einstein Condensation*

$$\begin{aligned} \text{Let } N &= N_c = \frac{V}{\lambda_c^3} g_{3/2}(z = e^{\beta\varepsilon_0}) \\ \Rightarrow n &= \lambda_c^{-3} \cdot 2.612 \end{aligned}$$

Critical Temperature T_c

$$T_c = \frac{\hbar^2 n^{(2/3)}}{2m} \cdot \frac{6.63}{k_B} \qquad (7)$$

Macroscopic occupation of the ground state

$$
\begin{aligned}
n &= \frac{2.612}{\lambda^3} + n_0 \\
&= \frac{2.612}{\lambda_c^3}
\end{aligned}
$$

$$
\begin{aligned}
n_0 &= n - \frac{2.612}{\lambda^3} \\
&= \left[1 - \left(\frac{\lambda_c}{\lambda}\right)^3\right] n \\
\frac{n_0}{n} &= \left[1 - \left(\frac{T}{T_c}\right)^{\frac{3}{2}}\right]
\end{aligned}
$$

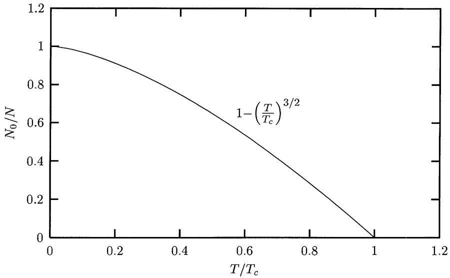


Figure: *from L.Pitaevskii, S.Stringari: Bose-Einstein Condensation*

Bose-Einstein Condensation

For $T < T_c$, the ground state is occupied macroscopically.

The phase-diagram

The Pressure can be calculated with the partition function:

$$p = -\frac{\Omega}{V} = \frac{T}{V}\ln Z = \frac{T}{\lambda^3} g_{5/2}(z)$$

$$\overset{T>>T_c}{=} Tn\left(1-\frac{n\lambda^3}{4\sqrt{2}}+\dots\right) \approx \frac{T}{v}\left(1-\frac{\lambda^3}{4\sqrt{2}v}\right)$$

$$\overset{T\leq T_c}{=} 1.342\frac{T}{\lambda^3}$$

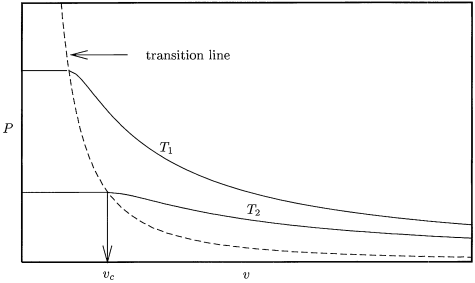
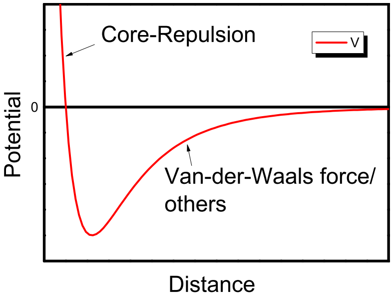


Figure: Phase diagram of the ideal Bose-Gas; $T_1 > T_2$, $v = n^{-1}$; *from L.Pitaevskii, S.Stringari: Bose-Einstein Condensation*

Introduction of interactions

Introduction of interactions adds a new term to the Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^{\,2}}{2m} + V(x_i) + \underbrace{\frac{1}{2}\sum_{i \neq j} U(x_i - x_j)}_{\text{interaction term}} \qquad (8)$$



- The shape of the potential doesn't allow the application of perturbation theory
- Solving the problem with the real interaction potential is impossible

The dilute gas

$\Rightarrow$ simplify!

Assumptions:

- The effective range r_0 of the interactions is much shorter than the average inter-particle distance d: $r_0 \ll d = n^{-1/3}$
- Gas is below the critical Temperature T_c

Consequences

- Only two-particle interactions have to be considered.
- The scattering amplitude $V(p) = \mathscr{F}(V(r))$ takes on a very simple form

The scattering amplitude

The scattering amplitude is the Fourier-transformed potential:

$$V(p) = \int V(r) e^{-ip\cdot r/\hbar} dr \tag{9}$$

With $T \leq T_c$ and $r_0 \ll d$ we get:

$$\frac{\hbar}{r_0} \gg \frac{\hbar}{d} \cdot 6.63 = \sqrt{2mk_B T_c}$$

$$\begin{aligned} p &\approx \sqrt{2mk_B T} \leq \sqrt{2mk_B T_c} = \hbar/d \ll \hbar/r_0 \\ \Rightarrow p &\ll \hbar/r_0 \end{aligned}$$

The scattering amplitude becomes independent of p:
($V(r) \approx 0$ for $r > r_0$)

$$V(p) = \int V(r) e^{-ip\cdot r/\hbar} dr \approx \int V(r) dr \tag{10}$$

The low-energy approximation

- The low energy approximation ("s-wave scattering") yields the s-wave scattering length a
- Interaction phenomena depend on a only in this regime
- This allows the use of a smooth effective potential V_{eff} which yields the same scattering length and -amplitude for small momenta $p \ll \hbar / r_0$
- Perturbation by the interaction potential must be small at all ranges to apply perturbation theory (Bogoliubov theory uses perturbation theory)
- A gas can be described as dilute if $|a| \ll n^{-1/3} = d$

Rewriting the Hamiltonian

Original Hamiltonian, expressed with field operators:

$$\hat{H} = \int \left(\frac{\hbar^2}{2m} \nabla \hat{\Psi}^\dagger \nabla \hat{\Psi} \right) d\mathbf{r} + \frac{1}{2} \int \hat{\Psi}^\dagger \hat{\Psi}^{\dagger\prime} V(\mathbf{r}' - \mathbf{r}) \hat{\Psi} \hat{\Psi}' d\mathbf{r}' d\mathbf{r} \quad (11)$$

Change of basis: $\left(\hat{\Psi}(\mathbf{r}) = \sum_{\mathbf{p}} \hat{a}_{\mathbf{p}} \frac{1}{\sqrt{V}} e^{i\mathbf{pr}/\hbar} \right)$

$$\hat{H} = \sum \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \frac{1}{2V} \sum V_{\mathbf{q}} \hat{a}^\dagger_{\mathbf{p_1}+\mathbf{q}} \hat{a}^\dagger_{\mathbf{p_2}-\mathbf{q}} \hat{a}_{\mathbf{p_1}} \hat{a}_{\mathbf{p_2}}$$

with $V_{\mathbf{q}} \approx V_0 = \int V(\mathbf{r}) d\mathbf{r}$ we get:

Basic Hamiltonian for Bogoliubov-Theory

$$\hat{H} = \sum \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \frac{V_0}{2V} \sum \hat{a}^\dagger_{\mathbf{p_1}+\mathbf{q}} \hat{a}^\dagger_{\mathbf{p_2}-\mathbf{q}} \hat{a}_{\mathbf{p_1}} \hat{a}_{\mathbf{p_2}}$$

The lowest-order approximation

In the dilute gas, occupation numbers at $T = 0$ are all small except for N_0:

$$\begin{aligned}\hat{H} = \; & \sum \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \frac{V_0}{2V} \sum \hat{a}^\dagger_{\mathbf{p_1}+\mathbf{q}} \hat{a}^\dagger_{\mathbf{p_2}-\mathbf{q}} \hat{a}_{\mathbf{p_1}} \hat{a}_{\mathbf{p_2}} \\ & \to \frac{V_0}{2V} \hat{a}^\dagger_0 \hat{a}^\dagger_0 \hat{a}_0 \hat{a}_0\end{aligned} \tag{12}$$

Bogoliubov prescription:

$$\hat{a}_0 \equiv \sqrt{N_0} \tag{13}$$

Which translates to $\hat{a}_0 \equiv \sqrt{N}$ and thus:

Ground state energy in lowest order approximation:

$$E_0 = \frac{N^2 V_0}{2V} \tag{14}$$

Lowest order approximation: Results

- Pressure remains finite, even for $T = 0$:

$$p \equiv -\frac{\partial E_0}{\partial V} = \frac{V_0}{2} n^2$$

- Thermodynamic stability requires $\frac{\partial n}{\partial p} = \frac{1}{V_0 n} > 0$
  $\Rightarrow$ BECs can only exist with repulsive V_0 (assuming no external potentials)
- $\mu = \frac{\partial E_0}{\partial N} = V_0 n$ is always positive or zero

BECs in external potentials

- BEC is often achieved by using magnetic traps
  $\Rightarrow$ external potential
- Gross-Pitaevskii-equation describes BECs in external potentials ("non-uniform Bose-Gases") in the lowest order approximation
- Assumes very low temperatures, so $N_0 \approx N$ and $V_{\mathbf{p}} \approx V_0$

Deriving the Gross-Pitaevskii-Equation

Starting Point:

$$i\hbar\partial_t\hat{\Psi}(\mathbf{r},t) = \begin{array}{l}[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r},t) \\ +\int\hat{\Psi}^\dagger(\mathbf{r}',t)V(\mathbf{r}'-\mathbf{r})\hat{\Psi}(\mathbf{r}',t)d\mathbf{r}']\hat{\Psi}(\mathbf{r},t)\end{array} \tag{15}$$

Replacing $\hat{\Psi}$ and $V(r)$:

$$i\hbar\partial_t\Psi_0(\mathbf{r},t) = \begin{array}{l}[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r},t) \\ +\int\Psi_0^*(\mathbf{r}',t)V_{eff}(\mathbf{r}'-\mathbf{r})\Psi_0(\mathbf{r}',t)d\mathbf{r}']\Psi_0(\mathbf{r},t)\end{array} \tag{16}$$

With $\Psi_0(\mathbf{r}',t) \approx \Psi_0(\mathbf{r},t)$ for $r' < r_0$:

$$i\hbar\partial_t\Psi_0(\mathbf{r},t) = \begin{array}{l}[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r},t) \\ +\int V_{eff}(\mathbf{r}'-\mathbf{r})d\mathbf{r}'|\Psi_0(\mathbf{r},t)|^2]\Psi_0(\mathbf{r},t)\end{array} \tag{17}$$

The Gross-Pitaevskii-Equation

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$$i\hbar\partial_t\Psi_0(\mathbf{r},t) = \left[-\frac{\hbar^2\nabla^2}{2m} + V_{ext}(\mathbf{r},t) + V_0|\Psi_0(\mathbf{r},t)|^2 d\mathbf{r}\right]\Psi_0(\mathbf{r},t) \tag{18}$$

- $n(\mathbf{r}) = |\Psi_0(\mathbf{r})|^2$
- Ψ_0 is classical limit of the de-Broglie wave
- GPE: Main tool for describing trapped gases theoretically
- Only valid for problems with many particles and length scales bigger than the scattering length a

Taking in higher orders: Bogoliubov approximation

- Lowest-order approximation: Only terms with $\mathbf{p} = 0$, Bogoliubov approximation also takes terms with $\mathbf{p} \neq 0$
- Terms violating conservation of momentum can be disregarded right away (neglected quadratic $\mathbf{p} \neq 0$ terms):

$$\begin{aligned}\hat{H} = \quad & \sum \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \frac{V_0}{2V} \sum \hat{a}^\dagger_{\mathbf{p_1}+\mathbf{q}} \hat{a}^\dagger_{\mathbf{p_2}-\mathbf{q}} \hat{a}_{\mathbf{p_1}} \hat{a}_{\mathbf{p_2}} \\ = \quad & \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \frac{V_0}{2V} \hat{a}^\dagger_0 \hat{a}^\dagger_0 \hat{a}_0 \hat{a}_0 \\ & + \frac{V_0}{2V} \sum_{\mathbf{p}\neq \mathbf{0}} (4 \hat{a}^\dagger_0 \hat{a}^\dagger_{\mathbf{p}} \hat{a}_0 \hat{a}_{\mathbf{p}} + \hat{a}^\dagger_{\mathbf{p}} \hat{a}^\dagger_{-\mathbf{p}} \hat{a}_0 \hat{a}_0 + \hat{a}^\dagger_0 \hat{a}^\dagger_0 \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}})\end{aligned}$$

Interaction term consists of:

1. "exchange" term $\hat{a}^\dagger_0 \hat{a}^\dagger_{\mathbf{p}} \hat{a}_0 \hat{a}_{\mathbf{p}} = N \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}}$
2. "excitation" terms
$\hat{a}^\dagger_{\mathbf{p}} \hat{a}^\dagger_{-\mathbf{p}} \hat{a}_0 \hat{a}_0 + \hat{a}^\dagger_0 \hat{a}^\dagger_0 \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}} = N(\hat{a}^\dagger_{\mathbf{p}} \hat{a}^\dagger_{-\mathbf{p}} + \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}})$

Quadratic term: higher accuracy

$$\hat{H} = \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{V_0}{2V} \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 + \frac{V_0 N}{2V} \sum_{\mathbf{p}\neq\mathbf{0}} (4\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}})$$

Second term requires higher accuracy:

$$\begin{aligned} \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 &\approx N_0^2 \\ &= (N - N_T)^2 \\ &= (N - \textstyle\sum_{\mathbf{p}\neq 0} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}})^2 \\ &\approx N^2 - 2N \textstyle\sum_{\mathbf{p}\neq 0} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} \end{aligned}$$

New Hamiltonian:

$$\hat{H} = \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{V_0 n N}{2} + \frac{V_0 n}{2} \sum_{\mathbf{p}\neq\mathbf{0}} (2\hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{-\mathbf{p}}^\dagger + \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}}) \quad (19)$$

The Bogoliubov-Transformation

$$\hat{H} = \sum_{\mathbf{p}} \frac{p^2}{2m} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \frac{V_0 n N}{2} + \frac{V_0 n}{2} \sum_{\mathbf{p}\neq\mathbf{0}} (2\hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} + \hat{a}^\dagger_{\mathbf{p}} \hat{a}^\dagger_{-\mathbf{p}} + \hat{a}_{\mathbf{p}} \hat{a}_{-\mathbf{p}})$$

The new Hamiltonian can be diagonalized via the Bogoliubov-transformation:

$$\begin{aligned} \hat{a}_{\mathbf{p}} &= u_{\mathbf{p}} \hat{b}_{\mathbf{p}} + v_{-\mathbf{p}} \hat{b}^\dagger_{-\mathbf{p}} \\ \hat{a}^\dagger_{\mathbf{p}} &= u_{\mathbf{p}} \hat{b}^\dagger_{\mathbf{p}} + v_{-\mathbf{p}} \hat{b}_{-\mathbf{p}} \end{aligned}$$

with $[\hat{a}_p, \hat{a}^\dagger_p] = [\hat{b}_p, \hat{b}^\dagger_p] = \delta_{pp'}$

Blackboard calculation: Bogoliubov-Transformation

Outline

Critical Temperature

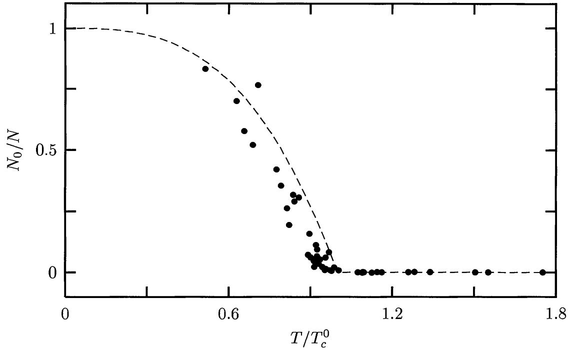


Figure: Condensate fraction vs Temperature (harmonic potential); Graph from *L.Pitaevskii, S.Stringari: Bose-Einstein Condensation*; Data from *Ensher et al., Phys.Rev.Let.77,25 (1996)*

Two-body interactions only contribute weakly to the condensation behaviour

Particle distribution

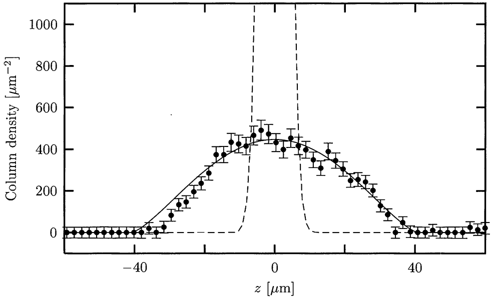


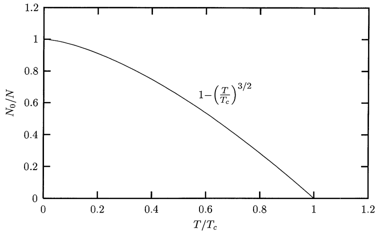
Figure: Dashed line: ideal gas; solid line: GP-equation - Graph from *L.Pitaevskii, S.Stringari: Bose-Einstein Condensation;* Data from *Hau et al., Phys.Rev. A 58,1 (1998)*

- Ideal Bose Gas' size depends only on the external potential
- real gases must expand with greater particle numbers

Summary: Mathematical results

Ideal Bose-Gas in the box:

- $T_c = \frac{\hbar^2 n^{(2/3)}}{2m} \cdot \frac{6.63}{k_B}$
- $N_0/N = 1 - \left(\frac{T}{T_c}\right)^{(3/2)}$
- Infinite compressibility



Weakly interacting Bose-Gas:

- Introduction of cold, dilute gases ($|a| \ll d$)
- Derived Gross-Pitaevskii-equation as main tool for investigating BEC
- Extended applicability with Bogoliubov-approximation

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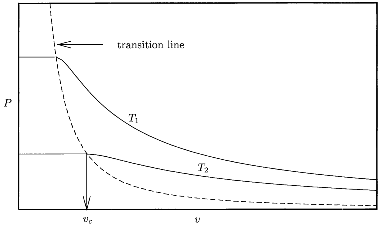

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