

Chapter 1

The non-interacting Bose gas

Learning goals

- What is a Bose-Einstein condensate and why does it form?
- What determines the critical temperature and the condensate fraction?
- What changes for trapped systems?

The ideal, i.e. non-interacting Bose gas is the starting point for our discussions. Its properties are determined by the quantum statistics of the particles. In the grand canonical ensemble, we can write down the Bose distribution function, which leads to a criterion for Bose-Einstein condensation. We define the critical temperature and the condensate fraction for the homogeneous gas before we turn to the experimentally relevant case of a gas trapped in a harmonic potential.

1.1 Introduction

1.1.1 Quantum statistics

Quantum statistics tells us how to distribute particles on possible quantum states. It is essentially determined by the symmetry of the wave function upon a permutation of the particles. As the most simple example, we consider two particles which can be distributed in two boxes (quantum states), see Fig. 1.1. If the particles are distinguishable, in total four different possibilities exist. The probability to find two particles in the same state is then $1/2$. This changes if we consider two indistinguishable bosons. Now, only three different combinations are possible, and the situation that two bosons occupy the same quantum state is enhanced to $2/3$ - bosons tend to stick together! This is in contrast to fermions, where the Pauli exclusion principle prohibits the possibility of two particles being in the same state and only one possibility to arrange the particles exists.

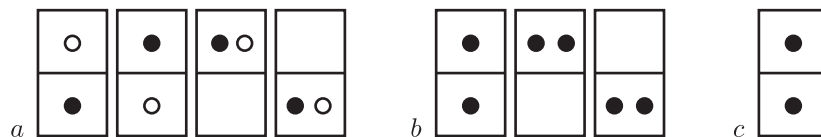


Figure 1.1: **Different possibilities to distribute two particles on two boxes.** (a) distinguishable particles have a probability of $1/2$ to find two particles in one box, (b) bosons have a probability of $2/3$ to find two particles in one box, (c) for fermions the Pauli principle excludes this possibility.

1.1.2 Grand canonical ensemble

Moving to a large system containing many particles and with many possible states, an ensemble description is needed to find the probabilities to populate certain states. The grand canonical ensemble is especially suited to derive the probability distribution of microscopic states. It holds for a system that is in contact with a large reservoir, such that it can exchange energy and particles with the reservoir. The constants in this ensemble are the chemical potential μ and the temperature T .

Applying the concept of the grand canonical ensemble to trapped gases is valid under the assumption of the local density approximation: as long as the correlation length of the gas is much shorter than the density variations, the gas may be thought as divided into small subsystems in which the thermodynamics of a homogenous gas can be applied, such that the following discussion is also true for trapped samples.

From the partition function of the grand canonical ensemble, the distribution function $f(\epsilon_\nu)$ for the average occupation of a single-particle state ν with energy ϵ_ν can be derived,

$$f(\epsilon_\nu) = \langle n_\nu \rangle = \frac{1}{e^{\frac{\epsilon_\nu - \mu}{k_B T}} \pm 1}. \quad (1.1)$$

The chemical potential μ corresponds to the energy required to add one particle to the thermally isolated system, $\mu = \left(\frac{\partial E}{\partial N}\right)_{S,V}$. It is determined by the total number of particles N and the temperature T of the gas. The sign in the nominator of the distribution function depends on the statistics of the particles. For bosons it is negative and for fermions it is positive, which results in the Bose- or Fermi-distribution, respectively. For high temperatures, the effect of the quantum statistics becomes negligible, and the distribution function can be approximated as

$$f(\epsilon_\nu) = \langle n_\nu \rangle = e^{-\frac{\epsilon_\nu - \mu}{k_B T}}, \quad (1.2)$$

which is the Boltzmann distribution known for classical particles.

Knowledge about the distribution function allows to derive basic quantities like the mean energy

$$E = \sum_{\nu} \epsilon_{\nu} f(\epsilon_{\nu}), \quad (1.3)$$

and the mean particle number

$$N = \sum_{\nu} f(\epsilon_{\nu}). \quad (1.4)$$

To move on in our discussion from this point on, it is very useful to replace the sum over the discrete energy levels in the above expression by an integral:

$$\bar{N} = \sum_{\nu} f(\epsilon_{\nu}) \approx \int_0^{\infty} d\epsilon f(\epsilon) g(\epsilon). \quad (1.5)$$

Here $g(\epsilon)$ is the density of states. While $f(\epsilon)$ describes the probability to populate a certain state, the density of states describes the states which are actually available in the system under consideration. The integral over the product of the two hence gives the total number of particles (see also Figure 1.2). Replacing the sum by an integral is usually a good choice if the density of states is high. However, for a vanishing density of states this might cause problems.

1.1.3 Density of states in three dimensions

Phase space in quantum mechanics can be quantized due to Heisenberg's uncertainty relation. Accordingly, there is one quantum state per phase space cell of volume $(2\pi\hbar)^3$. Describing the real space volume of a phase space region with $V = \Delta x \Delta y \Delta z$ and the volume in momentum

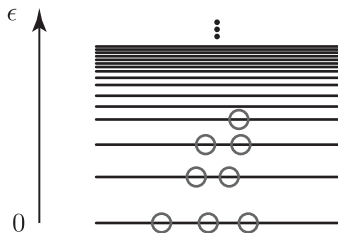


Figure 1.2: **Visualization of the density of states.** Starting at zero energy, the density of states $g(\epsilon)$ describes the number of available states in a system in a certain energy interval ϵ to $\epsilon + d\epsilon$. The distribution function $f(\epsilon)$ then describes the mean occupation of a certain level with energy ϵ .

space which contains states with momenta smaller than p with $\frac{4}{3}\pi p^3$, one can write the total number of states with energy less than $\epsilon = \frac{p^2}{2m}$ as

$$G(\epsilon) = \frac{V \frac{4}{3}\pi p^3}{(2\pi\hbar)^3} = V \frac{\sqrt{2}}{3\pi^2\hbar^3} (m\epsilon)^{3/2}. \quad (1.6)$$

The density of states $g(\epsilon)$ for a homogeneous system in three dimensions can thus be found to be

$$g(\epsilon) = \frac{dG(\epsilon)}{d\epsilon} = V \frac{\sqrt{2}}{3\pi^2\hbar^3} (m)^{3/2} \sqrt{\epsilon}. \quad (1.7)$$

In most cases, the density of states can be written as a power of the energy

$$g(\epsilon) = C_\alpha \epsilon^{\alpha-1}, \quad (1.8)$$

where C_α is a constant. For the homogeneous case in d dimensions, $\alpha = d/2$, while for the harmonic oscillator in d dimensions $\alpha = d$. Note that the density of states for the homogenous two-dimensional system becomes independent of the energy; Bose condensation in a 2 dimensional box can thus only occur at zero temperature. For the most important case of a three dimensional harmonic trapping potential, the density of states is given by

$$g(\epsilon) = C_3 \epsilon^{3-1} = \frac{1}{2\hbar^3 \omega_x \omega_y \omega_z} \epsilon^2. \quad (1.9)$$

1.2 Bose Einstein Condensation

We will now investigate the behavior of the expression

$$N = \int_0^\infty d\epsilon f(\epsilon) g(\epsilon), \quad (1.10)$$

assuming that we keep the temperature T fixed but add more and more particles to the system. The density $n = N/V$ thus will rise and we write

$$n = \frac{N}{V} = A \int_0^\infty d\epsilon \frac{\epsilon^{1/2}}{e^{\frac{\epsilon-\mu}{k_B T}}}, \quad (1.11)$$

with the prefactor $A = m^{3/2}/(\sqrt{2}\pi^2\hbar^3)$. In order to increase the density, we have to increase the chemical potential. As the chemical potential can only be negative (otherwise unphysical negative occupation numbers would occur in $f(\epsilon)$), the maximum value it can approach is zero

if we set the minimum energy ϵ_{\min} to zero. This implies that also the density of the system seems to be bound to a maximum value

$$n_c = n(\mu = 0) = A \int_0^\infty d\epsilon \frac{\epsilon^{1/2}}{e^{\frac{\epsilon}{k_B T}}} = A(k_B T)^{3/2} \int_0^\infty dx \frac{x^{1/2}}{e^x - 1}, \quad (1.12)$$

where we made the substitution $x = \epsilon/(k_B T)$. This integral can be evaluated with help of the Gamma function $\Gamma(\alpha)$ and the Riemann zeta function $\zeta(\alpha)$: $\int_0^\infty dx \frac{x^{\alpha-1}}{e^x - 1} = \Gamma(\alpha)\zeta(\alpha)$. Here, $\alpha = 3/2$ and we find

$$n_c = \Gamma(3/2)\zeta(3/2)A \approx 2.3A. \quad (1.13)$$

Obviously something is unphysical here, as the density of the system is bound although we increase the particle number. So what happens to the particles we add?

The error we made happened when we replaced the sum by an integral, which is not valid if the density of states becomes small – which it actually does for a homogeneous three-dimensional system. To fix this mistake, we now separate the lowest energy state from all other (excited) states, such that

$$n = n_0 + n_{\text{exc}} = \frac{1}{V} \frac{1}{e^{-\frac{\mu}{k_B T}} - 1} + A \int_0^\infty d\epsilon \frac{\epsilon^{1/2}}{e^{\frac{\epsilon - \mu}{k_B T}}}. \quad (1.14)$$

If we now let μ approach zero, i.e. increase the number of particles in the system, the second term will be limited to n_c , the critical density, while the first term n_0 can grow without any limit as $\frac{1}{e^{-\frac{\mu}{k_B T}} - 1} \rightarrow \infty$. Any additional particle in excess to the critical density will thus be accommodated in the ground state of the system which becomes macroscopically occupied. This phenomenon is called Bose-Einstein condensation.

The existence of a BEC is a spectacular result, as in a normal gas there is no particle at a specific energy, only in a certain energy interval. This is similar to the fact that finding a particle at a specific point in space has zero probability. A point has no volume and will in a continuum of states never be occupied. Here the ground state is a specific point in phase space that is macroscopically occupied!

1.2.1 Phase space density at the phase transition

It is instructive to express the critical density n_c with help of the thermal deBroglie wavelength $\lambda_T = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}$, which can be interpreted as the spatial extend of a particles wave function. We can then write

$$n_c = 2.3A(k_B T)^{3/2} = 2.3 \frac{m^{3/2}}{\sqrt{2\pi^2\hbar^3}} = 2.3 \frac{2}{\sqrt{\pi}} \frac{1}{\lambda_T^3}. \quad (1.15)$$

The critical density at which BEC sets in is thus reached if the interparticle distance is on the order of the thermal de Broglie wavelength. At this density the wave packets of the individual particles start to overlap and the influence of quantum statistics forces the system to Bose condense.

1.2.2 Transition temperature and condensate fraction

We now want to derive expressions for the critical temperature T_c at which the ground state of the system becomes macroscopically occupied, and for the according fraction of condensed atoms $n_0 = N_0/N$ if the temperature is below the critical temperature. To simplify, we keep $\epsilon_{\min} = 0$. The critical temperature can be found if we evaluate the system at the critical point, where we know that all particles are still occupying the excited states:

$$n = \frac{N}{V} = \frac{N_{\text{exc}}}{V} = A\Gamma(3/2)\zeta(3/2)(k_B T_c)^{3/2}, \quad (1.16)$$

such that we find

$$k_B T_c \approx 3.31 \frac{\hbar^2 n^{2/3}}{m}. \quad (1.17)$$

The condensate fraction n_0 can then be found from

$$n = n_0(T) + n_{\text{exc}}(T) = n_0(T) + A\Gamma(3/2)\zeta(3/2)(k_B T)^{3/2}. \quad (1.18)$$

where again, if a BEC is present in the system, the second term will be stuck at the critical density n_c . The prefactors of the second term can now be replaced with help of equation 1.16, and we find

$$n = n_0(T) + n \left(\frac{T}{T_c} \right)^{3/2}, \quad (1.19)$$

such that we get for the condensate fraction

$$n_0 = \frac{N_0}{N} = 1 - \left(\frac{T}{T_c} \right)^{3/2}. \quad (1.20)$$

1.3 Trapped atomic gases

1.3.1 Density- and momentum distributions

We now turn to the experimentally important topic of harmonically trapped atomic gases. Typically a gas of 10^4 to 10^7 atoms is prepared in such traps, and one is interested at the very basic level to understand the density and momentum distribution of the gas. While the density distribution in the trap can be measured by an *in-situ* absorption imaging, the momentum distribution is typically measured by time of flight imaging, where an absorption image is taken after abruptly switching off the trapping potential and allowing the atomic cloud to expand for a certain time.

We consider a harmonic trap which is described by the according trapping frequencies $\omega_x, \omega_y, \omega_z$:

$$V(\mathbf{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \quad (1.21)$$

If all atoms of a non-interacting gas occupy the ground state of the trapping potential (i.e. we consider a pure BEC), the density distribution $n(\mathbf{r})$ is determined by the single particle ground state wave function $\phi_0(\mathbf{r})$ of a particle in the trap:

$$n(\mathbf{r}) = N|\phi_0(\mathbf{r})|^2. \quad (1.22)$$

$\phi_0(\mathbf{r})$ for the anisotropic harmonic oscillator potential $V(\mathbf{r})$ is given by

$$\phi_0(\mathbf{r}) = \frac{1}{\pi^{3/4}(a_x a_y a_z)^{1/2}} e^{-\frac{x^2}{2a_x^2}} e^{-\frac{y^2}{2a_y^2}} e^{-\frac{z^2}{2a_z^2}}, \quad (1.23)$$

where $a_i = \sqrt{\frac{\hbar}{m\omega_i}}$ is the harmonic oscillator length for the trapping frequency ω_i .

We find the density distribution in momentum space $n(\mathbf{p}) = N|\phi_0(\mathbf{p})|^2$ by taking the Fourier transform of $\phi_0(\mathbf{r})$ which yields $\phi_0(\mathbf{p})$:

$$\phi_0(\mathbf{p}) = \frac{1}{\pi^{3/4}(c_x c_y c_z)^{1/2}} e^{-\frac{p_x^2}{2c_x^2}} e^{-\frac{p_y^2}{2c_y^2}} e^{-\frac{p_z^2}{2c_z^2}}, \quad (1.24)$$

with $c_i = \hbar/a_i = \sqrt{m\hbar\omega_i}$. We see that the momentum distribution for a BEC in an anisotropic trap is also anisotropic. The gas will thus expand anisotropically after switching off the trapping potential which is an important experimental signature for a BEC.

In contrast, for a thermal gas with temperature $T \gg T_c$ the density distribution is given by

$$n_{\text{th}}(\mathbf{r}) = \frac{N}{\pi^{3/2} R_x R_y R_z} e^{-\frac{x^2}{2R_x^2}} e^{-\frac{y^2}{2R_y^2}} e^{-\frac{z^2}{2R_z^2}}, \quad (1.25)$$

with the temperature dependent widths $R_i = \sqrt{\frac{2k_B T}{m\omega_i^2}}$.

The momentum distribution for a thermal gas is

$$n_{\text{th}}(\mathbf{p}) \propto e^{-\frac{p^2}{2mk_B T}}, \quad (1.26)$$

which is an isotropic distribution. A thermal cloud released from a harmonic trap will thus after sufficiently long expansion look spherically symmetric, very different from the image of a BEC after time of flight.

1.3.2 Semi-classical approximation

While we now found an expression for the density distribution of a bosonic gas at high temperatures, it is of interest to see how this distribution develops if the critical point is approached. If we compare the typical sizes of a thermal cloud with the extent of a BEC in the same trap, we find that the thermal cloud will be much larger than the BEC: $R_i/a_i = (2k_B T/\hbar\omega_i)^{1/2} \gg 1$. The energy scale set by the temperature of the gas is thus much larger than the level spacing of the trapping potential, and a semi-classical description of the system is valid. We can thus write down for a trapped gas the distribution function in phase space as

$$f(\mathbf{r}, \mathbf{p}) = \frac{1}{e^{(\epsilon(\mathbf{r}, \mathbf{p}) - \mu)/k_B T} \pm 1}, \quad (1.27)$$

with $\epsilon(\mathbf{r}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})$. Again, the different signs correspond to fermions and bosons, respectively. $f(\mathbf{r}, \mathbf{p})$ thus describes the occupation of a phase space cell. Integration over either momentum or real space then gives the according distribution in density or momentum. E.g.

$$n_{\text{exc}}(\mathbf{r}) = \int \frac{d^3 \mathbf{p}}{(2\pi\hbar)^3} f(\mathbf{r}, \mathbf{p}) = \pm \frac{1}{\lambda_T^3} g_{3/2} \left(\pm e^{(\mu - V(\mathbf{r}))/k_B T} \right). \quad (1.28)$$

The function $g_\gamma(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\gamma}$ is the Polylogarithm, a function which frequently appears when carrying out these types of integrals. In Fig. 1.3 we show $n_{\text{exc}}(r)$ for a gas at condensation. While for high temperatures only the first, Gaussian term in the sum of the Polylogarithm contributes, the density distribution becomes increasingly peak when the critical point is approached.

The critical temperature and the condensate fraction for a trapped system can be found with similar arguments as used in section 1.2.2. The number of thermal atoms occupying the excited states of the trap is given by

$$N_{\text{exc}} = \int d^3 \mathbf{r} n_{\text{exc}}(\mathbf{r}) = \left(\frac{k_B T}{\hbar\bar{\omega}} \right)^3 g_3(e^{\mu/k_B T}). \quad (1.29)$$

Setting now $T = T_c$ and $\mu \approx 0$ we find

$$k_B T_c = \hbar\bar{\omega} \left(\frac{N}{g_3(1)} \right)^{1/3} \approx 0.94 \hbar\bar{\omega} N^{1/3}, \quad (1.30)$$

where $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$ is the mean trapping frequency of the potential.

Using the number of thermal atoms $N_{\text{exc}}(T) = \left(\frac{k_B T}{\hbar\bar{\omega}} \right)^3 g_3(e^{\mu/k_B T})$ and the total number of atoms $N = N_{\text{exc}}(T_c) = \left(\frac{k_B T_c}{\hbar\bar{\omega}} \right)^3 g_3(e^{\mu/k_B T})$, we can find the condensate fraction

$$\frac{N_0}{N} = \frac{N - N_{\text{exc}}}{N} = 1 - \left(\frac{T}{T_c} \right)^3. \quad (1.31)$$

Note that we derived this expression already earlier in section 1.2.2. The condensate fraction as a function of temperature is plotted in Fig. 1.4.

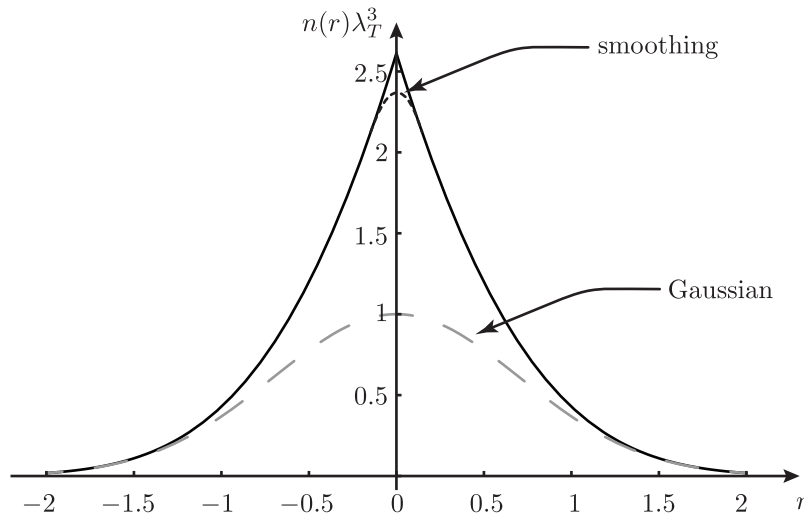


Figure 1.3: **Density distribution of trapped thermal atoms.** The gray dashed line shows the Gaussian distribution expected for a trapped thermal gas in a isotropic harmonic trap well above the critical temperature. The density distribution becomes increasingly peaked once T approaches T_c . The solid black line shows $n_{\text{exc}}(r)$ for a gas at the critical temperature ($\mu = 0$). In reality, the sharp central peaked will be smoothed on the length scale given by the thermal de Broglie length.

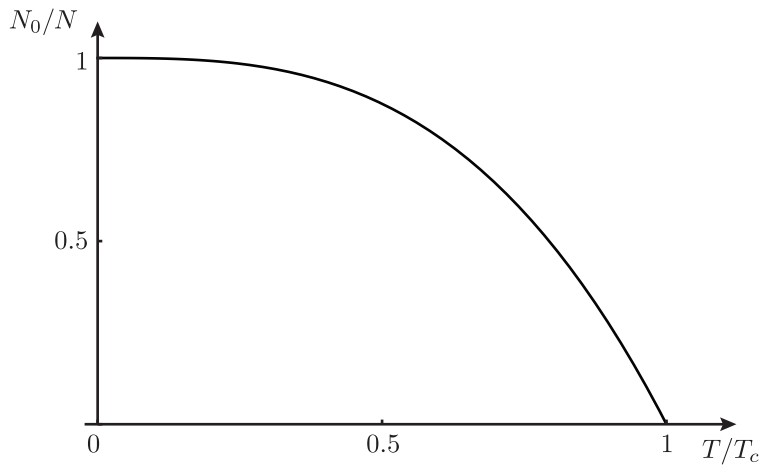


Figure 1.4: **Condensate fraction as function of temperature.** The condensate fraction for a trapped gas increases rapidly with decreasing temperature. E.g. at $T/T_c = 0.5$, the condensate fraction is already almost 90%.