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Bose-Einstein Condensate of Bosonic Atoms

Gross-Pitaevskii Equation and Hydrodynamic Expansion

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Abstract: In this seminar paper Bose-Einstein condensates of bosonic atoms are investigated. In detail, the theoretical foundation of cold ideal Bose gases is introduced and then expanded onto interacting Bose-Einstein condensates by deriving the Gross-Pitaevskii equation. It is shown that this equation describes dilute, interacting Bose gases at zero temperature and a few properties of it are discussed. Finally, the hydrodynamic expansion of initially trapped Bose-Einstein condensates is theoretically explained. Thereby, the results of theoretical predictions and measurements are compared.

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1 Motivation

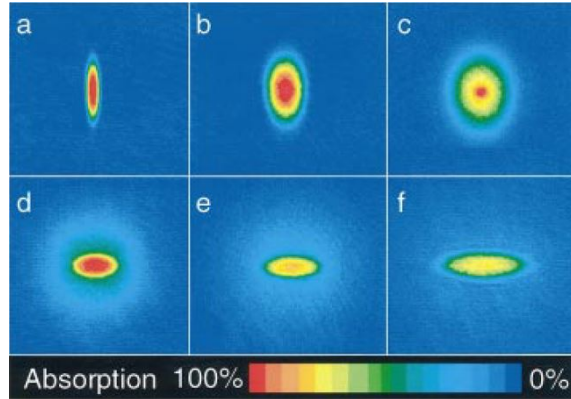


Figure 1: This image is taken from an experiment by the Ketterle Group at MIT in 1996 [1]. Depicted is a Bose-Einstein condensate of sodium-23 atoms that is initially trapped in an axially-symmetric harmonic potential generated by magnets. The trap is then switched off, so that the condensate can expand freely. The flight times for (a)–(f) are 1, 5, 10, 20, 30, and 45 ms, respectively.

This seminar paper is concerned with Bose-Einstein condensates of bosonic atoms and more concretely with the dynamics of condensates in harmonic traps governed by the Gross-Pitaevskii equation. To justify the assumptions and derivations as much as possible we want to compare the use and applications of the following computations with experiments. For comparison, we pick the first experiment where the expansion of a condensate was observed (cf. Fig. 1). In this experiment, conducted by the Ketterle Group at MIT in 1996, a condensate of sodium-23 atoms was produced and trapped in an axially-symmetric harmonic potential. After switching the trap off, it was observed that the condensate expands in a specific way. The aim of this seminar paper will be to understand and predict this expansion precisely.

Therefore, we start by sketching the most important facts and features of Bose-Einstein condensates in section 2, followed by the introduction and derivation of the Gross-Pitaevskii equation in section 3. As it turns out the Gross-Pitaevskii equation describes the time-evolution of nonuniform, dilute, interacting Bose gases at zero temperature. Since this equation is a nonlinear partial differential equation, it has a rich and complicated structure. However, we will investigate a few properties of it in section 4 in order to conduct the following computations appropriately. Finally, the established framework will be used to describe the hydrodynamic expansion of the condensate in section 5 and compare our results with the experiment.

2 Bose-Einstein condensate of bosonic atoms

In order to investigate the dynamics and expansion of a Bose-Einstein condensate it seems sensible to firstly remind ourselves what a Bose-Einstein condensate is and how it is theoretically explained and experimentally achieved. Therefore, we start by briefly introducing the historic development of Bose-Einstein condensates.

2.1 Bose-Einstein condensates in theory

In 1900 Max Planck initially introduced his hypothesis that energies on small scales only exists in discrete packages, thus laying the foundation of quantum theory. Almost a quarter

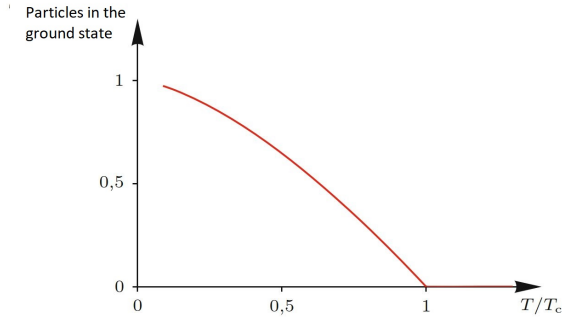


Figure 2: Occupation of the ground state in an ideal Bose gas in dependence of temperature.

of a century later in 1924 Satyendranath Bose working at the university of Dhaka found the same radiation law of photons by Planck, however, without the use of classical physics [2]. Afterwards, he sent his paper to Albert Einstein who, being impressed by his work, translated it to German and started working on the thermal properties of quantum gases aswell. In the same year he found that at low temperatures all gas particles will occupy the ground state at the same time meaning that they share the same quantum state [3], hence the gas transforms into a new phase, which is called, referring to the physicists who found that peculiar behavior, *Bose-Einstein condensate*.

In more detail, Bose and Einstein considered an ideal bosonic gas to derive its thermal properties at low temperatures. Bosons, contrary to fermions, can occupy the same state any number of times. Following this idea, it can be shown that below a certain critical temperature T_c all particles will gather in the ground state of the system (cf. Fig. 2). This critical temperature can be derived, for example in the framework of quantum statistics, to be

$$T_c = \frac{2\pi\hbar^2}{k_B m} \left(\frac{\rho}{2.612} \right)^{2/3}, \quad (1)$$

where ρ is the density of the Bose gas and m the particle mass. Experimentally it is well established, that this critical temperature does not often match the measured value. This hints towards the fact, that the consideration of a non-interacting, ideal Bose gas is not sufficient to quantitatively describe the properties of a Bose-Einstein condensate. Therefore, we will establish the framework of interacting Bose gases in the next sections, which will firstly lead us to the Gross-Pitaevskii equation. Beforehand, the experimental realization of Bose-Einstein condensates is discussed.

2.2 Bose-Einstein condensates in experiments

More than 70 years later in 1995, the experimental realization of a Bose-Einstein condensate was achieved, independently by E. A. Cornell and C. E. Wieman at the Joint Institute for Laboratory Astrophysics in Colorado with rubidium atoms [4] and by W. Ketterle at the MIT in Massachusetts with sodium atoms [5]. They used evaporative cooling in order to establish temperatures of a few nanokelvins. In 2001 they received the Nobel prize in physics “for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates”¹.

This achievement lead to a whole new field investigated in physics, namely the theory of ultra cold quantum gases. New phenomena were measured, such as the formation of quantum vortices in condensates, different collective oscillation modes of the condensate and the hydrodynamic expansion, which is the topic of this seminar paper. However, a

¹The Nobel Prize in Physics 2001. www.nobelprize.org/prizes/physics/2001/summary/

lot of the theoretical framework had not been developed yet, so that theoretical physicists started to research on ultra cold quantum gases in the following years. In particular, this led to a reuse of the Gross-Pitaevskii equation, that was already formulated in 1961, in order to describe the dynamics of Bose-Einstein condensates. The derivation of this equation will be sketched in the next section.

3 Gross-Pitaevskii equation

So far we have seen that below a certain critical temperature bosons form the so-called Bose-Einstein condensate by occupying the ground state of the system, so that the majority of the particles share the same quantum state. To that end, only non-interacting bosons were considered which led indeed to the right qualitative description. Quantitatively, however, we will see that a theory of non-interacting bosons is not sufficient to explain the measurements of an experiment accurately. Considering that a condensate possesses a denser profile than a gas, meaning that the particles are closer together, this is not surprising.

It turns out that in order to describe the dynamics of a Bose-Einstein condensate interaction necessarily needs to be considered, which leads naturally to a more complicated mathematical framework. Nevertheless, the foundation of the description of condensates has been already delivered by Lev P. Pitaevskii [6] and Eugene P. Gross [7] in 1961. The physicists researched independently of each other, Pitaevskii at the Academy of Sciences in the Soviet Union and Gross at CERN in Geneve, on the formation of quantum vortices in Bose-Einstein condensates, which led them to a formulation of an equation that describes the dynamics of condensate. Therefore, this equation is called the *Gross-Pitaevskii equation* and, as we will see, describes the behavior of nonuniform, interacting, dilute Bose condensates at zero temperature.

In this section, the derivation of the Gross-Pitaevskii equation is sketched, as it was originally done by Gross and Pitaevskii. Therefore, we firstly need to remind ourselves of the general notion of quantum many-body systems, since a system of many bosonic particle is exactly that.

3.1 Second quantization

Quantum many-body systems were initially introduced by Dirac [8] in 1926 in order to quantize the electromagnetic field. Thereby, classical fields are replaced by field operators, thus, elevating quantum mechanics to a theory that respects the spacetime structure of relativity. A natural consequence thereof is that particles can be created and annihilated in quantum many-body systems. A thorough discussion of the development from quantum mechanics to the description of quantum field theories would go beyond the constraints of this seminar paper. Therefore, we concentrate on the the most important aspects of this notion in order to derive the Gross-Pitaevskii equation by making certain assumptions.

As already mentioned, the number of particles is not a fixed value in quantum systems. Thus, a new Hilbert space needs to be introduced to describe the states a many-body system can obtain. The general idea is to consider ordinary Hilbert spaces of fixed particle numbers, e.g. the zero-particle Hilbert space \mathcal{H}_0 , one-particle Hilbert space \mathcal{H}_1 , etc., and then construct the so-called *Fock space* \mathcal{F} as a tensor sum of all these Hilbert spaces

$$\mathcal{F} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \dots \quad (2)$$

States in this Fock space can then simply be thought of as a set of occupation numbers that describe the number of particles that share the same energy within the system. To

describe the dynamics of the system it is useful to introduce the so-called *creation* and *annihilation operators* \hat{a}_i^\dagger and \hat{a}_i , where the index i numerates the different energy eigenvalues of the system. These operators create and annihilate particles which are in the i^{th} energy eigenstates, respectively. It turns out that further useful operators, that are convenient to define, are the *quantum field operators*. There are defined by the following equations

$$\hat{\Psi}(\mathbf{r}) = \sum_i \phi_i(\mathbf{r}) \hat{a}_i \quad \text{and} \quad \hat{\Psi}^\dagger(\mathbf{r}) = \sum_i \phi_i^*(\mathbf{r}) \hat{a}_i^\dagger, \quad (3)$$

where the sum goes over all energy eigenvalues and the ϕ_i describe the respective energy eigenstates in position space. Historically, these field operators were thought of as quantized versions of the wave functions in quantum mechanics. Hence, the term ‘Second quantization’, which suggests that quantum mechanics is somehow quantized even further. However, the interpretation has changed so that the modern view is quite different. Quantum field operators are now thought of as operators which create and annihilate particles of all energies in specific points in space, respectively.

One of the most important distinctions between the quantum field operators is whether they describe bosonic or fermionic states. As it is well known all bosonic particles obey specific commutation laws which directly transfer to the commutation laws of the bosonic field operators

$$\left[\hat{\Psi}(\mathbf{r}, t), \hat{\Psi}^\dagger(\mathbf{r}', t) \right] = \delta(\mathbf{r} - \mathbf{r}'), \quad (4)$$

$$\left[\hat{\Psi}(\mathbf{r}, t), \hat{\Psi}(\mathbf{r}', t) \right] = 0 \quad \text{and} \quad \left[\hat{\Psi}^\dagger(\mathbf{r}, t), \hat{\Psi}^\dagger(\mathbf{r}', t) \right] = 0. \quad (5)$$

Having introduced the operators to describe quantum many-body systems, we now have to consider their time evolution. Therefore, it is useful to formulate the Hamilton operator of the system and then, subsequently, derive the time evolution of the field operators in terms of the Heisenberg picture. In order to work out the Hamilton operator one can think of ordinary operators in quantum mechanics and transfer their action onto many particles by the framework established above. This is not done in detail here but rather simply stated and motivated by its form

$$\begin{aligned} \hat{H} = & \int d\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}, t) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}, t) \right) \hat{\Psi}(\mathbf{r}, t) \\ & + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}^\dagger(\mathbf{r}', t) U(\mathbf{r} - \mathbf{r}') \hat{\Psi}(\mathbf{r}', t) \hat{\Psi}(\mathbf{r}, t). \end{aligned} \quad (6)$$

In the first line of the equation one sees the action of the kinetic energy and an external potential $V_{\text{ext}}(\mathbf{r}, t)$ on every particle of the system which is established by the annihilation and creation of a particle at a specific point \mathbf{r} that is then integrated over all space. Further, in the second line a two-particle interaction $U(\mathbf{r} - \mathbf{r}')$ is described by the creation and annihilation of two particles at \mathbf{r} and \mathbf{r}' . In total, the Hamilton operator therefore describes the dynamics of a quantum many-body system with external potential and two-particle interaction.

Finally, the time evolution of the quantum field operator can be derived by using the Heisenberg equation

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\mathbf{r}, t) = \left[\hat{\Psi}(\mathbf{r}, t), \hat{H} \right], \quad (7)$$

and applying the bosonic commutation relations (4) and (5). This directly leads to a partial differential equation for the field operator

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}, t) + \int d\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r}', t) U(\mathbf{r} - \mathbf{r}') \hat{\Psi}(\mathbf{r}', t) \right) \hat{\Psi}(\mathbf{r}, t). \quad (8)$$

So far, only the general concepts of quantum many-body systems were introduced. From here on, the Gross-Pitaevskii equation can be derived by making two important assumptions about the system.

3.2 Derivation of the Gross-Pitaevskii equation

First assumption: Zero temperature approach. The first assumption concerns the temperature of the system. Since we are interested in a description of Bose-Einstein condensates, it seems appropriate to investigate the system at very low temperatures. To that end, the field operator introduced above is expanded in its expectation value and the quantum fluctuations of it

$$\hat{\Psi}(\mathbf{r}, t) = \Phi(\mathbf{r}, t) + \hat{\psi}(\mathbf{r}, t) \quad \text{with} \quad \langle \hat{\Psi}(\mathbf{r}, t) \rangle = \Phi(\mathbf{r}, t). \quad (9)$$

As mentioned, considering low temperatures it is known that most of the bosonic particles will occupy the ground state of the system. Hence, one can assume that the expectation values of the field operators correspond to the creation and annihilation operators of the ground state. The disturbances $\hat{\psi}(\mathbf{r}, t)$ can then be interpreted as thermal fluctuations from that ground state.

Such an expansion was initially introduced by Bogoliubov in 1947 [9] in order to describe the superfluid properties of Bose-Einstein condensate. He assumed the condensate itself to be uniform and time-independent, thus being a fixed number $\Phi(\mathbf{r}, t) = \text{const.}$, and only looked at the linear fluctuations of it. Thereby, he found the famous Bogoliubov quasi-particle excitation explaining the basics of the superfluid properties of condensates at very low temperatures. The ansatz Gross and Pitaevskii made is exactly the opposite. They considered nonuniform, time-dependent Bose-Einstein condensates, thus searching for properties of the condensate itself. Therefore, all thermal fluctuations are neglected, e.g. $\hat{\psi}(\mathbf{r}, t) = 0$, meaning that the system is assumed to be at zero temperature.

Consequently, the field operator can be replaced by its expectation value, which is then called the *order parameter* or simply *wave function* of the condensate. It describes the particle number density of the system and fixes its total particle number

$$|\Phi(\mathbf{r}, t)|^2 = n(\mathbf{r}, t) \quad \text{with} \quad \int d\mathbf{r} n(\mathbf{r}, t) = N. \quad (10)$$

As can be seen, the operator is replaced by a classical complex field, meaning that all quantum features of the condensate are neglected. The reasoning for this is that at zero temperature all particles are in the same state, so that the noncommutivity of the particle operators are not important. In fact, this is analogous to the transition from quantum electrodynamics to classical electrodynamics. If the majority of the photons share the same state, the electromagnetic fields can be describe, employing classical functions instead of operators.

Second assumption: Pseudo-potential. As established, we consider the system to be at very low temperatures. Hence it can be assumed that the de Broglie wave number k of the particles is large compared to other characteristic length of the system. Most importantly, one can expect the variations of the interaction potential to be much smaller than the wave number of the particles, so that the interaction between two particles can be characterized by a single number, the so-called (*s-wave*) *scattering length* a . In detail, the general scattering of a particle is described by an incoming plane wave and an outgoing spherical wave that amplitude is fixed by the scattering amplitude $f(\mathbf{k}, \mathbf{r}/r)$. Because of

the reasons above, at low temperatures this amplitude can be replaced by the scattering length

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}, \mathbf{r}/r) \frac{e^{ikr}}{r} \longrightarrow 1 - \frac{a}{r}.$$

Figuratively, one can interpret the scattering length a as the radius of hard spheres that scatter with each other, so that the length corresponds to the typical distance two particles need to have in order to interact with each other.

The important assumption that is then made, is to assume the condensate to be *dilute*, which means that on average there is always much less than one particle per scattering volume $\bar{n}|a|^3 \ll 1$, where \bar{n} denotes the particle density on average. Firstly, this justifies that only two-particle interactions have to be examined because the interaction of three particles is too unlikely. Secondly, the potential then needs to be assumed to be a pseudo-potential, so that any bound states between two particles can be prevented. Further this is justified because the specific shape of the potential can be ignored as already mentioned. The interaction strength can then be related to the scattering length

$$U(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}') \quad \text{with} \quad g = \frac{4\pi a\hbar^2}{m}. \quad (11)$$

The specific value and sign of a solely depends on the considered particles. If a is positive the interaction between particles is repulsive, if a is negative the interaction is attractive. In 1996 the scattering length of sodium-23 was measured to be $a = 2.75$ nm by Tiesinga et al. at the University of Chicago, so that the interaction between sodium particles is repulsive, which is going to be important later.

Before we finally set up the Gross-Pitaevskii equation, we want to convince ourselves that the dilution condition is actually fulfilled by most condensates. With scattering lengths of order of a few nanometres and density values ranging from 10^{13} cm^{-3} to 10^{15} cm^{-3} the dilution parameter is typically of order $\bar{n}|a|^3 < 10^{-3}$, which is sufficient for assuming the condensate to be dilute.

With these assumption the Gross-Pitaevskii equation can finally be formulated. Therefore, one simply starts with the equation of motion of the quantum field operator (8) and replaces the operator by the classical wave function of the condensate. Subsequently, replacing the general interaction potential by the pseudo-potential and integrating over it, leaves one with the Gross-Pitaevskii equation as it was originally formulated

$$i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}, t) + g|\Phi(\mathbf{r}, t)|^2 \right) \Phi(\mathbf{r}, t). \quad (12)$$

Looking at this equation, the resemblance to the Schrödinger equation is quite obvious. The only different feature is the last term in the brackets, which arose from the interaction of the system. This term leads to a non-linearity of the equation which gives rise to completely new and rich features of the condensate compared to non-interacting ones, as we will see. However, it also makes it almost impossible to solve the equation analytically since non-linearities always make dynamics vastly more complicated. Therefore, we deal with a few properties of the equation in the next section.

4 Properties of the Gross-Pitaevskii equation

4.1 Scales of the Gross-Pitaevskii equation and Thomas-Fermi approximation

Having discussed the derivation of the Gross-Pitaevskii equation, it is now time to choose the external potential to fit the problem that is considered here. As mentioned in the

motivation the external potential is a harmonic oscillator

$$V_{\text{ext}}(\mathbf{r}) = \frac{m}{2} \sum \omega_i^2 r_i^2, \quad (13)$$

where m denotes the mass of the particles. The potential is described by three different oscillation frequencies corresponding to the different space dimensions. With these frequencies a new length scale is introduced, the so-called harmonic oscillator length

$$a_{\text{ho}}^2 = \frac{\hbar}{m\omega_{\text{ho}}} \quad \text{with} \quad \omega_{\text{ho}} = \sqrt[3]{\omega_1\omega_2\omega_3}. \quad (14)$$

This length scale can be used to make the Gross-Pitaevskii equation (12) dimensionless by rescaling the dimensional variables, for example $\mathbf{r}^2 \rightarrow a_{\text{ho}}^2 \tilde{\mathbf{r}}^2$, $t \rightarrow \omega_{\text{ho}}^{-1} \tilde{t}$, $\Phi(\mathbf{r}, t) \rightarrow a_{\text{ho}}^{-3/2} \sqrt{N} \tilde{\Phi}(\tilde{\mathbf{r}}, \tilde{t})$. Here, $\tilde{\Phi}(\tilde{\mathbf{r}}, \tilde{t})$ was also chosen to be normalized to 1. The resulting equation can then be derived to be

$$2i \frac{\partial}{\partial \tilde{t}} \tilde{\Phi}(\tilde{\mathbf{r}}, \tilde{t}) = \left(-\tilde{\nabla}^2 + \tilde{\mathbf{r}}^2 + 8\pi \frac{Na}{a_{\text{ho}}} |\tilde{\Phi}(\tilde{\mathbf{r}}, \tilde{t})|^2 \right) \tilde{\Phi}(\tilde{\mathbf{r}}, \tilde{t}). \quad (15)$$

As can be seen, the only relevant scale left is the dimensionless ratio of the total particle number times the scattering length divided by the harmonic oscillator length Na/a_{ho} . In fact, it can be shown that this ratio is proportional to the ratio of the total kinetic energy E_{kin} to the total interaction energy E_{int} that the condensate possesses. From the Gross-Pitaevskii equation it can be inferred that the total interaction energy is proportional to $|g|N\bar{n}$, where the average density can be expressed by $\bar{n} = N/a_{\text{ho}}^3$. On the other side, the kinetic energy is of the order of $N\hbar\omega_{\text{ho}}$, which is then proportional to N/a_{ho}^2 . In total, the ratio of the energies is then indeed proportional to the dimensionless value found in the dimensionless Gross-Pitaevskii equation (15)

$$\frac{E_{\text{int}}}{E_{\text{kin}}} \propto \frac{N|a|}{a_{\text{ho}}}. \quad (16)$$

The order of the value of this ratio is strongly dependent on the experimental setup and type of particles used. For the experiments with sodium at MIT condensates were established with a comparatively large number of atoms of order from 10^6 to 10^7 [1, 5]. Therefore, this ratio is of order of $Na/a_{\text{ho}} \propto 10^3 - 10^4$, meaning that the interaction between the sodium atoms is much larger than the kinetic energy the atoms possess on average. Considering that the repulsive interaction as well as the kinetic energy drives the condensate apart, one can neglect the effect of the kinetic term in the Gross-Pitaevskii equation, since it is at least thousand times smaller than the effect of the interaction. This seemingly crude approximation is called the *Thomas-Fermi approximation* and simplifies the Gross-Pitaevskii equation extremely

$$i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) = \left(V_{\text{ext}}(\mathbf{r}) + g|\Phi(\mathbf{r}, t)|^2 \right) \Phi(\mathbf{r}, t). \quad (17)$$

Another way to justify the Thomas-Fermi-approximation is by visualizing it. As can be seen in Fig. 3, the effect of the interaction flattens the density profile strikingly. Hence, the variation of the particle number density described by the laplacian of the kinetic term can be neglected compared to the effect of the repulsive interaction.

At this point, it should be stressed that the application of the Thomas-Fermi approximation is very limited by the experiment that is considered. For example, experiments with rubidium as conducted at JILA by Wieman and Cornell [4] cannot produce condensates with an equally high number of atoms, so that the ratio (16) turns out to be much smaller.

Thus, this approximation cannot be used to deliver a quantitative description of the condensate. Moreover, for experiments with bosons that attract each other, as for example with lithium [12], the approximation also cannot be applied. The reason for that is that the kinetic energy counteracts the attractive interaction between the particles. Hence, a neglect of the kinetic term would immediately lead to a collapse of the Bose-Einstein condensate.

4.2 Static solutions of the Gross-Pitaevskii equation

Using the Thomas-Fermi approximation, searching for static solutions of condensates becomes a simple task. Considering the Gross-Pitaevskii equation (17) with the approximation enforced one sees that the differential equation became ordinary, since the kinetic term is neglected. By applying a simple separation ansatz for the wave function

$$\Phi(\mathbf{r}, t) = \Phi(\mathbf{r}) e^{-i\frac{\mu}{\hbar}t}, \quad (18)$$

where μ denotes the energy per particle, i.e. the chemical potential, the Gross-Pitaevskii equation reduces to

$$\mu \Phi(\mathbf{r}) = \left(V_{\text{ext}}(\mathbf{r}) + g|\Phi(\mathbf{r})|^2 \right) \Phi(\mathbf{r}). \quad (19)$$

Rearranging this equation and inserting the external potential (13) lead to an expression for the particle number density, which is called *Thomas-Fermi density* referring to the application of the Thomas-Fermi approximation

$$n(\mathbf{r}) = |\Phi(\mathbf{r})|^2 = \frac{1}{g} \left(\mu - \frac{m}{2} \sum \omega_i^2 r_i^2 \right). \quad (20)$$

This equation only holds when the chemical potential is greater than the external potential so that the particle number density does not become zero. As can be seen, the static shape of the condensate is fully determined by the form of the external potential. In the case of a harmonic trap, one obtains a parabolic shape for the density profile of the

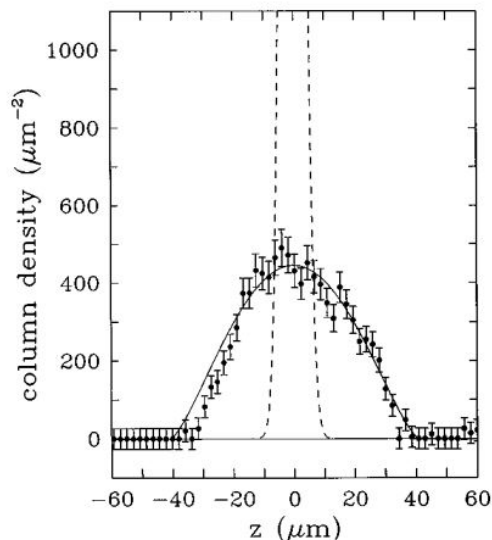


Figure 3: Density distribution of 80 000 sodium atoms in a trap of Hau et al. (1998) [10] as a function of the axial coordinate. Points describe the measured value, the solid line the theoretical prediction by the Gross-Pitaevskii equation and the dashed line the case for non-interacting bosons. (Figure from [11])

condensate (cf. Fig. 3).

Moreover, using (20) the chemical potential of the static configuration can be determined by enforcing that the total particle number N is fixed

$$N = \int d\mathbf{r} n(\mathbf{r}) \quad \rightarrow \quad \mu = \frac{\hbar\omega_{\text{ho}}}{2} \left(\frac{15Na}{a_{\text{ho}}} \right)^{2/5}. \quad (21)$$

The fact that the chemical potential depends on $N^{2/5}$ is indeed well fitted by experimental measurements [1].

4.3 Collisionless hydrodynamics and superfluidity

Having discussed the static solutions of the Gross-Pitaevskii equation we take a step back and examine again the full equation (12). Considering that we are interested in describing the dynamics of many particles that are interacting with each other, a hydrodynamic description of the condensate would be convenient. In order to establish such a description the wave function of the condensate is written in the following way

$$\Phi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)} e^{i\theta(\mathbf{r}, t)}, \quad (22)$$

where it is used that the modulus of the wave function is equal to the square root of the number density. Inserting this expression into the Gross-Pitaevskii equation and computing the spatial and time derivatives in terms of derivatives acting on n and θ , leads to differential equations for the number density of the condensate and the phase of the wave function by splitting the equation into its real and imaginary part

$$\frac{\partial}{\partial t} n(\mathbf{r}, t) = -\frac{\hbar}{m} \nabla [n(\mathbf{r}, t) \nabla \theta(\mathbf{r}, t)], \quad (23)$$

$$\hbar \frac{\partial}{\partial t} \theta(\mathbf{r}, t) = \frac{\hbar^2}{2m} \left(\frac{\nabla^2 \sqrt{n(\mathbf{r}, t)}}{\sqrt{n(\mathbf{r}, t)}} - (\nabla \theta(\mathbf{r}, t))^2 \right) - V_{\text{ext}}(\mathbf{r}, t) - g n(\mathbf{r}, t). \quad (24)$$

Firstly, the Thomas-Fermi approximation is again applied, so that the first term in the brackets on the right-hand side of the second equation, which is called kinetic pressure, can be neglected. Secondly, one notices that the first equation can be rewritten as a continuity equation if a velocity field is introduced in the following way

$$\mathbf{v}(\mathbf{r}, t) = \frac{\hbar}{m} \nabla \theta(\mathbf{r}, t). \quad (25)$$

In fact, this definition coincides with the particle current density of the wave function. Moreover, it becomes apparent that the velocity field itself is a gradient field. Using this definition, (24) can be written in terms of the velocity field, which then reads as follows

$$m \frac{\partial}{\partial t} \mathbf{v}(\mathbf{r}, t) + \nabla \left(\frac{m\mathbf{v}^2(\mathbf{r}, t)}{2} + V_{\text{ext}}(\mathbf{r}, t) + g n(\mathbf{r}, t) \right) = 0. \quad (26)$$

Using that the rotation of the velocity vanishes due to the fact that it is a gradient field, the first term in the brackets can be rewritten as a directional derivative of the velocity field. Additionally, one can interpret the gradient of the external potential as the external force and define a pressure field by $p = gn^2/2$. The differential equation of the velocity field then takes the form of an Euler equation. In total, one achieves from (23) and (24) the following equations

$$\frac{\partial}{\partial t} n + \nabla \cdot (n\mathbf{v}) = 0, \quad (27)$$

$$m \left(\frac{\partial}{\partial t} + (\mathbf{v} \cdot \nabla) \right) \mathbf{v} = -\frac{\nabla p}{n} - \nabla V_{\text{ext}}. \quad (28)$$

To conclude, one recognizes by starting from the Gross-Pitaevskii equation and applying the Thomas-Fermi approximation a continuity equation and Euler equation of the condensate can be derived. From the first one immediately total particle number conservation follows. More interestingly, in the second equation are no terms proportional to the laplacian of the velocity field, hence meaning that the condensate possesses zero viscosity, making it a superfluid. Moreover, the pressure of the condensate is fully determined by the repulsive particle interaction.

These important equations describe the superfluid nature of Bose-Einstein condensate and were derived by Stringari in 1996 [13] starting from the Gross-Pitaevskii equation. They will be the starting point in our discussion about the hydrodynamic expansion of Bose-Einstein condensates.

5 Hydrodynamic expansion

In the last sections the Gross-Pitaevskii equation was derived and it was shown that it describes the dynamics of nonuniform, dilute, interacting Bose gases at low temperature. Thus, it is able to describe the time evolution of a Bose-Einstein condensate. Subsequently, a few properties of the equation were discussed, for example the Thomas-Fermi approximation, that can be taken, and a static solution, that can be analytically computed. Most importantly, the hydrodynamic equations of a superfluid were deduced from the Gross-Pitaevskii equation. After having established all of this framework, we are finally able to come back to the main problem of this paper namely to theoretically explain the expansion of a freed condensate.

The motivation to consider such an expansion of a condensate is a simple practical one. A condensate is typically produced while being trapped in a harmonic potential. However, many important properties of the condensate are measured only after it is being freed. For example, the temperature of the condensate or collective excitations. Moreover, the measurements of the expansion itself can be used to compare theoretical results, as is the topic of this seminar paper.

5.1 Time evolution of an expanding condensate

Generally, one naturally assumes that the hydrodynamic equations (27) and (28) are a promising starting point in order to describe the time evolution of a Bose-Einstein condensate, since it is dealt with an interacting system of many particles. Beforehand, however, one needs to specify the external potential, which is following the experiment, a harmonic potential. Assuming the most general case, we choose an anisotropic oscillator with time dependent frequencies

$$V_{\text{ext}}(\mathbf{r}, t) = \frac{m}{2} \sum \omega_i^2(t) r_i^2. \quad (29)$$

The static values $\omega_i(t=0) = \omega_{0i}$ then determine the initial equilibrium distribution which is given by the Thomas-Fermi density, as was discussed in the previous section

$$n(\mathbf{r}, t=0) = \frac{1}{g} \left(\mu - \frac{m}{2} \sum \omega_{0i}^2 r_i^2 \right). \quad (30)$$

Thus, the equilibrium density profile exhibits a parabolic shape. As an ansatz, it is assumed that this parabolic shape is conserved during the expansion, so that the density profile and velocity profile should possess the following form

$$n(\mathbf{r}, t) = a_0(t) - a_x(t) x^2 - a_y(t) y^2 - a_z(t) z^2, \quad (31)$$

$$\mathbf{v}(\mathbf{r}, t) = \frac{1}{2} \nabla (\alpha_x(t) x^2 + \alpha_y(t) y^2 + \alpha_z(t) z^2), \quad (32)$$

where the a_i and α_i determine the time evolution of this configuration. Again, the number density is everywhere zero, where (31) gives a negative value. Thereby, the velocity profile is constructed to be a gradient field as is demanded by the hydrodynamic equations. Further, one notices the enormous simplification this ansatz delivers, namely that now only the time evolution has to be computed, since the spatial distribution is fixed. The Thomas-Fermi density determines the boundary conditions of the $a_i(t)$, whereas the $\alpha_i(t)$ are initially zero since the equilibrium density profile possesses no velocity field

$$a_i(t=0) = \frac{m\omega_{0i}^2}{2g} \quad \text{and} \quad \alpha_i(t=0) = 0. \quad (33)$$

The coefficient $a_0(t)$ can be at all times determined by fixing the total particle number to be N

$$a_0 = (15N/8\pi)^{2/5} (a_x a_y a_z)^{1/5}. \quad (34)$$

Plugging the ansatz into the continuity equation (27) and the Euler equation (28) yields a scalar and vector equation for the different coefficients

$$\dot{a}_0 - \sum \dot{a}_i r_i^2 + \left(a_0 - \sum a_i r_i^2 \right) \sum \alpha_j - 2 \sum \alpha_i a_i r_i^2 = 0, \quad (35)$$

$$\sum \mathbf{e}_i (m\dot{\alpha}_i r_i + m\alpha_i^2 r_i + m\omega_i^2 r_i - 2ga_i r_i) = 0, \quad (36)$$

where a dot above the coefficients denotes a time derivative. Since the equations need to hold for any values of the spatial coordinates, one can compare the prefactors in front of them and set them to zero independently. Thus, one achieves six coupled differential equations for the time evolution of the coefficients

$$\dot{a}_i + 2a_i\alpha_i + a_i \sum \alpha_j = 0, \quad (37)$$

$$\dot{\alpha}_i + \alpha_i^2 + \omega_i^2 - \frac{2g}{m}a_i = 0. \quad (38)$$

It should be mentioned that in the above equations the sums go over the spatial indices and the Einstein sum convention is not implied.

Although the original problem is already vastly simplified by these equations one can reduce the amount of equations even further by considering a different parameterization.

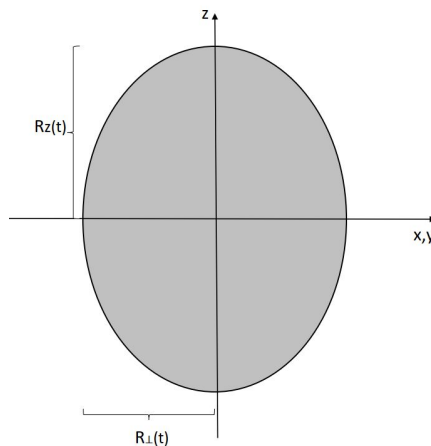


Figure 4: Schematic density profile of a bosonic condensate cloud, that is trapped in an axially symmetric potential. Sketched are the classical radii R_z and R_\perp .

To that end, the parabolic shape is characterized by its classical radii, i.e. the radii in each spatial direction where the number density vanishes (cf. Fig. 4). Comparing them with the ansatz (31), these radii are given by $R_i(t) = \sqrt{a_0(t)/a_i(t)}$. Following the idea, that the parabolic shape of the density profile is conserved, scaling functions $b_i(t)$ are introduced that govern the time evolution of the classical radii

$$R_i(t) = R_i(0) b_i(t) = \sqrt{\frac{2\mu}{m\omega_{0i}^2}} b_i(t), \quad (39)$$

where the initial values of the radii are again fixed by the static Thomas-Fermi density (20). Relating the initially introduced coefficients in the ansatz with the scaling parameters and solving for the coefficients yield

$$a_i = \frac{m\omega_{0i}^2}{2gb_x b_y b_z b_i^2}. \quad (40)$$

Using these expressions, the time evolution of the initial parameterization by a_i and α_i (cf. (37) and (38)) reduces to $\alpha_i = \dot{b}_i/b_i$ and the following equations that describe the time evolution of the new scaling parameters

$$\ddot{b}_i + \omega_i^2 b_i - \frac{\omega_{0i}^2}{b_i b_x b_y b_z} = 0. \quad (41)$$

These equations are the end result of the derivation and describe the dynamics of the hydrodynamic expansion of Bose-Einstein condensates completely. By making the ansatz that the parabolic shape of the density profile is conserved and choosing the right parameterization, the initial coupled partial differential equation of hydrodynamics reduces to three ordinary coupled differential equations which simplifies the problem to a great extent. Equations (41) were firstly derived by Castin and Dum at the École Normale Supérieure in Paris in 1996 [14], in the same year that the experiment at the MIT was conducted. Shortly after that also Kagan, Surkov and Shlyapnikov [15] and finally Dalfovo, Minniti, Stringari and Pitaevskii [16] derived the same equations.

5.2 Comparison to the experiment

With the equations (41) we are finally able to predict the measurements of the experiment [1] and compare the theoretical and experimental results. Therefore, the experimental setup needs to be specified further. The condensate is initially trapped in an axially symmetric harmonic potential, meaning that only two independent frequencies need to be considered $\omega_\perp = \omega_x = \omega_y$ and ω_z . At the time $t = 0$ the trap is switched off completely so that the free expansion can be observed. In terms of the equations (41) this means that they reduce from three independent ones to two, and additionally, that the second terms can be canceled since the external potential is switched off. In total, the following equations are obtained

$$\ddot{b}_\perp - \frac{\omega_\perp^2}{b_\perp^3 b_z} = 0 \quad \text{and} \quad \ddot{b}_z - \frac{\omega_z^2}{b_\perp^2 b_z^2} = 0, \quad (42)$$

where $b_\perp = b_x = b_y$. The boundary conditions are $b_\perp(t = 0) = 1$, $b_z(t = 0) = 1$, $\dot{b}_\perp(t = 0) = 0$ and $\dot{b}_z(t = 0) = 0$, since the initial scaling is normalized and static.

To effectively compare the theory with the experimental results, it is aimed to derive the so-called *aspect ratio* of the condensate, which is given by the ratio off the two classical radii R_\perp and R_z

$$\frac{R_\perp(t)}{R_z(t)} = \frac{R_z(0) b_\perp}{R_\perp(0) b_z} = \frac{\omega_z b_\perp}{\omega_\perp b_z} = \lambda \frac{b_\perp}{b_z}, \quad (43)$$

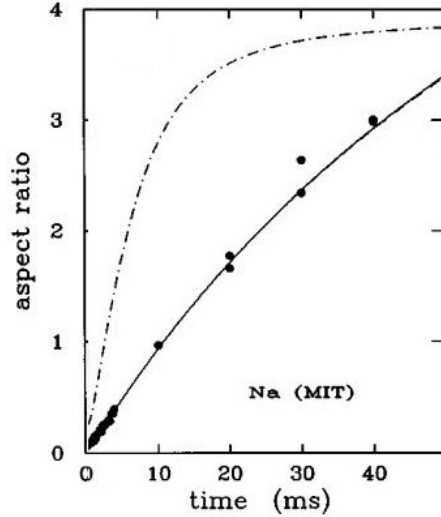


Figure 5: Aspect ratio of the expanding Bose-Einstein condensate at MIT [1] (Figure from [11]). The points correspond to the experimentally measured data points, the solid line to the exact numerical result of the hydrodynamic expansion equations, the dashed line (not seen because it almost completely matches the solid line) is the analytical result in the limit $\lambda \ll 0$ and the dashed-dotted line corresponds to the expansion of a non-interacting condensate.

where in the second equality it is used that the initial classical radii are inversely proportional to the static frequencies of the harmonic trap. Furthermore, the ratio $\lambda = \omega_z/\omega_\perp$ that describes the configuration of the trap is defined. Equations (42) can be rewritten in terms of λ by introducing the dimensionless time $\tau = \omega_\perp t$

$$\frac{d^2}{d\tau^2} b_\perp = \frac{1}{b_\perp^3 b_z} \quad \text{and} \quad \frac{d^2}{d\tau^2} b_z = \frac{\lambda^2}{b_\perp^2 b_z^2}. \quad (44)$$

This form has the advantage that the ratio λ can be computed from the experimental setup before solving the equations. The experimental values of the trap are given by $\omega_z = 2\pi \times 16.23 \text{ Hz}$ and $\omega_\perp = 2\pi \times 248 \text{ Hz}$, which explains why the initial profile has a cigar-like shape since the condensate is much tighter confined in the radial direction than in the axial one. The ratio then calculates to be $\lambda = 0.065$, which is much smaller than one. Using this limit the equations (44) can be even solved perturbatively as shown by the authors in [14]. The solutions up to second order in λ read

$$b_\perp(\tau) = \sqrt{1 + \tau^2}, \quad (45)$$

$$b_z(\tau) = 1 + \lambda^2 \left(\tau \arctan \tau - \ln \sqrt{1 + \tau^2} \right). \quad (46)$$

Plugging them into the formula for the aspect ratio (43) yield the final result

$$\frac{R_\perp}{R_z} = \frac{\lambda \sqrt{1 + \tau^2}}{1 + \lambda^2 \left(\tau \arctan \tau - \ln \sqrt{1 + \tau^2} \right)}, \quad (47)$$

which predicts the hydrodynamic expansion of the condensed gas quite perfectly as can be seen in Fig. 5. At longer times the condensate obtains again a static aspect ratio given by $\lim_{\tau \rightarrow \infty} (R_\perp/R_z) = 2/(\pi\lambda) = 9.794$. In particular, this means that the expansion is faster in that direction the trap was initially tighter confining. As can also be seen in Fig. 5 a non-interacting condensate would behave extremely different. In that case, the wave function of the condensate would simply obey the Schrödinger equation so that it would

diffuse according to the dispersion relation of a massive wave packet.

All in all, we see that the Gross-Pitaevskii equation delivered a precise theoretical explanation for the expansion of the condensate. Remarkably, even an analytical result is obtained by making right assumptions that are justified by experiments, as we have seen.

6 Conclusion and outlook

In this seminar paper, Bose-Einstein condensates of bosonic atoms were investigated. These are a peculiar phase of Bose gases at low temperatures, where the majority of the particles occupy the same quantum state. With the first achievements of Bose-Einstein condensates by Ketterle [5] and Cornell and Wieman [4] a whole new field in physics was established, namely the field of ultra-cold quantum gases. Following this experimental milestone new theoretical explanations were developed based on the Gross-Pitaevskii equation, that was 1961 derived by Gross [7] and Pitaevskii [6] independently. In a few words, the Gross-Pitaevskii equation describes the dynamics of nonuniform, dilute, interacting bosonic condensates at zero temperature. In particular, it was observed that Bose-Einstein condensates expand after being released from a trap [1]. This seminar paper followed the theoretical explanation by Castin and Dum [14] in order to describe this hydrodynamic expansion starting from the Gross-Pitaevskii equation. One of the main features of the expansion are that the initial shape of the density profile is conserved, which is in the case of an initially harmonic trap a parabolic shape. Moreover, it was shown that the expansion is in those spatial directions faster the trap was initially tighter confining. At last, the theoretical results were compared with the measurements and it was shown that they fit perfectly (cf. Fig. 5).

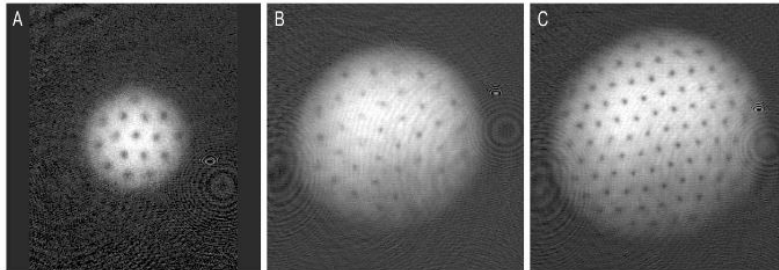


Figure 6: Experimentally realized vortex formation in a Bose-Einstein condensate of sodium atoms by [17]. The vortices are produced by stirring the condensate with a laser.

Further interesting properties that can be investigated in Bose-Einstein condensates using the Gross-Pitaevskii equation are for example soliton solutions or different oscillation modes. In particular, one can show that the Bogoliubov dispersion relation can be recovered from the Gross-Pitaevskii equation. Another property that can be examined are quantum vortices, as was the initial motivation for the derivation of the Gross-Pitaevskii equation. In fact, such vortices can nowadays even be experimentally realized (cf. Fig. 6). There are many more applications of the Gross-Pitaevskii equation and features of trapped Bose-Einstein condensates that are interesting to investigate. For a nice introduction to this topic the review by Dalfovo, Giorgini, Pitaevskii and Stringari [11] is recommended.

References

- [1] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee and W. Ketterle, *Bose-Einstein Condensation in a Tightly Confining dc Magnetic Trap*, *Phys. Rev. Lett.* **77** (1996) 416.
- [2] S. Bose, *Plancks Gesetz und Lichtquantenhypothese*, *Zeitschrift für Physik* **26** (1924) 178.
- [3] A. Einstein, *Quantentheorie des einatomigen idealen Gases. Zweite Abhandlung*, *Sitz.ber. Preuss. Akad. Wiss. Phys.* **23** (1924) 245 .
- [4] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman and E. A. Cornell, *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor*, *Science* **269** (1995) 198 [<https://science.sciencemag.org/content/269/5221/198.full.pdf>].
- [5] K. B. Davis, M. O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn et al., *Bose-Einstein Condensation in a Gas of Sodium Atoms*, *Phys. Rev. Lett.* **75** (1995) 3969.
- [6] L. P. Pitaevskii, *Vortex Lines in an Imperfect Bose Gas*, *JETP* **13** (1961) 451.
- [7] E. P. Gross, *Structure of a quantized vortex in boson systems*, *Il Nuovo Cimento (1955-1965)* **20** (1961) 454.
- [8] P. A. M. Dirac, *The Quantum Theory of the Emission and Absorption of Radiation*, *Proceedings of the Royal Society of London* **114** (1927) 243.
- [9] N. Bogolyubov, *On the theory of superfluidity*, *J. Phys. (USSR)* **11** (1947) 23.
- [10] L. Vestergaard Hau, B. D. Busch, C. Liu, Z. Dutton, M. M. Burns and J. A. Golovchenko, *Near-resonant spatial images of confined Bose-Einstein condensates in a 4-Dee magnetic bottle*, *Phys. Rev. A* **58** (1998) R54.
- [11] F. Dalfovo, S. Giorgini, L. P. Pitaevskii and S. Stringari, *Theory of Bose-Einstein condensation in trapped gases*, *Rev. Mod. Phys.* **71** (1999) 463.
- [12] E. R. I. Abraham, W. I. McAlexander, C. A. Sackett and R. G. Hulet, *Spectroscopic Determination of the s-Wave Scattering Length of Lithium*, *Phys. Rev. Lett.* **74** (1995) 1315.
- [13] S. Stringari, *Collective Excitations of a Trapped Bose-Condensed Gas*, *Phys. Rev. Lett.* **77** (1996) 2360.
- [14] Y. Castin and R. Dum, *Bose-Einstein Condensates in Time Dependent Traps*, *Phys. Rev. Lett.* **77** (1996) 5315.
- [15] Y. Kagan, E. L. Surkov and G. V. Shlyapnikov, *Evolution of a Bose-condensed gas under variations of the confining potential*, *Phys. Rev. A* **54** (1996) R1753.
- [16] F. Dalfovo, C. Minniti, S. Stringari and L. Pitaevskii, *Nonlinear dynamics of a Bose condensed gas*, *Physics Letters A* **227** (1997) 259–264.
- [17] J. R. Abo-Shaeer, C. Raman, J. M. Vogels and W. Ketterle, *Observation of Vortex Lattices in Bose-Einstein Condensates*, *Science* **292** (2001) 476 [<https://science.sciencemag.org/content/292/5516/476.full.pdf>].