1. Institut für Theoretische Physik

Seminar in theoretical physics: Non-linear and non-hermitian quantum mechanics

Bose-Einstein Condensation: Basics, Gross-Pitaevskii equation and Interactions

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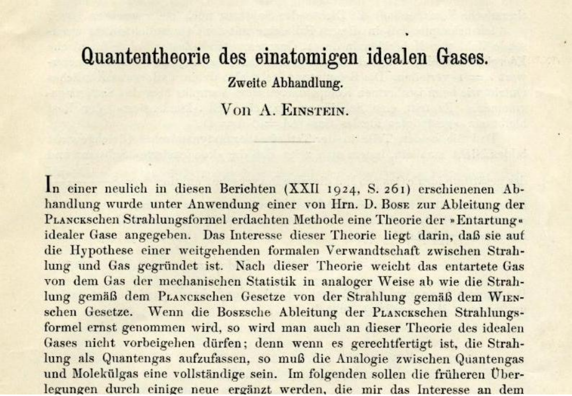
Introduction



Quantentheorie des einatomigen idealen Gases.

Zweite Abhandlung.

Von A. Einstein.

In einer neulich in diesen Berichten (XXII 1924, S. 261) erschienenen Abhandlung wurde unter Anwendung einer von Hrn. D. Bose zur Ableitung der Planckschen Strahlungsformel erdachten Methode eine Theorie der »Entartung« idealer Gase angegeben. Das Interesse dieser Theorie liegt darin, daß sie auf die Hypothese einer weitgehenden formalen Verwandtschaft zwischen Strahlung und Gas gegründet ist. Nach dieser Theorie weicht das entartete Gas von dem Gas der mechanischen Statistik in analoger Weise ab wie die Strahlung gemäß dem Planckschen Gesetze von der Strahlung gemäß dem Wienschen Gesetze. Wenn die Bosesche Ableitung der Planckschen Strahlungsformel ernst genommen wird, so wird man auch an dieser Theorie des idealen Gases nicht vorbeigehen dürfen; denn wenn es gerechtfertigt ist, die Strahlung als Quantengas aufzufassen, so muß die Analogie zwischen Quantengas und Molekülgas eine vollständige sein. Im folgenden sollen die früheren Überlegungen durch einige neue ergänzt werden, die mir das Interesse an dem

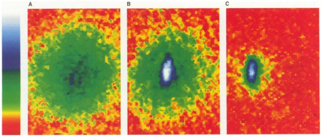
Figure: Theoretical prediction of Bose-Einstein condensation in 1924. from [1]

Introduction

Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor

M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman,* E. A. Cornell

A Bose-Einstein condensate was produced in a vapor of rubidium-87 atoms that was confined by magnetic fields and evaporatively cooled. The condensate fraction first appeared near a temperature of 170 nanokelvin and a number density of 2.5×10^{12} per cubic centimeter and could be preserved for more than 15 seconds. Three primary signatures of Bose-Einstein condensation were seen. (i) On top of a broad thermal velocity distribution, a narrow peak appeared that was centered at zero velocity. (ii) The fraction of the atoms that were in this low-velocity peak increased abruptly as the sample temperature was lowered. (iii) The peak exhibited a nonthermal, anisotropic velocity distribution expected of the minimum-energy quantum state of the magnetic trap in contrast to the isotropic, thermal velocity distribution observed in the broad uncondensed fraction.



First experimental Observation in 1995. Typically the velocity distribution is shown before the condensate appears (A), shortly afterwards (B) and very pure condensate (C). from [2]

Ideal Bose Gas

The Gross-Pitaevskii equation

Scattering theory

Ideal Bose gas

Bosons

- spin s is integer
- bosons may occupy the same single-particle state (symmetric wave function $\rightarrow$ no Pauli-principle)
- for $T = 0$ all bosons are in the ground state $N = N_0$ and the total wave function is a product of the single-particle wave functions: $\psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \prod_{i=1}^{N} \phi_0(\mathbf{r}_i)$
- for $T > 0$ bosons are in the thermal component as well $N = N_0 + N_T$
- Bose-Einstein condensate when ground state is occupied macroscopically

Ideal Bose gas

neglect interaction between particles

grand canonical ensemble:

- chemical potential μ and temperature T are fixed
- ε_i energies of single-particle states in the system
- total energy: $\varepsilon = \sum_i \varepsilon_i N_i$
  total number of particles: $N = \sum_i N_i$
- the chemical potential μ can be seen as:

$$\mu = \varepsilon(n) - \varepsilon(n-1)$$

  it can never exceed the energy of the ground state: $\mu \leq \varepsilon_0$

Finding T_c and fraction of particles in the condensate

- grand canonical partition function Z for bosons

$$Z = \prod_i \frac{1}{1 - \exp\left[(\mu - \varepsilon_i)/kT\right]}$$

- thermal occupation of the ith energy eigenstate

$$\begin{aligned} N_i =& kT \frac{\partial}{\partial \mu} \ln Z_i \\ =& \frac{1}{\exp\left[(\varepsilon_i - \mu)/kT\right] - 1} \end{aligned}$$

Finding T_c and fraction of particles in the condensate

- total number of particles

$$N = N_0 + \sum_{i \neq 0} \frac{1}{\exp\left[(\varepsilon_i - \mu)/kT\right] - 1}$$

$\sum_{i \neq 0} \quad \rightarrow \quad \int_{>0}^{\infty} d\varepsilon$ with the density of states $D(\varepsilon) = C_\alpha \varepsilon^{\alpha - 1}$

- density of states:
  free particle:

$$D(\varepsilon) = \frac{V}{2\pi} \left(\frac{2m}{\hbar^2} \right)^{3/2} \varepsilon^{1/2} = C_{3/2} \varepsilon^{3/2 - 1}$$

  harmonic trap:

$$D(\varepsilon) = \frac{\varepsilon^2}{2\hbar^3 \omega_x \omega_y \omega_z} = C_3 \varepsilon^{3 - 1}$$

Finding T_c and fraction of particles in the condensate

- total number of particles

$$N = N_0 + C_\alpha \int_{>0}^{\infty} \frac{\varepsilon^{\alpha-1}}{\exp[(\varepsilon-\mu)/kT]-1} d\varepsilon$$

- At T_c all particles are in the thermal component and $\mu_c = 0$

$$\begin{aligned} N_T(T_c, \mu = 0) &= C_\alpha \int_{>0}^{\infty} \frac{\varepsilon^{\alpha-1}}{\exp[\varepsilon/kT_c]-1} d\varepsilon \\ &= C_\alpha (kT_c)^\alpha \Gamma(\alpha) \zeta(\alpha) = N \end{aligned}$$

with $\Gamma(\alpha) = \int_0^\infty x^{\alpha-1} \exp(-x) dx$ and $\zeta(\alpha) = \sum_{n=1}^{\infty} n^{-\alpha}$

Finding T_c and fraction of particles in the condensate

- Therefore T_c is for a free particle given by:

$$kT_c = \frac{2\pi\hbar^2}{m}\left(\frac{N/V}{\zeta(3/2)}\right)^{2/3}$$

- compare to the thermal de-Broglie wavelength:

$$\lambda_c = \sqrt{\frac{2\pi\hbar^2}{mkT_c}} = \zeta(3/2)^{1/3}\frac{1}{(N/V)^{1/3}}$$

- Bose-Einstein condensation takes place when the mean free path and the de-Broglie wavelength are of the same order of magnitude

Finding T_c and fraction of particles in the condensate

- T_c is for a harmonic trap given by:

$$kT_c = \hbar(\omega_x\omega_y\omega_z)^{1/3}\left(\frac{N}{\zeta(3)}\right)^{1/3}$$

  typical critical temperatures in harmonic traps are $10^{-7}K$

- For $T < T_c$ the chemical potential stays $\mu = 0$

$$\begin{aligned} N_T(T,\mu=0) &= C_\alpha(kT)^\alpha\Gamma(\alpha)\zeta(\alpha) \\ &= N\left(\frac{T}{T_c}\right)^\alpha \end{aligned}$$

Finding T_c and fraction of particles in the condensate

The number of particles in the condensate is:

$$N_0 = N\left(1 - \left(\frac{T}{T_c}\right)^{\alpha}\right)$$

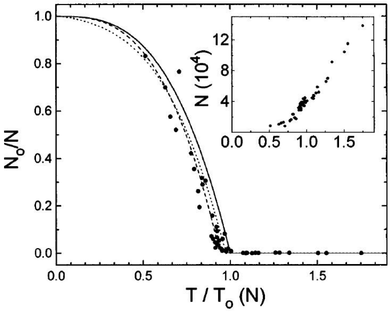


Figure: Total number N and ground state fraction N_0 as a function of scaled temperature T/T_c. from [3]

Ideal Bose Gas

The Gross-Pitaevskii equation

Scattering theory

Derivation of the Gross-Pitaevskii equation

many-particle Schrödinger equation

$$\sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\Delta_i + V_{ext}(\mathbf{r_i}) + \frac{1}{2}\sum_{\substack{j=1\\ j\neq i}}^{N} W(\mathbf{r_i},\mathbf{r_j})\right]\psi(\mathbf{r_1},..,\mathbf{r_N}) = E\psi(\mathbf{r_1},..,\mathbf{r_N})$$

Not solvable exactly! Assume that all particles are in the ground state and use mean-field theory:

- ground state wave function is product of identical single-particle wave functions:

$$\psi(\mathbf{r_1},..,\mathbf{r_N}) = \prod_{i=1}^{N}\phi(\mathbf{r_i})$$

- neglect correlations between particles

Derivation of the Gross-Pitaevskii equation

- vary single-particle wave function to minimize the total energy

$$
\begin{aligned}
E_{mf} &= \langle \psi(\mathbf{r_1}, ..., \mathbf{r_N}) | \, H \, | \psi(\mathbf{r_1}, ..., \mathbf{r_N}) \rangle \\
&= \int d\mathbf{r_1} ... \int d\mathbf{r_N} \left(\prod_{i=1}^{N} \phi^*(\mathbf{r_i}) \right) \\
&\quad \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \Delta_i + V_{ext}(\mathbf{r_i}) + \frac{1}{2} \sum_{\substack{j=1 \\ j \neq i}}^{N} W(\mathbf{r_i}, \mathbf{r_j}) \right] \left(\prod_{i=1}^{N} \phi(\mathbf{r_i}) \right) \\
&= -N \frac{\hbar^2}{2m} \int d\mathbf{r} \phi^*(\mathbf{r}) \Delta \phi(\mathbf{r}) + N \int d\mathbf{r} \, V_{ext}(\mathbf{r}) |\phi(\mathbf{r})|^2 \\
&\quad + \frac{1}{2} N(N-1) \int d\mathbf{r} \int d\mathbf{r'} W(\mathbf{r}, \mathbf{r'}) |\phi(\mathbf{r})|^2 |\phi(\mathbf{r'})|^2
\end{aligned}
$$

Derivation of the Gross-Pitaevskii equation

- vary $\phi(\mathbf{r})$ but respect normalization

$$\int d\mathbf{r}\phi^*(\mathbf{r})\phi(\mathbf{r}) = 1$$

  by using a Lagrange parameter μN
- the first variation with respect to $\phi^*(\mathbf{r})$ should be zero
- first variation of a functional:

$$\delta F(y)(f) = \frac{d}{d\varepsilon} F(y + \varepsilon f)\Big|_{\varepsilon=0}$$

Derivation of the Gross-Pitaevskii equation

$$
\begin{aligned}
&\delta\left(E_{mf} - \mu N\left(\int d\mathbf{r}\phi^*(\mathbf{r})\phi(\mathbf{r}) - 1\right)\right)(f) \\
&= \int d\mathbf{r} \;\; f\left(-N\frac{\hbar^2}{2m}\Delta\phi(\mathbf{r}) + NV_{ext}(\mathbf{r})\phi(\mathbf{r})\right. \\
&\quad \left. + N(N-1)\int d\mathbf{r'}|\phi(\mathbf{r'})|^2 W(\mathbf{r},\mathbf{r'})\phi(\mathbf{r}) - \mu N\phi(\mathbf{r})\right) = 0
\end{aligned}
$$

has to be zero for every test function f

- for a big number of particles $N \approx N - 1$
- Gross-Pitaevskii equation

$$
\left[-\frac{\hbar^2}{2m}\Delta + V_{ext}(\mathbf{r}) + N\int d\mathbf{r'}|\phi(\mathbf{r'})|^2 W(\mathbf{r},\mathbf{r'})\right]\phi(\mathbf{r}) = \mu\phi(\mathbf{r})
$$

The Gross-Pitaevskii equation is a non-linear differential equation

- existence and uniqueness of solutions of non-linear differential equations are hard to show
- the superposition of two solutions of a non-linear differential equation is not necessarily a solution to it as well
- usually symmetries of the problems have to be used to solve a non-linear differential equation
- two solutions ϕ_a, ϕ_b corresponding to different values μ_a, μ_b are not orthogonal: $\int d\mathbf{r}\phi_a^*\phi_b$ can be different from zero.
- for large values of N the many-particle wave functions become orthogonal:

$$\left(\int d\mathbf{r}\phi_a^*\phi_b\right)^N \stackrel{N\to\infty}{\longrightarrow} 0$$

Ideal Bose Gas
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Scattering theory

Interactions in the condensate

- Gross-Pitaevskii equation:

$$\left[-\frac{\hbar^2}{2m}\Delta + V_{ext}(\mathbf{r}) + N\int d\mathbf{r'}|\phi(\mathbf{r'})|^2 W(\mathbf{r},\mathbf{r'})\right]\phi(\mathbf{r}) = \mu\phi(\mathbf{r})$$

- up to here: $W(\mathbf{r},\mathbf{r'})$ is any arbitrary interaction between two particles
- in the condensate both long-range and short-range interactions take place
- scattering (short-range interaction) will be discussed

Scattering Theory

- Scattering between two particles is described in relative coordinates with the reduced mass μ
- Schrödinger-equation for the relative motion

$$\left[-\frac{\hbar^2}{2\mu}\Delta + V(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

- Two particle interaction is described by Lennard-Jones potential:

$$V(r) = \frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}$$

  Second part describes Van-der-Waals interaction
- Schrödinger equation for the relative motion is solved by:

$$\psi(\mathbf{r}) = e^{i\mathbf{kr}} + f(\theta)\frac{e^{ikr}}{r}$$

  incoming plane wave and a scattered spheric wave
  $f(\theta)$:scattering amplitude depending on the potential

Scattering Theory

The scattering cross section is given by:

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

with the phase shifts δ_l

- for short-range interaction (here $1/r^6$) phase shifts become small for small k
- s-wave scattering ($l = 0$) becomes dominant

in this limit:

$$\tan \delta_0 = -ak$$

$$\sigma = 4\pi \frac{\delta_0^2}{k^2} = 4\pi a^2$$

The constant a is called the scattering length.

Scattering Theory

the scattering amplitude is given by:

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)P_l(cos\theta)(e^{2i\delta_l} - 1)$$

with the Legendre polynoms P_l

- consider s-wave scattering $(l = 0) \rightarrow P_0 = 1$
- use $\tan\delta_0 = -ak$

in this limit:

$$f(\theta) = \frac{1}{2ik}(e^{2i\delta_0} - 1) = -\frac{a}{1 + iak}$$

Effective Potential

- Use an effective potential V_{eff} which leads to the same $f(\theta)$ and σ section as the original potential:

$$V_{eff} = V_0 \delta(\mathbf{r})$$

- Solving the Schrödinger equation shows:

$$V_0 = \frac{2\pi\hbar^2 a}{\mu} = \frac{4\pi\hbar^2 a}{m}$$

- For the Gross-Pitaevskii equation we do not use relative coordinates:

$$W_{eff}(\mathbf{r}, \mathbf{r'}) = \frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r} - \mathbf{r'})$$

Trapped Bose-Einstein Condensate with interactions

- The Gross-Pitaevskii equation including a harmonic trapping potential and the effective scattering potential:

$$\left[-\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m\omega_0^2 r^2 + N\frac{4\pi\hbar^2 a}{m}|\phi(\mathbf{r})|^2\right]\phi(\mathbf{r}) = \mu\phi(\mathbf{r})$$

  can not easily be solved.

- For $a = 0$ the ground state of the harmonic oscillator is:

$$\phi_0(\mathbf{r}) = \frac{1}{\pi^{3/4} a_{osc}^{1/2}} \exp\left[-\frac{r^2}{2a_{osc}^2}\right]$$

  with $a_{osc} = \sqrt{\hbar/m\omega_0}$.

- We assume that the interatomic interactions change the dimensions of the cloud: replace a_{osc} by b

Trapped Bose-Einstein Condensate with interactions

- To find b: Same approach as derivation of Gross-Pitaevskii equation. Minimize mean-field energy with respect to b.
- The total energy of the system is given by:

$$E(b) = 3N\hbar\omega_0 \left(\frac{a_{osc}^2}{b^2} + \frac{b^2}{a_{osc}^2} \right) + \frac{N^2 U_0}{2(2\pi)^{3/2} b^3}$$

- For large N: interaction energy per particle large compared to $\hbar\omega_0 \rightarrow$ neglect kinetic energy term

Trapped Bose-Einstein Condensate with interactions

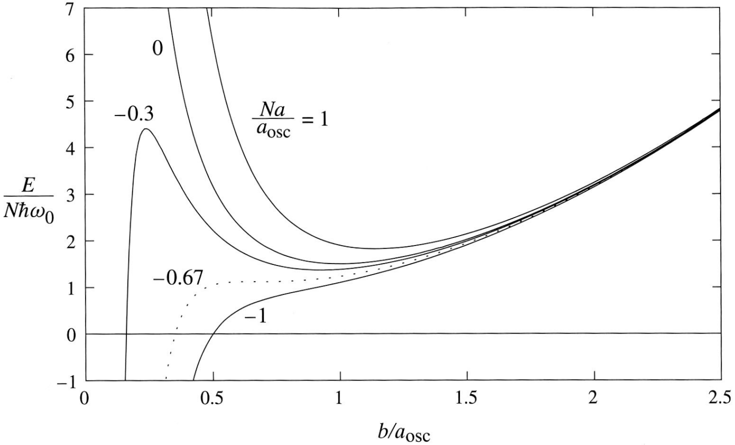

Figure: Mean-field energy of the Bose-Einstein Condensate including a harmonic trapping potential and scattering. from [4]

Trapped Bose-Einstein Condensate with interactions

- Solution is given by ground state wave function of the harmonic potential:

$$\psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \prod_{i=1}^{N} \frac{1}{\pi^{3/4} b^{1/2}} \exp\left[-\frac{r_i^2}{2b^2}\right]$$

with the new oscillator length:

$$b = \left(\frac{2}{\pi}\right)^{1/10} \left(\frac{Na}{a_{osc}}\right)^{1/5} a_{osc}$$

- And the total energy is given by:

$$E = \frac{5N}{4} \left(\frac{2}{\pi}\right)^{1/5} \left(\frac{Na}{a_{osc}}\right)^{2/5} \hbar\omega_0$$

- but no solution for $\frac{Na}{a_{osc}} \leq -0.671$

Conclusions

- Below a critical temperature T_c Bose-Einstein condensation takes place: The ground state is occupied macroscopically.
- A mean-field approach leads to the Gross-Pitaevskii equation which has to be fulfilled by the single-particle wave functions in order to minimize the total energy in the system.
- Using an effective potential to describe scattering the energy and wave function of the system can be found.

A. Einstein.
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Thanks for your attention!