Bose-Einstein condensation into non-equilibrium states

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Chapter 2

Theoretical background

In this chapter we compile main theoretical expressions relevant to the Bose-Einstein condensation. We also sketch some theoretical ideas underlying phase coherence and formation of a BEC. Further, we introduce the bare fundamentals of evaporative cooling and derive several results specific to the experiments described further in this work. A separate section is dedicated to the scaling description of the gas clouds in harmonic traps. For a complete review on the theory of Bose-Einstein condensation in trapped gases one can, for example, refer to [27].

2.1 Rubidium

The diagram of energy levels of $^{87}\text{Rb}$ isotope is shown in Figure 2.1. Cooling and trapping is performed with laser light red-detuned with respect to the $|5S_{1/2}, F = 2 \rightarrow |5P_{3/2}, F = 3\rangle$ transition of the D2 line. This light also induces non-resonant pumping of the atoms to the $|5P_{3/2}, F = 2\rangle$ state, from where they decay according to the transitions' strengths to $F = 1$ and $F = 2$ hyperfine states. To prevent atoms from accumulating in the $F = 1$ state, another laser – the repumper – tuned to a $|5S_{1/2}, F = 1 \rightarrow |5P_{3/2}, F = 2\rangle$ transition is used. Another laser is employed for optical pumping of the atoms into a $|5S_{1/2}, F = 2, m_F = 2\rangle$ Zeeman state.

2.2 Magnetic trapping

Trapping of neutral atoms in magnetic fields arises from Zeeman interaction of the magnetic moment $\mu$ of the atom with the external field $\mathbf{B}$. The energy of the interaction is given by

$$E = -\mu \cdot \mathbf{B}(\mathbf{r}), \quad (2.1)$$

where $\mu = m_F g_F \mu_B$, $\mu_B$ is the Bohr magneton. The Zeeman energy of the different magnetic sublevels can be expressed by the Breit-Rabi formula in the approximation of the Zeeman splitting $g_s \mu_B B$ being much smaller than the hyperfine splitting $\hbar \omega_{hf}$

$$E_{F,m_F} = (-1)^F \left( \frac{1}{2} \hbar \omega_{hf} + m_F g_F \mu_B B + \frac{1}{16} \left( 4 - m_F^2 \right) \frac{(g_s \mu_B B)^2}{\hbar \omega_{hf}} \right) + \text{const.} \quad (2.2)$$
Figure 2.1. Energy level scheme of $^{87}$Rb. The data was taken from refs. [7] and [84].

\[ g_F = (-1)^F \frac{1}{2I+1} g_x. \]  

(2.3)

Different Zeeman states can be divided into “low-field seekers” and “high-field seekers”. Since the Maxwell equations do not allow for the existence of a local magnetic field maximum, only the atoms in the low-field seeking states can be trapped. For rubidium these are the $|F = 1, m_F = -1\rangle$, $|F = 2, m_F = 1\rangle$ and $|F = 2, m_F = 2\rangle$ states. All experiments described in this thesis were done with the $|F = 2, m_F = 2\rangle$ state.

The magnetic field minimum is created by the current coils of the Ioffe trap schematically shown in Figure 2.2. Four parallel current bars created by four elongated “racetrack” coils produce a quadrupole magnetic field in the x-y plane. Small circular dipole coils in the centre (“pinch” coils) create the confining potential along the z-axis. Large outer compensation coils are used for reduction of the large offset field created by the pinch coils. This setup allows to avoid regions where the magnetic field crosses zero value. If an atom were to cross such a point it would experience a spin flip and would be lost from the trapping field. Such spin flips are referred to as Majorana losses.
2.2 Magnetic trapping

![Diagram of magnetic trap](image)

**Figure 2.2.** Coils of the magnetic trap in an Ioffe-quadrupole configuration. Arrows indicate the directions of the currents.

The magnetic field of the Ioffe trap can be written down in the following form \([10, 73]\)

\[
\begin{align*}
B_\rho (\rho, \phi, z) &= -\alpha \rho \sin(2\phi) - \frac{1}{2} \beta \rho (z - z_0) \\
B_\phi (\rho, \phi, z) &= -\alpha \rho \cos(2\phi) \\
B_z (\rho, \phi, z) &= B_0 + \frac{1}{2} \beta (z - z_0)^2 - \frac{1}{4} \beta \rho^2.
\end{align*}
\]  

\[(2.4)\]

Here \(\alpha\) is the radial field gradient of the quadrupole field and \(\beta = \partial^2 B_z(0,0,z)/\partial z^2\) at \(z = z_0\) – the curvature of the field. Close to the centre of the trap the field can be approximated by the harmonic potential

\[
B(\rho, z) = B_0 + \frac{1}{2} \left( \frac{\alpha^2}{B_0} - \frac{\beta}{2} \right) \rho^2 + \frac{1}{2} \beta z^2.
\]  

\[(2.5)\]

One can further write down the frequencies of the harmonic potential

\[
\omega_z = \left[ \frac{\mu_B g_e m_F}{m} \beta \right]^{1/2}
\]  

\[(2.6)\]
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\[ \omega_p = \left[ \frac{\mu_B g_F m_F}{m} \left( \frac{\alpha^2}{B_0} - \frac{\beta}{2} \right) \right]^{1/2}. \]  \hspace{1cm} (2.7)

Note that for strong confinement in the radial direction the term \( \alpha^2/B_0 \) is dominant and the radial frequency can thus be adjusted by changing the value of the offset field \( B_0 \).

### 2.3 Bose-Einstein condensation

In this section we summarize the main theoretical results required for the description of trapped Bose gases. Among these are the expressions for the critical temperature \( T_C \) and the density distribution above and below the phase transitions. Detailed description and reviews can be found in refs. [8, 27, 53, 105].

The energy spectrum of an individual atom in a harmonic potential \( U(r) \) is characterized by a set of three non-negative integer quantum numbers \( \{n\} = \{n_x, n_y, n_z\} \) and is given by

\[ \varepsilon_{\{n\}} = \sum_{i=x,y,z} \hbar \omega_i \left( n_i + \frac{1}{2} \right), \]  \hspace{1cm} (2.8)

where \( \omega_i \) are the trap frequencies. The average number of particles in the state \( \{n\} \) is given by the Bose distribution:

\[ N_B = \left[ \exp \left( \frac{\varepsilon_{\{n\}} - \mu}{k_B T} \right) - 1 \right]^{-1}. \]  \hspace{1cm} (2.9)

The value of the chemical potential is fixed by the condition

\[ \sum_{\lambda} N_B (\varepsilon_{\lambda}) = N, \]  \hspace{1cm} (2.10)

where \( N \) is the total number of particles. For this system the density distribution \( n(r) \) above the phase transition can be calculated as

\[ n(r) = \frac{1}{\Lambda_T^3} g_{3/2} \left( \bar{\varepsilon} \exp \left[ \frac{U(r)}{k_B T} \right] \right), \]  \hspace{1cm} (2.11)

with fugacity \( \bar{\varepsilon} = \exp \left( \frac{\mu}{k_B T} \right) \), where \( g_{3/2}(x) \) is a polylogarithm function

\[ g_{3/2}(x) = \sum_{l=1}^{\infty} \frac{x^l}{l^3}. \]  \hspace{1cm} (2.12)
2.3 Bose-Einstein condensation

(Note that \( g_n(1) = \zeta(n) \), where \( \zeta(n) \) is Riemann zeta-function.) The thermal de Broglie wavelength is defined as

\[
\Lambda_T = \left[ \frac{2\pi \hbar^2}{mk_B T} \right]^{1/2} .
\]  
(2.13)

Independently of trap geometry, BEC occurs if the so-called degeneracy parameter reaches the critical value:

\[
n(0) \Lambda_T^3 = g_{3/2}(1) \approx 2.61 ,
\]  
(2.14)

where \( n(0) \) is the peak density in the centre of the trap. In the case of harmonic potential one can obtain an expression for the critical temperature:

\[
T_C = \frac{\hbar \bar{\omega}}{k_B} \left( \frac{N}{g_3(1)} \right)^{1/3} ,
\]  
(2.15)

where \( \bar{\omega} = [\omega_x^2 \omega_z^2]^{1/3} \) is the mean trap frequency.

For a trapped Bose gas in the classical regime, where the chemical potential \( \mu < 0 \) and \( |\mu| \gg k_B T \) one can find that the density distribution has a Gaussian shape

\[
n(\mathbf{r}) = \frac{N}{\pi^{3/2} \prod_i r_{i,0}} \exp \left[ -\sum_i \left( \frac{r_i}{r_{i,0}} \right)^2 \right] ,
\]  
(2.16)

where \( r_{i,0} \) is the \( 1/e \) radius of the cloud in the \( i \)-direction:

\[
r_{i,0} = \left( \frac{2k_B T}{m\omega_i^2} \right)^{1/2} .
\]  
(2.17)

Appearance of the condensate in a trapped weakly interacting gas is characterised by the macroscopic wavefunction, which is determined by the Gross-Pitaevskii (GP) equation \([45, 54]\)

\[
\left( -\frac{\hbar^2 \Delta}{2m} + U(\mathbf{r}) + \tilde{U}|\Psi_0(\mathbf{r})|^2 \right) \Psi_0(\mathbf{r}) = \mu \Psi_0(\mathbf{r}) ,
\]  
(2.18)

where \( \tilde{U} = 4\pi \hbar^2 a/m \) is the coupling constant, \( a \) is s-wave scattering length (\( a = 5.238(1) \) nm \([103]\)), and the chemical potential \( \mu \) is determined by the normalisation condition

\[
N_0 = \int d^3 r |\Psi_0|^2 .
\]  
(2.19)
The density profile of the condensate is given by $n_0(r) = |\Psi_0|^2$. When the maximum level spacing is much smaller than the chemical potential the interactions smear out the discrete structure of the trap levels. In this case the mean field term $\bar{U}n_0$ becomes dominant compared to the kinetic term, which can be neglected in what is referred to as the Thomas-Fermi approximation. In the case of a harmonic trap the density profile of the condensate assumes a parabolic shape

$$n_0(r) = \max \left\{ \frac{1}{g} \left[ \mu - U(r) \right], 0 \right\},$$  

(2.20)

and the Thomas-Fermi radius of the condensate $L_f$ is given by

$$L_{f0} = \frac{1}{\omega} \sqrt{\frac{2\mu}{m}}.$$  

(2.21)

The total number of particles in the condensate can be calculated to be

$$N_0 = \int d^3 r n_0(r) = \left( \frac{2\mu}{\hbar\omega} \right)^{5/2} \frac{r_h}{15a},$$  

(2.22)

where $r_h = [\hbar/ma]^{1/2}$ is the harmonic oscillator length.

### 2.4 BEC formation and phase coherence

Phase coherence properties of a BEC are closely related to the formation process of a quantum degenerate state. Studies of novel Bose-condensed gases, such as phase-fluctuating condensates, can provide new fundamental insights into the nature of macroscopic quantum states and are important for applications in atom optics. So far, phase coherence has been studied for equilibrium trapped Bose-condensed gases [6, 15, 31, 48, 82, 95], and these studies were decoupled from the experiments on the kinetics of growth of BECs [65, 78]. Evolution of the phase coherence properties during formation of a condensate is a matter of particular interest.

It is important to identify regimes of the formation kinetics of a trapped condensate. One expects the existence of two regimes, depending on the trap geometry and the mean-field interatomic interaction near the BEC transition temperature $T_C$. In the first regime, the interatomic interaction is much smaller than the spacing between the lowest trap levels. Then, by doing evaporative cooling and crossing $T_C$ from above one has straightforward formation of a true condensate in the trap ground state, which then grows and acquires the Thomas-Fermi density profile. This regime requires a comparatively small number of particles as in the work at MIT on the growth of a condensate in real time [78] and related
2.4 BEC formation and phase coherence

Figure 2.3. Schematic time diagram of BEC formation in a simplified RF-truncation experiment.

Theoretical work [38]. In our experiments we expect the second regime, where already above \( T_C \) the discrete structure of the lowest trap levels is smeared out by the interatomic interaction, and, similarly to the spatially homogeneous case [57, 58, 61, 62], one expects the formation of a condensate with fluctuating phase (quasicondensate). The quasicondensate will have the same density profile and local correlation properties as a true condensate but will have drastically different phase coherence properties. This regime requires either a very large number of particles or a strongly elongated trapping geometry. In the latter case, already for a moderate particle number (\( \sim 10^5 \) or \( 10^6 \)) the interparticle interaction at \( T_C \) exceeds the spacing between the axial trap levels. Then the axial fluctuations of the phase of the appearing Bose-condensed state acquire a 1D character and can be large, similar to the case of equilibrium 3D elongated quasicondensates discussed in ref. [82]. This regime is likely to be realized in the Munich experiment [65] on the formation and growth of a condensate in an elongated trap as well as in the experiments described in this thesis.

A schematic time diagram of the condensate formation based on ref. [57] is presented in Figure 2.3. Here the process of formation is triggered by an abrupt truncation of the evaporation barrier performed with a system just above the critical temperature. The first kinetic stage, where no condensate is yet present, is described by the Boltzmann kinetic equation and is characterised by the time

\[
\tau_{\text{kin},1} = \frac{1}{n \sigma v_T},
\]  

(2.23)

where \( n \) is the total density of the gas, \( \sigma \) is the scattering cross-section and \( v_T \) is the thermal velocity. The next, coherent stage, is much shorter than the kinetic stage and has a characteristic time.
Theoretical background

\[ \tau_c = \frac{m}{4\pi\hbar n_0 a}, \quad (2.24) \]

where \( a \) is the scattering length, and \( n_0 \) is the density of the condensate. In this evolution stage the non-equilibrium density fluctuations die out. Finally, the second kinetic stage is also characterised by an expression identical to (2.23), with the density \( n \) replaced by the condensate density \( n_0 \). During this stage the number of particles in the condensate grows to its equilibrium value. Further damping of phase fluctuations leads to formation of an equilibrium BEC.

2.5 Evaporative cooling

2.5.1 Evaporative cooling

Evaporative cooling plays a key role in the path towards BEC and has been used in all BEC experiments up to date. The basic principles of evaporative cooling are presented to the extent required for understanding of the experiments described in Chapter 5 and Chapter 6. For an extensive review on evaporative cooling one can refer to [105] and [63].

The description of evaporative cooling presented here is based on the model introduced in [74] and [105]. Evaporative cooling is a powerful cooling method based on the preferential removal of atoms with energy higher than average energy per atom. Subsequent thermalization by elastic collisions leads to an energy distribution with a lower temperature than the one before removal of the atoms.

For constant truncation barrier \( \varepsilon_i \) ("plain evaporation") evaporation rate per atom can be written as

\[ \tau_{ev}^{-1} = \frac{\dot{N}_{ev}}{N} = n(0)\nu_r \sigma \frac{V_{ev}}{V_e} e^{-\eta}, \quad (2.25) \]

where \( \sigma = 8\pi a^2 \) is the elastic collisional cross section,

\[ \eta = \frac{\varepsilon_i}{k_B T}, \quad (2.26) \]

is the truncation parameter, and \( V_{ev} \approx V_e \) is the effective evaporation volume [105]. If the truncation barrier is constantly reduced one enters regime of forced evaporative cooling. If truncation parameter \( \eta \) is kept constant it can be shown that the temperature behaves as

\[ T \propto N^\gamma, \quad (2.27) \]
2.5 Evaporative cooling

where efficiency parameter $\alpha$ depends only on $\eta$. In the course of evaporative cooling it is possible to enter the so-called "runaway" regime, when, despite the particle loss, the density of atoms increases. In the runaway regime the increase in density is sufficiently strong to compensate the dropping temperature and the elastic collision rate increases leading to ever faster evaporation. The efficiency of the evaporative cooling is limited by the loss mechanisms from the trap such as collisions with background gas or collisions with the products of three-body recombination. The figure of merit in this case is the ratio of "good" to "bad" collisions:

$$ R = \frac{\dot{N}_{ev}}{\dot{N}_{i-body}} = \frac{1}{\lambda_i} \frac{V_{ev}}{V_e} e^{-\eta}, $$  

(2.28)

where $\lambda_i = \tau_i^{-1}/\tau_{col}^{-1}$, with $\tau_i^{-1}$ being the $i$-body atomic loss rate and $\tau_{col}^{-1} = n(0)\nu_T\sigma$ – the elastic collision rate.

2.5.2 Local critical temperature in a cylindrical geometry

Unlike a familiar result for the critical temperature in quasi-static systems (Section 2.3), experiments on non-equilibrium formation of a Bose-Einstein condensate described further in this thesis require understanding of a local critical temperature related to the local density of the sample. This concept becomes important if collisions occur on a length scale much shorter than the (axial) size of the cloud. We start calculation of local $T_C$ with writing down an expression for the density of states in a truncated harmonic trap [105]:

$$ \rho(\epsilon) = \frac{2\pi(2m)^{3/2}}{(2\pi\hbar)^3} \int_{r(\epsilon) \leq r_0} dr \sqrt{\epsilon - U(r)}. $$

(2.29)

Here $U(r) = m\omega^2 r^2/2$, and $\epsilon$ is the truncation energy. By integrating out the radial dimensions, we get for an infinitely long cylinder:

$$ \rho_{1D}(\epsilon) = \frac{2\pi(2m)^{3/2}}{(2\pi\hbar)^3} r_0 \int_0^{r_0} 2\pi r dr \sqrt{\epsilon - m\omega^2 r^2/2} = \frac{(2m)^{3/2}}{3\pi\hbar^3 m\omega^2_\rho} \epsilon^{3/2}, $$

(2.30)

where $r_0 = 2\epsilon/m\omega^2_\rho$.

Further, we can write down the total one-dimensional density of an ideal Bose gas [105] (see also Section 6.4.1), and substitute in Equation (2.30)

$$ n_{1D} = \int_0^{\infty} d\epsilon \rho_{1D}(\epsilon) \frac{1}{\exp(\epsilon/k_BT_C)-1} = \left(\frac{m}{2\pi}\right)^{1/2} \frac{(k_BT_C)^{5/2}}{\hbar^3 \omega^2_\rho} g_{5/2}(1), $$

(2.31)

where $g_{5/2}(1)$ is a polylogarithm function.
Finally, the local critical temperature is

\[ T_C(z) \approx \frac{1.28 \hbar \omega_p}{k_B} \left[ n_{1D}(z) r_p \right]^{2/5}, \quad (2.32) \]

where \( r_p = [\hbar/m\omega_p]^{1/2} \) is the radial oscillator length.

### 2.5.3 Development of temperature gradients

Investigation of a temperature profile induced in an elongated cloud by an abrupt lowering of the RF barrier (what we further refer to as RF truncation) is of particular interest with regard to the experiments described in Chapter 6.

To the zero approximation a gas above \( T_C \) can be described by a simple model of a Boltzmann gas. To calculate the temperature profile in the thermal gas after truncation we write down the ratio of one-dimensional truncated density distribution \( n'_{1D} \) to the initial, non-truncated density distribution \( n_{1D} \):

\[
\frac{n'_{1D}}{n_{1D}} = \frac{\int_0^{\infty} d\varepsilon \rho_{1D}(\varepsilon) \exp\left(-\varepsilon/k_B T_0\right)}{\int_0^{\infty} d\varepsilon \rho_{1D}(\varepsilon) \exp\left(-\varepsilon/k_B T_0\right)}, \quad (2.33)
\]

where the density of states \( \rho_{1D} \) is defined by Equation (2.30), and \( \varepsilon(z) = \varepsilon - m\omega^2 z^2/2 \) is the local trap depth. The same ratio can be written down for the total energies excluding the axial component of the potential energy:

\[
\frac{E'}{E} = \frac{\int_0^{\infty} d\varepsilon \varepsilon \rho_{1D}(\varepsilon) \exp\left(-\varepsilon/k_B T_0\right)}{\int_0^{\infty} d\varepsilon \rho_{1D}(\varepsilon) \exp\left(-\varepsilon/k_B T_0\right)}, \quad (2.34)
\]

Combining Equations (2.34), (2.33) and (2.30) we can write down a local temperature of the Boltzmann gas as a function of the axial coordinate:

\[
T_{loc}(z) = \frac{2}{5} \frac{E'}{n'_{1D}} = \frac{2}{5} \frac{E}{n_{1D}} \frac{P(7/2, \eta)}{P(5/2, \infty)} \frac{P(5/2, \eta)}{P(7/2, \infty)} = \frac{P(7/2, \eta)}{P(5/2, \eta)} \frac{P(5/2, \infty)}{P(7/2, \infty)} T_0 \quad (2.35)
\]

where

\[
\eta = \frac{\varepsilon - m\omega^2 z^2/2}{k_B T_0}. \quad (2.36)
\]
Scaling theory of gas evolution

2.6 Scaling theory of gas evolution

2.6.1 Evolution of a condensate

Let us consider a condensate with a fixed number of particles in an anisotropic harmonic potential \( V(r) = m \sum \alpha_i^2 r_i^2 / 2 \) with time-dependent frequencies \( \omega_i(t) \). Neglecting the thermal cloud, the condensate wave function follows a time-dependent Gross-Pitaevskii equation

\[
\frac{i\hbar}{2} \frac{\partial \Psi_0}{\partial t} = \left( -\frac{\hbar^2 \Delta}{2m} + \sum_i \omega_i^2(t) r_i^2 + \bar{U} \right) \Psi_0.
\]  

(2.38)

Here \( \bar{U} = 4\pi \hbar^2 a / m \), with \( a \) being the scattering length and \( m \) the atom mass. To describe the evolution of the Bose gas we follow the method described in ref. [21, 59, 60] and turn in Equation (2.38) to new coordinates \( \rho_i = r_i / b_i(t) \). Here \( b_i = L_i(t) / L_{0i} \) are the scaling parameters, where \( L_{0i} \) is the initial size of the condensate in the trap, as defined by Equation (2.21). We then search for a solution in a density-phase representation. When equation of motion (2.38) in the new coordinates is reduced to a stationary GP equation (2.18), it sets the following condition on the scaling parameters:

\[
\ddot{b}_i + \omega_i^2(t) b_i = \frac{\omega_{0i}^2}{b_i \Pi_i b_i(t)},
\]  

(2.39)

where \( \omega_{0i} = \omega_i(0) \). Considering the case of a cylindrical geometry and an abrupt switch-off of the trap Equations (2.39) can be rewritten in the form

\[
\ddot{b}_\rho = \frac{\omega_{0\rho}^2}{b_{\rho}^2 b_i},
\]  

(2.40)

\[
\ddot{b}_z = \frac{\omega_{0z}^2}{b_{z}^2 b_i^2},
\]  

(2.41)

with initial conditions \( b_i(0) = 1, \dot{b}_i(0) = 0 \).
2.6.2 Evolution of a hydrodynamic thermal cloud

Evolution of the thermal gas in the hydrodynamic regime is in many aspects similar to the evolution of the condensate. The Euler equation of motion for the gas in an anisotropic parabolic potential has the form

$$\frac{\partial \nu_i}{\partial t} + \sum_j v_j \frac{\partial \nu_i}{\partial r_j} + \omega_i^2(t) r_i + \frac{1}{mn(r,t)} \frac{\partial P(r,t)}{\partial r_i} = 0,$$

(2.42)

where $n(r,t)$ and $P(r,t)$ are the density and pressure profiles, and $v_i(r,t)$ the velocity field. Like in Section 2.6.1 using a scaling approach which reduces Equation (2.42) to the equations for the scaling parameters:

$$\ddot{b}_i + \omega_i^2(t) b_i = \frac{\omega_{0i}^2}{b_i \left[ \Pi, b_i(t) \right]^{2/3}},$$

(2.43)

where $\omega_{0i} = \omega_i(0)$ and $b_i = b_i(t)/l_{0i}$, with $l_i$ is the 1/e radius of the thermal cloud and $l_{0i} = l_i(0) = \left[2k_B T_0/m \omega_i^2\right]^{1/2}$ is the initial size in the trap. Considering the case of a cylindrical geometry and an abrupt switch-off of the trap Equations (2.39) can be rewritten in the form

$$\ddot{b}_\rho = \frac{\omega_\rho^2}{b_\rho^{7/3} b_z^{2/3}},$$

(2.44)

$$\ddot{b}_z = \frac{\omega_z^2}{b_z^{5/3} b_\rho^{4/3}},$$

(2.45)

with initial conditions $b_i(0) = 1$, $\dot{b}_i(0) = 0$. 

\[ \text{Theoretical background} \]