Bose-Einstein Condensation

Kim-Louis Simmoteit

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1 Introduction

For several hundred years it is known that matter can have various states of aggregation, including solid, liquid and gaseous. Apart from them further states of matter exist, which were discovered in the last 100 years within the introduction of quantum physics. A major discovery was made by the physicist Albert Einstein(1925)[1] based on a paper of Bose(1924)[2] . He firstly noticed a condensation of a macroscopic number of Bosons into the ground state for an ideal gas of Bosons, referred to as Bose-Einstein condensation (BEC). Finally after 70 years, the first experimental creation of a Bose-Einstein condensate was achieved in a trap. For their work Cornell,Wiedmann and Ketterle were awarded with the Nobel prize of physics 2001 [3]. Since then, further development was pushed into the subject of

Bose-Einstein condensation by several working groups and people to gain a better understanding and experimental progress. As an example the proper realization of an Atom-Laser is one of the main goals.

2 Condensation of Trapped Ideal Bose Gas

Trapping of a Bose Gas is important for the experimental realization of Bose-Einstein condensation. Therefore this section shows the basic mechanism of Bose-Einstein condensation with using a uniform, non-interacting gas of Bosons confined in an external harmonic potential, as it is described in [4, 5, 6, 7] and [8].

2.1 Trapped Bose Gas

In the following a system of a trapped noninteracting ideal Bose gas with spin $s = 0$ is examined with help of statistical physics. The single particle Hamiltonian of the system is expressed as

$$\mathcal{H} = \frac{p^2}{2m} + V_{ext}, \qquad V_{ext} = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \tag{2.1}$$

with eigenvalues

$$\begin{aligned} \epsilon &= (n_x + \frac{1}{2})\hbar\omega_x + (n_y + \frac{1}{2})\hbar\omega_y + (n_z + \frac{1}{2})\hbar\omega_z \\ &= \epsilon_{000} + \hbar(\omega_x n_x + \omega_y n_y + \omega_z n_z) \end{aligned} \tag{2.2}$$

where $n_i, i = 1, 2, 3$ being integer numbers from 0 to infinity. The groundstate energy $\epsilon_{000} = \frac{1}{2}\hbar(\omega_x + \omega_y + \omega_z)$ is directly pulled out for later usage. Starting point is the average particle number

$$< N >= \sum_i < n_i > \tag{2.3}$$

which can be obtained from the grandcanonical ensemble. Due to having a system of Bosons, particles in each state are distributed after the Bose-Einstein distribution:

$$< n_B >= \frac{1}{e^{\beta(\epsilon-\mu)} - 1} \tag{2.4}$$

Characteristic for this distribution is its divergence close at μ, which is the underlying principle of the Bose-Einstein condensation. Also important to mention is the constraint of the chemical potential μ

$$\mu \leq \epsilon_0 \tag{2.5}$$

to prevent an outcome of negative particle numbers. From (2.3) one now obtains

$$< N >= \sum_{n_x=0}^{\infty} \sum_{n_y=0}^{\infty} \sum_{n_z=0}^{\infty} \frac{1}{e^{\beta(\epsilon(n_x,n_y,n_z)-\mu)} - 1} \tag{2.6}$$

If the thermal energy $k_B T$ is much higher than the harmonic oscillator energy $\hbar\omega_i$ between single oscillator states, one obtains a semiclassical approximation [4]

$$\frac{\hbar\omega_i}{k_B} \ll T \tag{2.7}$$

and the sums can be replaced by integrals. For low temperatures this approximation is not valid anymore and one need to go back to summation. The number of particles in the groundstate $< N_0 >$ is listed separately, but can be neglected at high temperatures. This leads to the following equation with μ' beeing defined as $\mu' = \mu - \epsilon_{000}$ [8]:

$$\begin{aligned} < N > &=< N_0 > + < N_T > \\ &=< N_0 > + \int_0^{\infty}\int_0^{\infty}\int_0^{\infty} \frac{1}{e^{\beta(\hbar(\omega_x n_x+\omega_y n_y+\omega_z n_z)-\mu')} - 1} \mathrm{d}n_x \mathrm{d}n_y \mathrm{d}n_z \end{aligned} \tag{2.8}$$

Rewriting the Bose-Einstein distribution as a geometric series, a simplification of this expression into easily solvable integrals is done [7]:

$$\begin{aligned} < N_T > &= \int_0^{\infty}\int_0^{\infty}\int_0^{\infty} \sum_{l=1}^{\infty} [e^{-\beta(\hbar(\omega_x n_x+\omega_y n_y+\omega_z n_z)-\mu')}]^l \mathrm{d}n_x \mathrm{d}n_y \mathrm{d}n_z \\ &= \sum_{l=1}^{\infty} e^{\beta\mu' l} \prod_{i=1}^{3} (\int_0^{\infty} e^{-\beta\hbar\omega_i n_i l} \mathrm{d}n_i) \\ &= \sum_{l=1}^{\infty} e^{\beta\mu' l} (\frac{1}{\beta\hbar l\bar{\omega}})^3 \end{aligned} \tag{2.9}$$

($\bar{\omega}$ is defined as the geometric average $\bar{\omega} = (\omega_x\omega_y\omega_z)^{\frac{1}{3}}$ of the oscillator frequencies [4]). In the next step the generalized Riemann-Zeta function is introduced:

Definition: *Generalized Riemann-Zeta function*

$$g_\nu(x) = \sum_{l=1}^{\infty} \frac{x^l}{l^\nu} \tag{2.10}$$

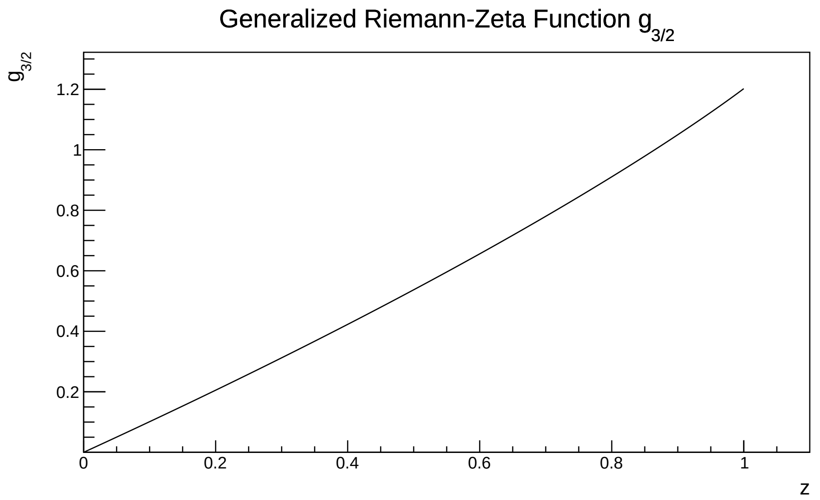

Figure 1: Plot of the generalized Riemann-Zeta function with $\nu = 3$ (own creation).

Riemann-Zeta function

$$\zeta(\nu) = g_\nu(1) \tag{2.11}$$

Equation (2.9) can now be simplified to

$$< N_T >= (\frac{1}{\hbar\beta\bar{\omega}})^3 g_3(z) \tag{2.12}$$

with z being a fugacity $z = e^{\beta\mu'}$. A visualization of $g_3(z)$ is shown in Figure 1.

An alternative way to solve (2.8) would be to rewrite the integral in terms of energy ϵ, yielding the density of states $D(\epsilon)$:

$$< N >=< N_0 > + \int_0^\infty D(\epsilon) < n_B > (\epsilon) \mathrm{d}\epsilon \tag{2.13}$$

With this, an integral representation of the generalized Riemann-Zeta function can be found.

2.2 Phase Transition

Assuming a large particle number N, the averages can be taken as direct particle numbers ($< N > \to N, < N_T > \to N_T$). The number of particles in the ground state is determined by

$$N_0 = N - N_T \tag{2.14}$$

Due to a total number of particles N, N_T can never exceed N. Therefore μ needs to decrease at high temperatures. However, at small temperatures $g_3(z)$ needs to rise to fulfill particle conservation. Since μ is limited by the Bose-Einstein distribution, only a maximal fugacity of $z = 1$ is possible. At this point the number of particles in excited states N_T now only depends on the temperature and therefore decreases. To conserve particle number N, the remaining Bosons have to occupy the ground state. For temperatures close to zero N_0 has a macroscopic occupation, whereas N_T gets negligibly small. This process is called Bose-Einstein condensation and the resulting system a Bose-Einstein condensate. The critical point $N = N_T$ with maximal chemical potential $\mu = \epsilon_{000}$ therefore gives rise to a phase transition. The corresponding critical temperature T_c can be calculated with (2.12) [7]:

$$k_B T_c = \hbar\bar{\omega}(\frac{N}{\zeta(3)})^{\frac{1}{3}} \approx 0.94\hbar\bar{\omega}N^{\frac{1}{3}} \tag{2.15}$$

($\zeta(3)$ is roughly 1.202)
Expected values of the critical temperature arise in the range of multiple $100nK$, if $\bar{\omega}$ lays in the range between $10^2\frac{1}{s}$ and $10^3\frac{1}{2}$ an rough estimate of $10^4 - 10^8$ particles are used [6].
Multiplying a one into equation (2.9) for the case $T \leq T_c$ yields the temperature dependence of the condensate fraction N_0/N:

$$N = N_0 + N_T = N_0 + (\frac{k_B T_c}{\hbar\bar{\omega}})^3(\frac{T}{T_c})^3\zeta(3) \implies \frac{N_0}{N} = 1 - (\frac{T}{T_c})^3 \tag{2.16}$$

A visualization of equation (2.16) can be found in Figure 2. The exact value of μ can be obtained by the Bose-Einstein distribution:

$$\mu = -(k_B T \ln(1 + \frac{1}{N_0}) + \epsilon_0) \tag{2.17}$$

2.3 Why are Interactions important ?

Interactions often play a crucial role in the treatment of multi-particle systems. In this section the interactions are motivated by looking at the Landau criterion of superfluidity following [4]. If a condensed ideal Bose liquid is moving in a capillary, it needs a minimum velcocity to create excitations. Excitations leads to energy dissipation which can be interpreted as friction.

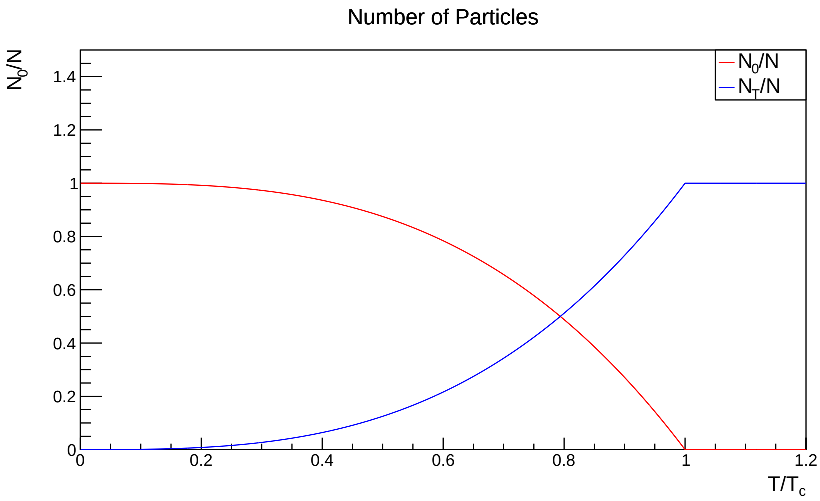

Figure 2: Particles in the groundstate N_0 and particles in thermal states N_T plotted depending on the relative temperature T towards the critical temperature T_c. (own creation)

For velocities lower than the critical velcocity v_c no excitations are created and thus the fluid behaves as a superfluid. The Landau criterion gives the following equation for the critical velocity:

$$v < v_c = \min_p \frac{\epsilon(p)}{p} \tag{2.18}$$

For the ideal Bose gas with $\epsilon(p) = \frac{p^2}{2m}$ the critical velocity is zero and thus no superfluidity is expected, albeit the existence of superfluidity in Helium-4. If now interactions are taken into account, as Bogoliubov did in treating the weakly interacting Bose gas, one obtains the following energy dispersion relation:

$$\epsilon(p) = \sqrt{\underbrace{(\frac{p^2}{2m})^2}_{\text{ideal}} + \underbrace{\frac{gn}{m}p^2}_{\text{interactions}}} \tag{2.19}$$

($g =$ interaction strength, $n =$ particle density)
One can clearly see, that the critical velocity is now given by

$$v_c = \sqrt{\frac{gn}{m}} \tag{2.20}$$

which is non zero. In this system superfluid behaviour can occur.

3 Interacting Bose Gas

In the following the Gross-Pitaevskii equation is derived by looking at a two body potential $V(\boldsymbol{r})$. To simplify things, one looks at a already fully condensed state ($T < T_c$), leading to low momenta in the system. For such a system the scattering length a is nearly constant due to s-wave scattering. An additional prequesite is the dilute gases limit $na \ll 1$, which motivates the usage of an effective potential $U_{eff} = U_0 \delta(\boldsymbol{r} - \boldsymbol{r}')$. U_0 is given by the Born-approximation and is $U_0 = \frac{4\pi\hbar^2 a}{m}$ [6].
The upcoming derivations in this section are based on a mean field theory presented mainly in [4, 5] and [9].

3.1 Bogoliubov Prescription and Mean-Field Approximation

For describing many body systems in quantum mechanics it is easier to use the formalism of second quantization. Therefore one introduces operators $\hat{a}_i$ and $\hat{a}_i{}^\dagger$, which describe the annihilation and creation of a particle in state i. The operators obey the commutation relations

$$[\hat{a}_i, \hat{a}_j{}^\dagger] = \delta_{ij}, \quad [\hat{a}_i, \hat{a}_j] = 0, \quad [\hat{a}_i{}^\dagger, \hat{a}_j{}^\dagger] = 0 \tag{3.1}$$

With these operators one can now define field operators:

Definition: *Field operator for annihilating/creating a particle at position* $\boldsymbol{r}$

$$\hat{\psi}(\boldsymbol{r}) = \sum_i \varphi_i \hat{a}_i, \quad \hat{\psi}^\dagger(\boldsymbol{r}) = \sum_i \varphi_i^* \hat{a}_i{}^\dagger \tag{3.2}$$

(φ_i being single particle wave functions for the state i)

Like the annihilation and creation operators, the field operators underly the same commutation relations. For Bose-Einstein condensation the ground state $i = 0$ plays an important role, which motivates to write it detached in the field operator representation. In the case of an condensate the number of particles in excited states is comparably small, leading to a negligible non-condensate part:

$$\hat{\psi}(\boldsymbol{r}) = \varphi_0(\boldsymbol{r})\hat{a}_0 + \sum_{i \neq 0} \varphi_i(\boldsymbol{r})\hat{a}_i = \psi_0(\boldsymbol{r}) + \delta\hat{\psi}(\boldsymbol{r}) \tag{3.3}$$

In equation (3.3) the macroscopic part of the field operator $\hat{\psi}(\boldsymbol{r})$ is treated as a classical field, which is referred to as the Bogoliubov approximation. This results in the mean field approach of

$$\psi_0(\boldsymbol{r}) = <\hat{\psi}(\boldsymbol{r})> \neq 0 \tag{3.4}$$

Definition: *The complex function $\psi_0(\boldsymbol{r})$ is the macroscopic wave function of the condensate and acts as an order parameter.*
It can be characterized by a magnitude and phase $S(\boldsymbol{r})$:

$$\psi_0(\boldsymbol{r}) = |\psi_0(\boldsymbol{r})| e^{iS(\boldsymbol{r})} \tag{3.5}$$

$S(\boldsymbol{r})$ plays a crucial role in the treatment of superfluids.

3.2 The Gross-Pitaevskii Equation

One starts with the Hamiltonian in field operator representation

$$\begin{aligned} \hat{H} = & \int \hat{\psi}^\dagger(\boldsymbol{r}) (\underbrace{-\frac{\hbar^2}{2m}\nabla^2}_{\text{kinetic energy}} + \underbrace{V_{ext}(\boldsymbol{r})}_{\text{potential energy}}) \hat{\psi}(\boldsymbol{r}) \mathrm{d}\boldsymbol{r} \\ & + \frac{1}{2} \int \hat{\psi}^\dagger(\boldsymbol{r}) \hat{\psi}^{\dagger\prime}(\boldsymbol{r}') \underbrace{V(\boldsymbol{r}' - \boldsymbol{r})}_{\text{interaction potential}} \hat{\psi}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}') \mathrm{d}\boldsymbol{r} \mathrm{d}\boldsymbol{r}' \end{aligned} \tag{3.6}$$

An expression of the field operator $\hat{\psi}(\boldsymbol{r}, t)$ is determined by changing to the Heisenberg description and applying the Heisenberg equation of motion $i\hbar\frac{\partial\hat{\psi}}{\partial t} = [\hat{\psi}, \hat{H}]$:

$$i\hbar\frac{\partial\hat{\psi}}{\partial t} = (-\frac{\hbar^2}{2m}\nabla^2 + V_{ext} + \int \hat{\psi}^{\dagger\prime}(\boldsymbol{r}') V(\boldsymbol{r}' - \boldsymbol{r}) \hat{\psi}\boldsymbol{r}') \mathrm{d}\boldsymbol{r}') \hat{\psi}(\boldsymbol{r}) \tag{3.7}$$

With the effective interaction potential a compact solution of the interaction integral is obtained. In the last step, the time-dependent Gross-Pitaevskii equation results from inserting the mean field approach:

$$\boxed{i\hbar\frac{\partial\psi_0}{\partial t} = (-\frac{\hbar^2\nabla^2}{2m} + V_{ext} + g|\psi_0|^2)\psi_0} \tag{3.8}$$

(with coupling constant $g = U_0 = \frac{4\pi\hbar^2 a}{m}$)
For stationary solutions of ψ_0 where one can apply time evolution (multiply with $e^{i\frac{\mu}{\hbar}t}$, $\mu = \frac{\partial E}{\partial N}$) and in the case of a time independent effective potential one arrives at the time independent Gross-Pitaevskii equation:

$$(-\frac{\hbar^2\nabla^2}{2m} + V_{ext} + g|\psi_0|^2 - \mu)\psi_0 = 0 \tag{3.9}$$

In most cases, the GP equation needs to be solved numerically. To still achieve analytical results one needs to take further approximations. For example the Thomas-Fermi limit in which the kinetic energy is neglected.

3.3 Ground State of Trapped Bose Gas

In this section an application of the GP equation is demonstrated to show exemplary changes when introducing interactions in the trap.
Before the groundstate is investigated another quantity has to be introduced:

Definition: *One-body density matrix*

$$n^{(1)}(\boldsymbol{r}, \boldsymbol{r'}) = <\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r'})> \tag{3.10}$$

With (3.10) one can obtain the density of the system, which gives the total number of particles when being integrated over the total volume:

$$n(\boldsymbol{r}) = <\hat{\psi}\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})>, \qquad N = \int n(\boldsymbol{r})\mathrm{d}\boldsymbol{r} \tag{3.11}$$

Now, one can obtain the following relation for the groundstate:

$$n_0(\boldsymbol{r}) = |\psi_0(\boldsymbol{r})|^2 = N|\varphi_0(\boldsymbol{r})|^2 \tag{3.12}$$

For the case of an ideal gas, one can directly calculate the density with the groundstate wave function of the quantum harmonic oscillator $\varphi_0 = (\frac{m\bar{\omega}}{\pi\hbar})^{\frac{3}{4}} e^{\sum_{k=1}^{3}\omega_k x_k^2}$. If instead interactions are considered, then one solves the GP equation with the Thomas-Fermi approximation, which results in

$$|\psi_0|^2 = \sqrt{n} = \frac{1}{g}(\mu - V_{ext}) \tag{3.13}$$

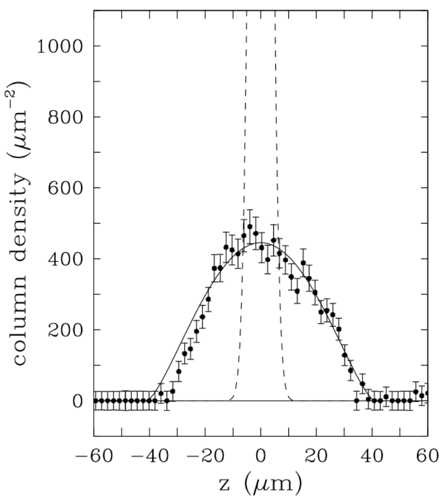

Figure 3: Column density of ideal and interacting Bose gas with data from measurements, taken from [5]

whereas μ is determined by the density normalization condition:

$$\mu = \frac{\hbar\bar{\omega}}{2}(\frac{15Na}{\bar{a}})^{\frac{2}{5}} \tag{3.14}$$

($\bar{a} = \sqrt{\frac{\hbar}{m\bar{\omega}}}$ being the oscillator length). Comparing both cases, one obtains a broader density distribution as expected when repulsive interactions occur. Figure 3 contains a plot comparing ideal and interacting column densities with measured data. Another interesting case is given by looking at attractive interactions $a < 0$. This gives rise to a unstable regime over a critical particle number N_{cr}.

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