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# Dynamics and excitations of Bose-Einstein condensates

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Academic dissertation

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## Preface

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Helsinki, December 19 2001

*Jani-Petri Martikainen*

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## Abstract

In this thesis I study some dynamical properties of Bose-Einstein condensates. Unlike superfluid He or superconductors, two other systems where Bose-Einstein condensation plays an essential role, the condensates in question are dilute and weakly interacting. Therefore they can be well understood from a microscopic theory and treated without too many approximations. They also provide a uniquely controlled environment for studying many important phenomena, such as spontaneous symmetry breaking and superfluidity.

In a scalar condensate the  $U(1)$  symmetry is broken which implies a complex-valued order parameter, the condensate wavefunction. This kind of condensate can have quantized vortices that play an important role in the breakdown of superfluidity. In this thesis I investigate vortex dynamics as well as shortly discuss a more exotic structure called “a coreless vortex” that can exist in a spinor condensate. While in a scalar condensate the breakdown of superfluid flow involves the creation of vortices, I will demonstrate that the breakdown of superfluid flow in a spinor condensate involves the creation of coreless vortices.

In an optical trap all different magnetic substates ( $m$  states) of some hyperfine  $F$  manifold can be trapped and thus the spin degree of freedom is not necessarily frozen and the system is described with a spinor. Normally the  $U(1)$  symmetry is broken, but topological properties of a spinor condensate can be more complex and entirely new topological excitations, such as monopoles and skyrmions, are expected. I find spinor condensates extremely interesting, promising, and rich area of research and therefore, I devote a large fraction of my thesis to study their properties. Some of the results in this thesis concerning spinor condensates, such as soliton stability, flow instability, and skyrmion dynamics, are previously unpublished.

## List of publications

This thesis consists of an introductory part, followed by five research publications. The introductory part includes some previously unpublished material.

- I *Bose-Einstein condensation in a shallow trap*  
J.-P. Martikainen  
Physical Review A **63**, 043602 (2001)
- II *Comment on “Bose-Einstein condensation with magnetic dipole-dipole forces”*  
J.-P. Martikainen, Matt Mackie, and K.-A. Suominen  
Physical Review A **64**, 037601 (2001)
- III *Generation and evolution of vortex-antivortex pairs in Bose-Einstein condensates*  
J.-P. Martikainen, K.-A. Suominen, L. Santos, T. Schulte, and A. Sanpera  
Physical Review A **64**, 063602 (2001)
- IV *Collective excitations in an  $F = 2$  Bose-Einstein condensate*  
J.-P. Martikainen and K.-A. Suominen  
Journal of Physics B **34**, 4091 (2001)
- V *Creation of a monopole in a spinor condensate*  
J.-P. Martikainen, A. Collin, and K.-A. Suominen  
submitted for publication

## Summary of the original publications

- I Usually the trap for the condensate atoms is a parabola or is approximated as such. It is not clear how well this approximation works in shallow optical traps, relevant for spinor Bose-Einstein condensates. In this paper I look into this matter and calculate condensate fraction, chemical potential, and the frequencies of the low lying collective excitations in a Gaussian shaped trap. Also, I compare these results to those obtained with the parabolic approximation and observe that differences can be noticeable.
- II We study condensates with dipole-dipole interactions and calculate the instability threshold in three different ways. Serious errors in often quoted paper are discovered.
- III We explore the creation and dynamics of vortices in a toroidal trap. Vortices are created using the instability of a soliton in two dimensions. Due to the restricted geometry the vortex anti-vortex dynamics is very different to the homogeneous gas. We explain the vortex dynamics using the method of images.
- IV We apply Bogoliubov theory to homogeneous  $F = 2$  condensate to calculate elementary excitations and conclude that all ground-state excitations have either Bogoliubov form or free-particle form (with a possible gap). We also observe the importance of spin-exchange terms for the cyclic state and consequently the importance of a well defined phase relationship between different  $m$  states.
- V We suggest a method to create a monopole in a spinor condensate and study how to observe it. Also, we investigate the dynamics of a monopole in a spin-1 condensate and observe some analogies to vortex precession in a scalar condensate.

## **Contribution by the author**

My role was central in all papers. I wrote all the programs, did all the computer simulations, and analytical work in all the papers except in paper III. In the paper III the method of images was applied to the vortex dynamics by L. Santos, T. Schulte, and A. Sanpera. My role was also essential in writing the papers.

# 1 Introduction

Most everyday phenomena involve interaction between light, or generally speaking an electro-magnetic field, and matter. Therefore it is hardly surprising that a large fraction of physics has been (and still is) related to light, matter and their interactions.

The question as to the nature of light has been addressed by the most famous physicists. Newton was a prominent proponent of the corpuscular theory of light, a theory that described light as particles along the lines of the atomic theory of matter. This was challenged from the beginning by Huygens and many others who favored a notion that light is really a wave phenomenon. Young's double slit experiment convinced most scientists that Newton had it wrong. The last nail in the coffin of a corpuscular theory was hammered by Maxwell. His theory of electro-magnetism predicted electromagnetic waves that had just the properties light had. Or so it was thought. Max Planck had to postulate a quantum of light to explain the spectra of black body radiation correctly and Albert Einstein explained photo-electricity assuming a particle of light carrying a certain amount of energy and being absorbed by the electron in the atom. A confusion as to the nature of light was back and has stayed with us ever since. Light behaves as a particle or as a wave, depending on what sort of experiments one conducts (*i.e.* what sort of interactions there are between the em-field and its surroundings).

And as if this was not enough, there were more puzzling results to come. The particle nature of matter was not seriously questioned at the beginning of the 20th century. From a large number of experiments and from the new theory of statistical physics one had deduced that matter consists of atoms. While the atoms were proved to be not quite so indivisible as Democritus had taught, for most practical reasons their role as building blocks of matter was beyond doubt. With no experiments on individual atoms, the belief that atoms would behave according to the dictates of Newtonian mechanics was generally accepted. Atom has a mass, position, and some velocity. There are forces acting on the atom and these forces change the velocity and the position of the atom in a known manner. And that is all there is! Louis de Broglie's idea that you should give a massive particle some wavelength, which implies delocalization and interference phenomena, was revolutionary. It was later embedded into the structure of quantum mechanics, the theory which explains most atomic phenomena, and it has been verified in many experiments. Not only is there wave-particle duality for light, but also for matter.

In this thesis I investigate certain dynamical properties of dilute Bose-Einstein condensates [1–3]. Bose-Einstein condensates (BEC:s) are coherent sources of atoms and they enable us to explore the analogies between light and matter even further. With BEC:s coherent matter wave sources (atom lasers) can be created and matter wave optics will come even closer to normal optics with light. We used to have coherent light sources, and mirrors and beam splitters made of atoms. We now have also coherent atom sources and mirrors and beam splitters made of light!

From the fundamental point of view condensates are extremely interesting. **The microscopic theory** [4] of BEC in a dilute gas is fairly well **understood** and, perhaps equally important, can be solved and the solution is expected to be in quantitative agreement with experiments. In condensates one can study a **phase transition** that gives rise to a **symmetry breaking** as the condensate acquires some unknown, but well defined phase. The BEC is a macroscopic system showing signs of **coherence** and **decoherence** allowing us to probe these fundamentally important properties of quantum systems in a controlled way. The BEC is also a **superfluid** and in a spinor condensate **spin-gauge symmetry** [5,6] is expected to play a very interesting role in our efforts to understand superfluidity in systems with topologically more complicated order parameters. The BEC offers a way to investigate topological excitations such as **quantized vortices** [7], **vortex lattices** [8,9], **skyrmions** [10,11], and **monopoles** [12] and also other excitations such as **solitons** [13,14] and **collective excitations** [15–17] experimentally. If this is not enough to convince the reader of the richness of this field, he/she should also note that the dynamics of condensates are governed by a nonlinear equation, which allows for many phenomena that have, until now, been encountered only in the field of non-linear optics. These include such fascinating phenomena as **four-wave-mixing** [18–21] and **phase-conjugation** [22].

In this thesis my emphasis is on the dynamics and excitations of Bose-Einstein condensates. These are studied in the mean field approximation by postulating a broken  $U(1)$  gauge symmetry (additional symmetries might exist in spinor condensates, see Section 3.6) and an accompanying complex valued order parameter, the condensate wavefunction. It can be shown that the time-evolution of the order parameter (in zero temperature) obeys a nonlinear Schrödinger equation also known as the **Gross-Pitaevskii equation** [23–25]. The validity of this equation has been experimentally tested under many different circumstances and it has been shown to be very precise.

A word of caution is still in place. In a realistic experiment there will naturally be some dissipation and this can be modeled with the Gross-Pitaevskii equation only phenomenologically (with imaginary time, for example). In an interacting Bose gas there will also be some non-condensate atoms, but at low enough temperatures the condensate fraction in a dilute-alkali gas can be very close to unity [4]. The non-condensate atoms can be included into the theory, but with the inclusion of the non-condensate atoms the computational demands will grow dramatically and only the case of the static mixture of the condensate and non-condensate atoms has been solved in some detail [26–28]. Given these warnings we can conclude that there are conditions when the Bose-Einstein condensate can be well described with a Gross-Pitaevskii equation and a complex valued wavefunction.

Considering small perturbations around some state one can calculate the excitation spectrum of the Bose-Einstein condensate. The excitation spectrum determines whether or not the condensate behaves as a superfluid, *i.e.* a fluid flowing without friction. Energetic (thermodynamic) stability of the flow requires a spectrum of elementary excitations, *i.e.* phonon spectrum, that is linear in momentum. For a weakly interacting scalar-condensate it has been shown [29] that the spectra behaves precisely in a way required for a superfluid. In one of the papers (paper IV) included in this Thesis we calculate the spectrum of elementary excitations also for a homogeneous spin-2 spinor condensate and observe that many properties of the scalar condensates are similar to the properties of order parameters with more complex topological properties. Especially the functional form of the spectra seems to be universal.

The excitation spectra can also predict the dynamical instability of certain states, for example soliton states in two dimensions. A signature of the dynamical instability is a complex valued excitation energy (with positive imaginary part). Excitations with complex eigenvalues can grow exponentially and drive the system far away from the initial state. At some point the linearization of the Gross-Pitaevskii equation fails and to predict the final state of the system one has to solve the Gross-Pitaevskii equation without approximations, and usually numerically. In this thesis I demonstrate how to calculate excitation spectra by linearizing Gross-Pitaevskii equations and apply this technique to study excitations around a soliton solution of a spin-1 spinor condensate.

A lot of my effort has gone into solving the Gross-Pitaevskii equation numerically. Typically the equations are so complex that analytical results are nearly impossible and not worth pursuing. Among other things the

Gross-Pitaevskii equation will be used to describe vortex dynamics in two dimensions and study the dynamics of the monopole and the skyrmion in a spin-1 spinor condensate.

A multicomponent spinor-condensate can display “spin-gauge” symmetry [5, 6], which implies that the superfluid velocity does not only depend on the gauge phase gradients, but also on the local spin rotations. This symmetry can have non-trivial consequences. For example, under certain conditions a BEC with a vortex can be a ground state even in the absence of a rotating trap [5]. Also for certain (ferromagnetic) states coreless vortices are allowed. This is in marked contrast to scalar condensates whose density must vanish at the vortex core due to a divergent superfluid velocity. In a spinor condensates spin-rotation can be used to have a vortex without divergent superfluid velocity at the vortex core.

Spinor condensates can be trapped in optical dipole traps [30], which are insensitive to the magnetic quantum number  $m$  of some hyperfine manifold  $F$ . These traps are much more shallow than magnetic traps typically used in BEC experiments and it is not clear how well they can be approximated as parabolic, an approximation usually done in this field. In this thesis I also explore the limits of parabolic approximation and demonstrate that this approximation can fail under reasonable experimental parameters.

This thesis is organized as follows. In Chapter 2 I present the “canonical” theory of Bose-Einstein condensation. This includes the formalism to study non-interacting BEC, the derivation of the Gross-Pitaevskii equation and the Bogoliubov theory of elementary excitations. I also briefly discuss the behavior of the condensate when condensate atoms interact via anisotropic long-range interactions (Sec. 2.4).

I give spinor condensates a chapter of their own, namely Chapter 3. There I present the model (Sec. 3.1) and discuss the ground state properties (Sec. 3.2). Linearization of the Gross-Pitaevskii equations is demonstrated in Section 3.3 and applied to study soliton stability in a spinor condensate. Effects due to the spin-gauge symmetry and the stability of the superfluid flow in spinor condensates are discussed in Sections 3.4 and 3.5. Topological properties of the order parameter are discussed in Section 3.6 and I end my Thesis with a summary and some concluding remarks in Chapter 4.

## 2 Canonical theory of Bose-Einstein condensate

In this chapter I present the standard theory of weakly interacting Bose-Einstein condensate. I introduce the theory of ideal Bose gas and also derive the Gross-Pitaevskii equation, the equation that forms the back bone of most studies in this thesis. To give the necessary tools to understand research in this field I also outline the Bogoliubov theory for excitations. I conclude this chapter with a short discussion on the role of contact interaction approximation in Bose-Einstein condensate.

### 2.1 Noninteracting condensate

The first step into the studies of Bose-Einstein condensation is naturally the study of noninteracting particles. Usually the text book examples of BEC only deal with the homogeneous system studied by Bose and Einstein [31, 32]. With an eye on the recent experiments, this case is somewhat irrelevant and it is more useful to study BEC in a trap. The textbook approach usually involves the calculation of the density of states. For a general potential this calculation can be difficult and analytic results might be impossible. For the parabolic trapping potential the density of states is known analytically and the condensate fraction can be calculated in the same way as for a homogeneous system, but instead of following the normal “textbook” approach I present the method used (for example) in the book by Pethick and Smith [33] since this method is easier to use with more complicated trapping potentials.

The phase space density of the ideal Bose gas is given by

$$f(\mathbf{r}, \mathbf{p}) = \frac{1}{\exp(\beta K) - 1}, \quad (1)$$

where  $K = H - \mu N$  and  $H$  is the Hamiltonian.  $\beta = 1/k_B T$ , where  $k_B$  is Boltzmann’s constant and  $T$  is the temperature. Let us use the continuum approach and therefore ignore the discrete nature of the motional states of a trapped atom. If the trap has only a few eigenstates, the continuum approach fails and the system should be modeled using a discrete spectrum. The Hamiltonian for a trapped atom is  $H = \frac{p^2}{2m} + V_{trap}(x, y, z)$  and below the critical temperature the chemical potential vanishes (in the continuum approach),

The number of noncondensed atoms  $N_T$  is the integral of the phase-space density over both momentum and position space (condensed atoms

occupy the lowest energy level and are ignored in the continuum approximation),

$$N_T = \frac{1}{(2\pi\hbar)^3} \int \int d\mathbf{p} d\mathbf{r} f(\mathbf{r}, \mathbf{p}). \quad (2)$$

Since the condensate vanishes at the transition temperature, the transition temperature can be calculated by setting  $N_T$  equal to the number of particles  $N$  and solving for the temperature.

For a parabolic trapping potential with trapping frequencies  $\omega_x$ ,  $\omega_y$ , and  $\omega_z$  the integral (2) can be simply calculated and the transition temperature is given by

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

where  $\zeta(n)$  is the Riemann  $\zeta$ -function. Using this result the condensate fraction as a function of temperature takes a simple form

$$\frac{N_c}{N} = 1 - \left( \frac{T}{T_c} \right)^3. \quad (4)$$

For homogeneous system the exponent would be 3/2 instead of 3 [33].

In paper I I studied the problem of BEC in a Gaussian potential. In that case the integral (2) cannot be calculated analytically, but numerical studies showed that the transition temperature could be much larger than transition temperature predicted when the Gaussian potential is approximated as a parabola. Qualitatively one can understand this behavior by remembering that in a shallow trap we only have a finite number of states. If the trap is shallow enough there is only one bound state and there are no bound states accessible to thermal atoms. Therefore all atoms must be in the lowest state, *i.e.* in a condensate and the condensate fraction must tend to unity as the trap depth is lowered. Of course, keeping an atom number constant in a realistic experiment can be quite a challenge. Also, the continuum approximation breaks down for traps with only few states, but the general behavior of the condensate fraction can be understood in this way. In paper I I also showed that the condensate fraction as a function of trap depth behaved qualitatively differently when the potential was approximated as a parabola.

## 2.2 Order parameter and Gross-Pitaevskii equation

A gas of bosons makes a transition into a BEC when the phase space density becomes of the order of one. When the transition occurs the gauge

symmetry is spontaneously broken, and the condensate acquires some well defined, although unknown, phase. This interpretation of the phase transition is very common, but it should be noted that the act of measurement can also give the appearance of symmetry breaking [34, 35]. The order parameter of the system is the condensate wavefunction  $\Phi$  [4], which is defined as an expectation value of the atomic annihilation operator  $\hat{\psi}$ . The condensate wave function is a classical field with a given amplitude and phase. It also characterizes the off-diagonal long-range behavior of the single-particle density matrix  $\rho_1(\mathbf{r}', \mathbf{r}) = \langle \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}) \rangle$ , since asymptotically

$$\lim_{|\mathbf{r}' - \mathbf{r}| \rightarrow \infty} \rho_1(\mathbf{r}', \mathbf{r}) = \Phi^*(\mathbf{r}')\Phi(\mathbf{r}). \quad (5)$$

Strictly speaking the expectation value of the annihilation operator can be non-vanishing only if the wavefunction of the system is an appropriate superposition of states corresponding to different number of atoms. Since the particle number is a conserved quantity this result is physically dubious. In practice this subtle point rarely matters and the definition of the order parameter as an expectation value of an annihilation operator streamlines many calculations. For enlightening discussion of condensate order parameter I recommend the review article by Leggett [36].

The many body Hamiltonian for system of  $N$  bosons is

$$\hat{H} = N \int d\mathbf{r} \left[ \hat{\psi}^\dagger \left( -\frac{\hbar^2}{2m} \nabla^2 + V_{trap} \right) \hat{\psi} + \frac{g}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \right], \quad (6)$$

where we have assumed that bosons are trapped and interact via contact interaction with some strength  $g = \frac{4\pi\hbar^2}{m}a$ , proportional to the scattering length  $a$ . (In Section 2.4 we discuss shortly the mean field theory without assuming a contact interaction.) The creation and annihilation operators for bosons satisfy the commutation relation

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'). \quad (7)$$

Once we know the Hamiltonian and the commutation relations it is a simple matter to derive the Heisenberg equation of motion for the annihilation operator:

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, t) = [\hat{\psi}, \hat{H}] = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{trap} + g\hat{\psi}^\dagger \hat{\psi} \right] \hat{\psi}. \quad (8)$$

In a broken symmetry description one assumes that the annihilation operator can be described as a sum of the “large” complex valued order parameter

$\Phi$  and “small” fluctuation  $\hat{\phi}$ . In the simplest case we can set the fluctuation to zero and get the Gross-Pitaevskii (GP) equation [23–25]

$$i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) + g|\Phi(\mathbf{r}, t)|^2 \right] \Phi(\mathbf{r}, t), \quad (9)$$

where the condensate wavefunction is normalized to the number of particles. This equation is the backbone of most of the studies in this thesis.

Gross-Pitaevskii equation can also be obtained a using variational procedure. The Hartree-Fock ansatz for the  $N$ -particle ground state is [36]

$$\Psi_N(\mathbf{r}_1 \cdots \mathbf{r}_N) = \prod_{i=1}^N \phi(\mathbf{r}_i), \quad (10)$$

where  $\phi$  is normalized to unity. Using this ansatz the expectation value of the energy takes the form

$$\begin{aligned} E[\phi] &= N \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla \phi(\mathbf{r})|^2 + V_{trap}(\mathbf{r}) |\phi(\mathbf{r})|^2 \right] \\ &\quad + \frac{1}{2} N(N-1)g \int d\mathbf{r} |\phi(\mathbf{r})|^4. \end{aligned} \quad (11)$$

Minimizing this energy subject to the constraint of normalization of  $\phi$  and ignoring the difference between  $N$  and  $N-1$  (experimentally  $N$  is  $10^5-10^7$ ) we get the Hartree equation for condensed bosons,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) + Ng|\phi(\mathbf{r})|^2 \right] \phi(\mathbf{r}, t) = \mu \phi(\mathbf{r}). \quad (12)$$

Multiplying Eq. (12) by  $\phi^*(\mathbf{r})$ , integrating over  $\mathbf{r}$ , and remembering that  $E$  is stationary against small variations of  $\phi(\mathbf{r})$ , we find that  $\mu = \delta E / \delta N$  is the chemical potential. If we define  $\Phi(\mathbf{r}) = \sqrt{N}\phi(\mathbf{r})$ , Eq. (12) is the time-independent version of the GP-equation (9).

The time-dependent GP-equation can also be derived variationally. This is done by calculating

$$i\hbar \frac{\partial \phi}{\partial t} = \frac{\delta E}{\delta \phi^*}. \quad (13)$$

This procedure gives the time-dependent GP-equation (9), but makes a nontrivial assumption. Namely, while calculating the time-dependent GP-equation variationally we assume that the number of condensate atoms is not a function of time. In reality interactions deplete the condensate and

the time-dependent GP-equation is only an approximation [37] – although often a very good one.

The Hamiltonian of the GP-equation has a  $U(1)$  gauge symmetry and consequently the phase of a lone condensate does not carry much meaning. Only a relative phase is of importance. While global phase-change is trivial, a local phase-change can have far reaching consequences. To preserve the single valuedness of the wave function, the phase change  $\Delta\phi$  when going around a closed contour must be  $2\pi N$ , where  $N$  is an integer called the winding number. When  $N \neq 0$  we have quantized vortices.

We studied the dynamics of a vortex-antivortex pair in a toroidal trap in paper III using the time-dependent GP-equation. In our setup the restrictions due to the trapping geometry were clearly visible. In a homogeneous system two vortices of opposite circulation move parallel, since each vortex will move with the velocity of the other one. In our system vortices moved along the torus and bounced from each other. While the GP-equation provides an accurate description, we found that the vortex dynamics could be well described assuming a homogeneous system with appropriate boundary conditions. The effects due to inhomogeneity were small and the question still remains: When does the inhomogeneity play an important role? Also the vortex dynamics in three-dimensional systems is an interesting topic for further research.

### 2.3 Bogoliubov- de Gennes equations and elementary excitations

We derived the Gross-Pitaevskii equation (9) by assuming that only one state is occupied and by describing such a state by a complex valued wavefunction. This approach is always an approximation since in an interacting Bose gas many states will be occupied even at zero temperature. A natural extension from the simple Gross-Pitaevskii theory is to assume that the deviations from the GP-theory are small. This is the essence of the Bogoliubov theory for a degenerate Bose gas.

We write the annihilation operator for the atoms as  $\hat{\psi} = \Phi + \hat{\phi}$ , where the first term is (presumably) a large complex valued wavefunction of the condensate and the last term is a (small) fluctuation. Bogoliubov's great insight was to make a canonical transformation of the fluctuation in such a manner that (in the homogeneous case) this quantum many body problem can be solved analytically [29]. The terms in the Hamiltonian that are

second order in  $\hat{\phi}$  can be diagonalized by the transformation

$$\hat{\phi}(\mathbf{r}) = \sum_j \left[ u_j(\mathbf{r})\hat{\alpha}_j + v_j^*(\mathbf{r})\hat{\alpha}_j^\dagger \right], \quad (14)$$

where  $\alpha_j$  is the annihilation operator for the elementary excitations.

If we define the condensate density as  $n_c = |\Phi|^2$ , the noncondensate density as  $n_T = \langle \hat{\phi}^\dagger \hat{\phi} \rangle$ , and anomalous terms  $m_T = \langle \hat{\phi} \hat{\phi} \rangle$ , and  $\tilde{m}_T = \langle \hat{\phi}^\dagger \hat{\phi}^\dagger \rangle$  then it can be shown that first order terms in  $\hat{H}$  vanish if the condensate wavefunction obeys the generalized GP equation:

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{trap} + g(n_c + 2n_T + \tilde{m}_T) \right] \Phi = \mu \Phi. \quad (15)$$

The second order terms in  $\hat{\phi}$  are diagonalized by the canonical transformation (14) if the amplitudes  $u_j$  and  $v_j$  are solutions of the Bogoliubov-de Gennes equations

$$\begin{aligned} \hat{A}u_j(\mathbf{r}) + \hat{B}v_j(\mathbf{r}) &= \epsilon_j u_j(\mathbf{r}) \\ \hat{A}v_j(\mathbf{r}) + \hat{B}u_j(\mathbf{r}) &= -\epsilon_j v_j(\mathbf{r}), \end{aligned} \quad (16)$$

where  $\hat{A} = -\frac{\hbar^2}{2m} \nabla^2 + V_{trap} - \mu + 2g(n_c + n_T)$ ,  $\hat{B} = g[n_c + m_T]$ , and  $\epsilon_j$  is the energy of the elementary excitation. These equations can be solved using various approximations [38], but in this thesis I use only the most simple approximation, namely ignoring the thermal component altogether. This is often a good approximation, especially well below the critical temperature. In paper III I also focused only on the lowest lying excitations.

In practice Eq (16) could be solved (for example) in a gapless Popov-approximation. In this approximation one ignores the anomalous terms and solves the generalized GP-equation in combination with (16) self consistently. The gaplessness of the approximation means that the spectra has an excitation with zero energy (Goldstone mode), which coincides with the solution of the generalized GP-equation. If one keeps the anomalous terms one is dealing within the Hartree-Fock-Bogoliubov (HFB) framework. In a variational sense, it is the best single-particle approximation for a Bose-condensed system [39], but unfortunately it does not obey the Hugenholtz-Pines theorem [40] that requires gapless excitation spectra.

Numerical solution of the Bogoliubov- de Gennes equations with finite differences leads to a sparse eigenvalue problem that can be solved with suitable numerical libraries (ARPACK was used in [28]). Once the amplitudes  $u$  and  $v$  have been solved (and normalized) the noncondensate density

can be calculated from

$$n_T(\mathbf{r}) = \sum_{j=1} \left[ N_j |u_j(\mathbf{r})|^2 + (N_j + 1) |v_j(\mathbf{r})|^2 \right], \quad (17)$$

where  $N_j$  is the occupation of the state and can be calculated from the Bose-Einstein distribution

$$N_j = \frac{1}{\exp(\beta\epsilon_j) - 1}. \quad (18)$$

It should be noted that in Eq. (17) the sum is set to start from 1 as an indication that the mode with zero energy (Goldstone mode) should not be included in the sum.

To incorporate temperature dependence in the problem increases the computational work dramatically but the static case is not beyond the capacity of modern computers. In this case one has to solve the condensate density and the density of the thermal cloud self consistently [27, 28, 41].

For the homogeneous BEC ( $V_{trap} = 0$ ,  $\Phi(\mathbf{r}) = \sqrt{n}$ ) the Bogoliubov-de Gennes equations can be solved analytically. In this case  $u_j(\mathbf{r})$  and  $v_j(\mathbf{r})$  are plane waves:  $u_j(\mathbf{r}) = A \exp(i(\mathbf{k} \cdot \mathbf{r} - \epsilon_j t/\hbar))$ ,  $v_j(\mathbf{r}) = B \exp(i(\mathbf{k} \cdot \mathbf{r} - \epsilon_j t/\hbar))$ . Explicit solution of (16) then yields the famous Bogoliubov dispersion relation

$$\epsilon = \sqrt{\frac{\hbar^2 k^2}{2m} \left( \frac{\hbar^2 k^2}{2m} + 2ng \right)}. \quad (19)$$

Therefore the spectra of elementary excitations in a homogeneous BEC has the sound-wave form  $\hbar c_s k$  for small values of  $k$ , but takes a single particle form  $\frac{\hbar^2 k^2}{2m}$  at the opposite limit of large momentum.

By analyzing the energy conservation in a moving liquid one can show [42] that the flow becomes thermodynamically unstable when the liquid velocity exceeds

$$v_c = \min_p \frac{\epsilon(p)}{p}, \quad (20)$$

where  $\epsilon(p)$  is the energy of the excitation with the momentum  $p = \hbar k$  in the laboratory frame. If the liquid velocity is less than  $v_c$  there are no states with a lower energy than that of the initial state. In the Bogoliubov theory the critical velocity is the sound velocity and the system is superfluid in the presence of repulsive interactions (positive scattering length) between atoms.

One should note that at the heart of the Bogoliubov theory lies the linearization of the Gross-Pitaevskii equation. This linearization is not

only useful to get the spectra of elementary excitations and the properties of the thermal cloud, two things of interest in Bogoliubov theory, but the same method can also be used to study dynamical stability of the steady-state solutions. In this thesis I study dynamical stability of certain steady states such as a soliton, for example. In this case one can extract useful information from the linearization of the Gross-Pitaevskii equation (see section 3.3). As a by-product of linear stability analysis one also obtains a linear response theory for the condensate, a theory of great importance when interpreting many experiments which apply a weak perturbation to the condensate.

## 2.4 Long-range interactions

Typically interactions between Bose condensed atoms is described only in terms of the scattering length. It is implicitly assumed that interactions can be described with isotropic contact interactions with some strength proportional to the scattering length. Often this works quite well and there is little reason to suspect its validity for the BEC:s currently available. But sometimes scattering theory results in a divergent scattering length or interactions might be anisotropic. The notable example of such an interaction is the dipole-dipole interaction. In references [43–47] the effect of dipole-dipole interactions in a Bose condensate were studied with a mean field theory. This consists of studying the GP-equation with the additional non-local term to include dipolar interactions.

$$i\hbar\frac{\partial\Psi}{\partial t} = \left\{ -\frac{\hbar^2\nabla^2}{2m} + \frac{1}{2}m\omega_0^2(x^2 + y^2 + \gamma^2z^2) + \frac{4\pi\hbar^2a}{m}|\Psi|^2 + \int V(\mathbf{r} - \mathbf{r}')|\Psi(\mathbf{r}')|^2d^3\mathbf{r}' \right\} \Psi. \quad (21)$$

Here  $a$  is the s-wave scattering length and wavefunction is normalized to the number of particles. The long-range potential due to the magnetic dipole-dipole interaction is given by

$$V(\mathbf{r} - \mathbf{r}') = \frac{\mu_0}{4\pi} \frac{\bar{\mu}_1(\mathbf{r}) \cdot \bar{\mu}_2(\mathbf{r}') - 3\bar{\mu}_1(\mathbf{r}) \cdot \mathbf{u} \bar{\mu}_2(\mathbf{r}') \cdot \mathbf{u}}{|\mathbf{r} - \mathbf{r}'|^3}, \quad (22)$$

where  $\mathbf{u} = (\mathbf{r} - \mathbf{r}')/|\mathbf{r} - \mathbf{r}'|$  and  $\mu_0$  is the magnetic permeability of the vacuum. Let us assume that all the magnetic moments point in the same direction ( $z$ -direction), *i.e.*  $\bar{\mu}_1 = \bar{\mu}_2 = \mu\hat{z}$ .

It should be noted that electric-dipole interactions are formally similar to magnetic ones. Some molecules have large electric dipoles and therefore

the theory of dipolar condensates might well find applications in the emerging field of molecular condensates. Also the electric dipole of the atoms will depend on the external electric field and if this field is strong enough, the dipolar interactions have to be taken into account.

The mean field theory presented above predicts modifications of the condensate density that can be dramatic. The dipole-dipole interactions causes the condensate to contract in the direction orthogonal to  $\bar{\mu}$ . In paper II we noticed that if the dipolar interaction is too large, it can even induce an instability that leads to the condensate collapse. This phenomenon is analogous to the collapse of the condensate when the scattering length is negative [48, 49].

In Fig. 1 I show an (unpublished) example of the possible dynamical behavior of the chromium condensate with scattering length 5% above the critical value and a soliton in the z-direction. the number of particles was 100000 and the trap frequency for the spherical trap was  $\omega = 2\pi 150$  Hz. One can clearly see a rapid decay of the soliton into two vortex rings, after this the inner vortex is destroyed as it merges with the second ring vortex. The decay of the three dimensional soliton into a vortex ring has been recently observed [50] and my results are therefore not all that surprising. However, what is somewhat unexpected is the qualitative change in the behavior if the soliton would have been in the  $xy$ -plane. In this case a soliton is stable considerably longer than in Fig. 1. It seems likely that in the absence of other factors it is stable indefinitely. Therefore not only do the dipolar interactions modify the condensate density dramatically, but also its excitation spectra. In particular, they can even stabilize structures that would normally be unstable.

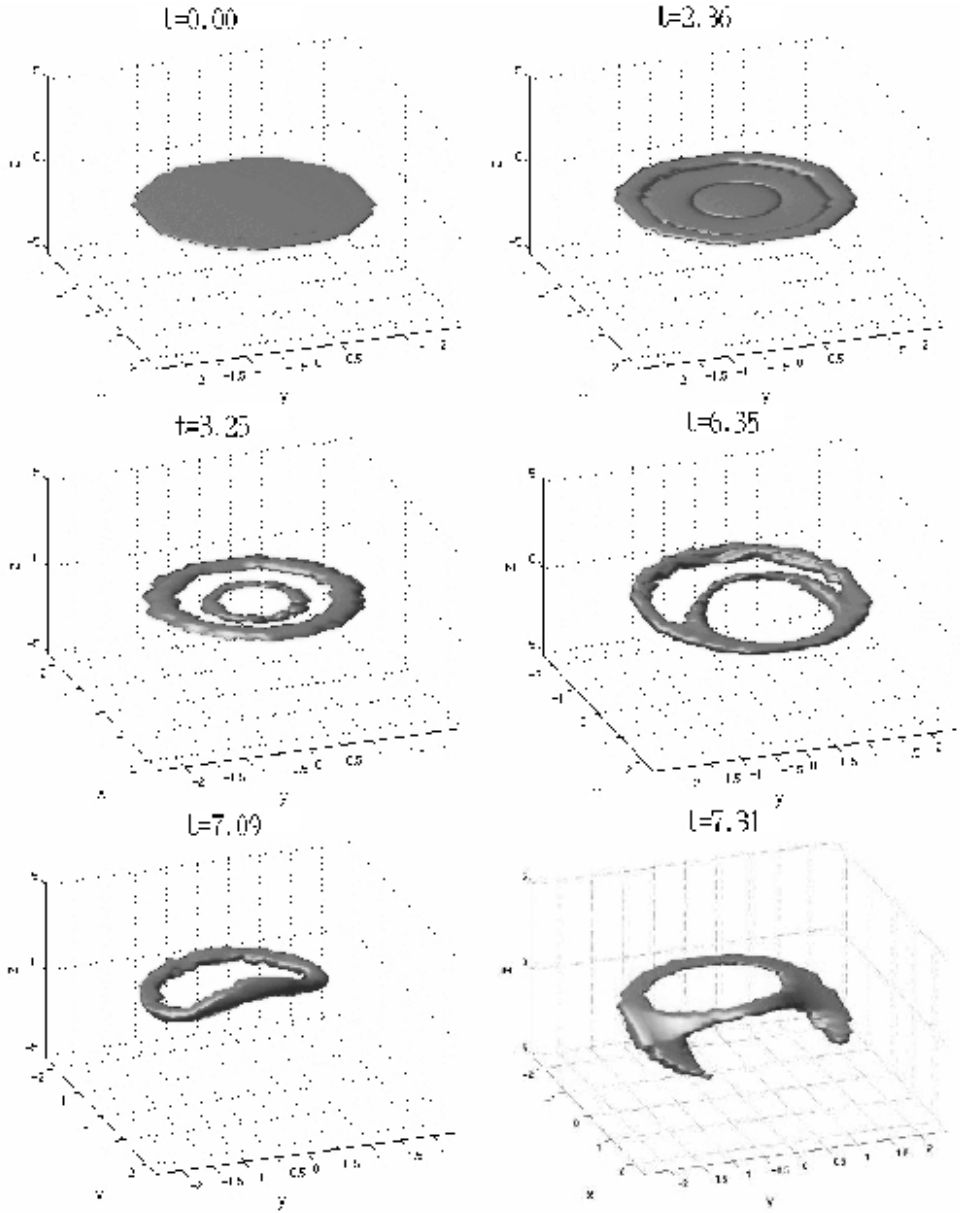


Figure 1: Soliton decay in a chromium condensate in the presence of dipolar interactions when trapping frequency is  $\omega = (2\pi) 150$  Hz, number of particles is 100000, and the scattering length is 5% above the critical value. Figure shows the low density regions inside the condensate.

### 3 Spinor condensates

In a magnetic trap only some of the  $2f + 1$  different  $m$  states of hyperfine spin  $f$  can be trapped and their degeneracy is lifted. Even though the atoms carry spin, their spins are frozen and therefore they behave almost as scalar particles. Some interesting effects might arise from the local spin-gauge symmetry [5], but usually such effects are small and can be ignored. This is in a marked contrast to an optical trap, where all states can be trapped and spin-degree of freedom is not necessarily frozen. In an optical trap the condensate should be described with a spinor having  $2f + 1$  components and this makes such systems very rich in new physics.

The condensate was trapped in an optical dipole trap for the first time in MIT in 1998 [30] and until this day most of the experiments with spinor condensates have been done in that same group. The MIT group was the first group to tune the scattering length using the Feshbach resonance [51], they have observed spin domains [52], and have studied metastability in a spinor condensate [53]. The recent all optical formation of a  $^{87}\text{Rb}$  BEC directly in an optical trap [54] indicates new possibilities for studies of spinor condensates.

In the relevant low energy limit, the interactions between atoms must be described by a pairwise interaction that is rotationally invariant in the hyperfine spin space and preserves the hyperfine spin of the individual atoms [6]. The general form of such an interaction is

$$V(\mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2) \sum_{F=0}^{2f} g_F \sum_{M=-F}^F |F, M\rangle \langle M, F|, \quad (23)$$

where  $g_F = 4\pi\hbar^2 a_F/m$  is the strength of the interaction in each total hyperfine spin- $F$  channel. For bosons, only even  $F$ -states contribute to the sum above. This interaction forms the backbone of most studies of spinor condensates. My work is not an exception to this rule. In a magnetic field rotational invariance is not, strictly speaking, required (and  $F$  is no longer a good quantum number) and the above interaction is only an approximation. Nonetheless, at low magnetic fields for which the Zeeman shifts are much smaller than the hyperfine splitting, one can expect the rotationally invariant interaction to provide a good description of the collisional properties.

### 3.1 Mean field theory

The total hyperfine spin- $F$  state  $|F, M\rangle$  can be expanded in the basis of atomic states  $|f, m\rangle$  [55] and doing that we will be led to an interaction Hamiltonian involving only the field operators  $\psi_m$  for different  $m$ -states. If  $f = 1$  the interaction Hamiltonian is

$$\begin{aligned}
 H_I = & \frac{\lambda_s}{2} \sum_{\alpha, \beta} \int d^3r \psi_\alpha^\dagger \psi_\beta^\dagger \psi_\alpha \psi_\beta + \frac{\lambda_a}{2} \int d^3r \left( \psi_1^\dagger \psi_1^\dagger \psi_1 \psi_1 + \psi_{-1}^\dagger \psi_{-1}^\dagger \psi_{-1} \psi_{-1} \right. \\
 & + 2\psi_1^\dagger \psi_0^\dagger \psi_1 \psi_0 + \psi_{-1}^\dagger \psi_0^\dagger \psi_{-1} \psi_0 - 2\psi_1^\dagger \psi_{-1}^\dagger \psi_1 \psi_{-1} + 2\psi_0^\dagger \psi_0^\dagger \psi_1 \psi_{-1} \\
 & \left. + 2\psi_1^\dagger \psi_{-1}^\dagger \psi_0 \psi_0 \right), \quad (24)
 \end{aligned}$$

where  $\lambda_s = (g_0 + 2g_2)/3$  and  $\lambda_a = (g_2 - g_0)/3$ . The total Hamiltonian is then  $H = \hat{K} + H_{trap} + H_I$ , where  $\hat{K}$  is the kinetic energy operator and  $H_{trap}$  is due to the trapping potential. In this thesis I will also investigate the spin-2 spinor condensate using mean field theory, but since the resulting expressions are fairly long I will give the Hamiltonian explicitly only for a spin-1 condensate.

In the mean field theory (MFT) operators are replaced with complex numbers. From now on we will implicitly assume that such an approximation has already been made. Using this Hamiltonian it is a simple matter to derive the appropriate generalized GP-equations for the spinor condensate. For the spin-1 condensate GP-equations are:

$$\begin{aligned}
 i\hbar \frac{\partial \psi_1}{\partial t} &= \mathcal{L} \psi_1 + \lambda_a \left( \psi_0^2 \psi_{-1}^* + |\psi_1|^2 \psi_1 + |\psi_0|^2 \psi_{-1} - |\psi_{-1}|^2 \psi_1 \right) \\
 i\hbar \frac{\partial \psi_0}{\partial t} &= \mathcal{L} \psi_0 + \lambda_a \left( 2\psi_1^* \psi_{-1}^* \psi_0 + |\psi_{-1}|^2 \psi_0 + |\psi_1|^2 \psi_0 \right) \\
 i\hbar \frac{\partial \psi_{-1}}{\partial t} &= \mathcal{L} \psi_{-1} + \lambda_a \left( \psi_0^2 \psi_1^* + |\psi_{-1}|^2 \psi_{-1} + |\psi_0|^2 \psi_{-1} - |\psi_1|^2 \psi_{-1} \right), \quad (25)
 \end{aligned}$$

where the operator  $\mathcal{L}$  is given by

$$\mathcal{L} = -\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(\mathbf{r}) + \lambda_s \sum_{k=-1}^1 |\psi_k(\mathbf{r})|^2. \quad (26)$$

### 3.2 Ground states and fragmentation

The ground state structures of spinor condensates with spins 1 and 2 have been studied by several authors [6, 56–60]. In the MFT of a spin-1 condensate the ground state is either ferromagnetic, when the spinor is

$\zeta_F^T = (1 \ 0 \ 0)$ , or anti-ferromagnetic (polar)  $\zeta_P^T = (0 \ 1 \ 0)$ , depending on the sign of  $\lambda_a$  [6]. If  $\lambda_a$  is positive, the energy is minimized with a non-magnetized spinor, and the polar-state is the ground state. In the opposite case of negative  $\lambda_a$  the ferromagnetic spinor is favored. (In the expressions above I used the basis where the spin operator  $\hat{S}_z$  is diagonal. Naturally, in zero magnetic field, one has a freedom to make a global rotation of the spinor without any changes in physics.)

For a spin-2 condensate the situation is more complicated. In zero magnetic field we have three degenerate polar states:  $P0 = (0 \ 0 \ 1 \ 0 \ 0)$ ,  $P1 = (0 \ e^{i\phi_1} \ 0 \ e^{i\phi-1} \ 0)$ , and  $P = (e^{i\phi_2} \ 0 \ 0 \ 0 \ e^{i\phi-2})$ , where all the phase factors are arbitrary. In a magnetic field the degeneracy of the polar states is lifted and the  $P$  state has the lowest energy [57]. In addition to polar states we also have the ferromagnetic state  $F = (1 \ 0 \ 0 \ 0 \ 0)$  and finally the cyclic state  $C = \frac{1}{2}(e^{i\phi} \ 0 \ \sqrt{2} \ 0 \ -e^{-i\phi})$ , a state that does not have an analog in the spin-1 condensate.

Superficially it would seem that the cyclic state is a superposition of  $P0$  and  $P$  states. As polar states are degenerate (in zero field) one would not, perhaps, expect cyclic state to have different energy. Nevertheless, it has a different energy due to the nonlinearity of the GP equations. Some contributions to the energy that vanish for polar states show up for their superpositions (see paper IV). Which one of these three classes of states is the ground state depends on the three different scattering lengths in a fairly complicated manner [57].

In the mean field theory the operators are replaced with complex valued (“classical”) wavefunctions. In the MFT for spinor condensate one also does not put any constraints on the total angular momentum of the spins. In reality the angular momentum must be quantized, but in the MFT angular momentum can be arbitrary. This might mask some subtle effects [58, 59]. The interaction Hamiltonian for the homogeneous spin-1 condensate can be written in terms of atomic field operators,

$$\begin{aligned}
H_I = & \mu\hat{N} - \lambda_s\hat{N}(\hat{N} - 1) + \lambda_a \left( \hat{\psi}_1^\dagger\hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_1 + \hat{\psi}_{-1}^\dagger\hat{\psi}_{-1}^\dagger\hat{\psi}_{-1}\hat{\psi}_{-1} \right. \\
& - 2\hat{\psi}_1^\dagger\hat{\psi}_{-1}^\dagger\hat{\psi}_1\hat{\psi}_{-1} + 2\hat{\psi}_1^\dagger\hat{\psi}_0^\dagger\hat{\psi}_1\hat{\psi}_0 + 2\hat{\psi}_{-1}^\dagger\hat{\psi}_0^\dagger\hat{\psi}_{-1}\hat{\psi}_0 \\
& \left. + 2\hat{\psi}_0^\dagger\hat{\psi}_0^\dagger\hat{\psi}_1\hat{\psi}_{-1} + 2\hat{\psi}_1^\dagger\hat{\psi}_{-1}^\dagger\hat{\psi}_0\hat{\psi}_0 \right). \tag{27}
\end{aligned}$$

Here  $\hat{N} \equiv \hat{\psi}_1^\dagger\hat{\psi}_1^\dagger\hat{\psi}_1\hat{\psi}_1 + \hat{\psi}_0^\dagger\hat{\psi}_0^\dagger\hat{\psi}_0\hat{\psi}_0 + \hat{\psi}_{-1}^\dagger\hat{\psi}_{-1}^\dagger\hat{\psi}_{-1}\hat{\psi}_{-1}$  is the total number of atoms (conserved quantity) and  $\lambda_{s,a}$  have been redefined so that  $\lambda_{s,a} \rightarrow \lambda_{s,a}/V$  where  $V$  is the quantization volume. This Hamiltonian can be diagonalized exactly [56]. If  $\lambda_a < 0$  the exact ground state energy coincides

with the predictions of the MFT (which amounts to Hartree-Fock approximation) and the mean field ground states are exact eigenstates of  $H_I$ . If, on the other hand,  $\lambda_a > 0$ , the exact ground state does not have the same energy as the polar state. The energy difference between the mean field result and the exact one is

$$\Delta E = E_{MFT} - E_{exact} = \lambda_a N. \quad (28)$$

As the energy of the system increases as  $E \sim N^2$  the relative error tends to zero in the thermodynamic limit ( $N \rightarrow \infty$ ).

For the exact ground state the single particle density matrix defined as  $\hat{\rho}_{\alpha\beta} = \langle \psi_\beta^\dagger \psi_\alpha \rangle$  is diagonal and has in general three macroscopic eigenvalues [59]. Since the density matrix has more than one macroscopic eigenvalue the exact ground state in the anti-ferromagnetic case corresponds to a *fragmented* condensate [61]. A fragmented condensate can be well approximated (we ignore the pathological superfragmentation [59]) by the Fock state  $|N_1; N_0, N_{-1}\rangle$  and for such a state the terms in the Hamiltonian responsible for spin-mixing dynamics average to zero. Therefore spin-mixing dynamics is not to be expected for a fragmented condensate, but the numbers of particles in different  $m$  states are separately constant [36]. In this case the GP equations take the form that is often used in the literature for studies of multicomponent condensates [62]:

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + V_m(r) + \sum_n g_{m,n} |\psi_n|^2 \right) \psi_m = \mu_k \psi_m. \quad (29)$$

In paper IV we noticed that ignoring spin-mixing dynamics can have important consequences for the cyclic state of the spin-2 condensate. The chemical potential of the cyclic state depends on the spin-mixing terms and therefore on the existence of a well defined relative phase between different  $m$  states.

Possible fragmentation of the condensate is an extremely interesting topic for further research. As the error of the MFT vanishes in the thermodynamic limit the relative stability of the fragmented and the (coherent) polar state is very delicate. Experimental preparation of the spinor condensate [30] seems to leave the spinor condensate in a coherent state where the relative phase of the components is initially well defined, and not in the true ground state. At present, very little is known about the relaxation towards the true ground state and even less about the robustness of the fragmented ground state to the measurement process. For two overlapping scalar condensates it has been shown [34,35,63] that the act of measurement can give

the appearance of a relative phase between two condensates even though there was no well defined relative phase initially. One might ask whether something similar might happen for a fragmented spinor condensate.

All the discussion until now has assumed the absence of an external magnetic field. In the presence of a magnetic field the degeneracy of the  $m$  states is lifted, but if the Zeeman shifts caused by the external magnetic field are much smaller than the hyperfine splitting, we can assume that the model presented here makes sense. One only has to add a term

$$H_B = -\gamma \mathbf{B} \cdot \mathbf{S} \quad (30)$$

into the Hamiltonian to account for the magnetic field, where  $\gamma$  is the gyromagnetic ratio,  $\mathbf{B}$  is the magnetic field, and  $\mathbf{S}$  is the spin operator. If the magnetic field is taken into account, it turns out that the fragmented state might be very fragile [59]. To explore the properties of the exact ground state will require a very high degree of magnetic shielding. The experiments that might realize this are currently in progress [64].

### 3.3 Linearization and soliton stability in a spinor condensate

As linearization of the Gross-Pitaevskii equation is used in many papers included in this Thesis it is prudent to familiarize the reader with the linearization procedure by applying it to study (unpublished) the stability of the soliton in a spin-1 condensate. the Gross Pitaevskii equation

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + \frac{4\pi\hbar^2 a}{m} |\psi|^2 \psi(x, t) \quad (31)$$

with repulsive interactions (*i.e.*  $a > 0$ ) has a well known dark soliton solution

$$\psi_s(x, t) = \sqrt{n_0} \tanh(x/\xi) e^{-i\mu t/\hbar}, \quad (32)$$

where  $\xi = 1/\sqrt{4\pi a n_0}$  is the coherence length and  $\mu = \frac{4\pi\hbar^2 a}{m} n_0$  is the chemical potential. A soliton in a homogeneous system with more than one dimension is expected to be dynamically unstable and exhibit a “snake instability” [65–70]. This means that disturbances with certain wavelengths will grow exponentially and deform an initially straight soliton front into a snake-like form. Finally, as the instability takes the system away from the initial state, the soliton decays into vortices [66, 67, 69, 71] (or possibly into vortex rings in a three-dimensional system [50]).

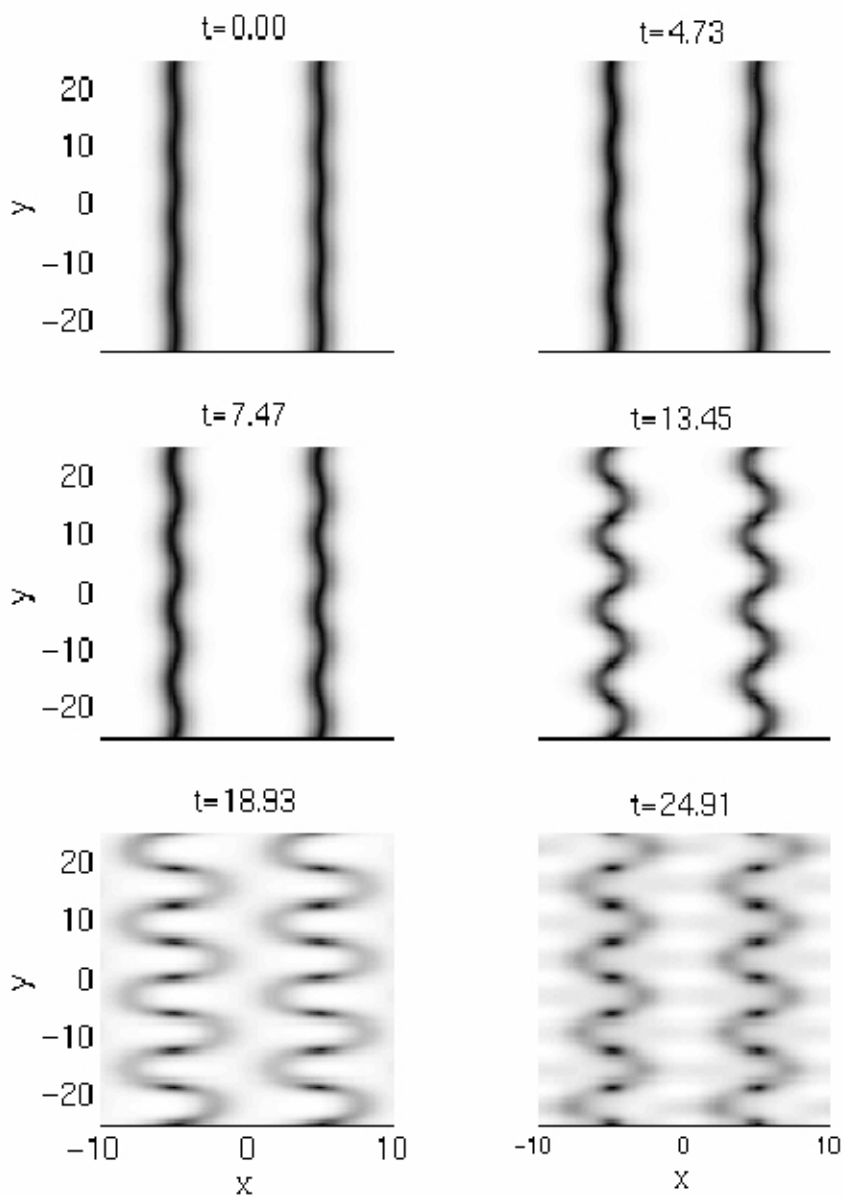


Figure 2: Snake instability of a two-dimensional soliton leads to the creation of vortices. In this figure a small disturbance was added to the initial state to speed up the instability. (Units of time and length are  $\tau = 0.19$  ms and  $l = 0.37 \mu\text{m}$ .)

Let us first study a soliton in a spin-1 condensate with antiferromagnetic interactions ( $^{23}\text{Na}$  for example). In this case a soliton in the ground state will be

$$\bar{\psi}(\mathbf{r}) = \psi_s(x) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \quad (33)$$

In order to explore excitations and stability of such a structure we linearize the Gross-Pitaevskii equations for different  $m$ -states by setting

$$\bar{\psi}(\mathbf{r}) = \begin{pmatrix} \delta\psi_1 \\ \psi_0(x) + \delta\psi_1 \\ \delta\psi_{-1} \end{pmatrix} \quad (34)$$

and ignoring all terms of higher order than one in the disturbance  $\delta\psi_m$ . To get rid of the large terms, the chemical potential must be  $\mu = \lambda_s n_0$  and with this choice we are left with three equations for the disturbances. It is natural to choose coherence length  $\xi$  as the unit of length and  $\mu$  as the unit of energy. With these choices the three equations are

$$\begin{aligned} i\delta\dot{\psi}_1 &= \left[ -\frac{1}{2}\nabla^2 + (1 + \Delta a) \tanh^2 x - 1 \right] \delta\psi_1 + \Delta a \tanh^2 x \delta\psi_{-1}^* \\ i\delta\dot{\psi}_0 &= \left[ -\frac{1}{2}\nabla^2 + 2 \tanh^2 x - 1 \right] \delta\psi_0 + \tanh^2 x \delta\psi_0^* \\ i\delta\dot{\psi}_{-1} &= \left[ -\frac{1}{2}\nabla^2 + (1 + \Delta a) \tanh^2 x - 1 \right] \delta\psi_{-1} + \Delta a \tanh^2 x \delta\psi_1^* \end{aligned} \quad (35)$$

where  $\Delta a$  is defined as

$$\Delta a = \frac{a_2 - a_0}{a_0 + 2a_2}. \quad (36)$$

Elementary excitations of the solitonic condensate are characterized by the momentum  $\mathbf{k}$  of the transverse ( $y, z$ ) motion and by the quantum number  $\nu$  of motion along the  $x$ -axis. With this in mind we write the disturbance as [70]

$$\delta\psi_m = \sum_{\nu, k} f_{m, k\nu}(x) \exp(i\mathbf{k} \cdot \mathbf{r}). \quad (37)$$

It is now straightforward to derive the equations for the amplitudes  $f_{m, k\nu}(x)$ . As the  $m = 0$  case coincides with studies done for an ordinary scalar condensate [70], let us focus only on  $m = \pm 1$  states. The equations for these amplitudes are:

$$\begin{aligned} i\frac{\partial}{\partial t} f_{1, k\nu} &= \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + (1 + \Delta a) \tanh^2 x - 1 + \frac{k^2}{2} \right] f_{1, k\nu} \\ &+ \Delta a \tanh^2 x f_{-1, -k\nu}^* \end{aligned} \quad (38)$$

$$i\frac{\partial}{\partial t}f_{-1,k\nu} = \left[ -\frac{1}{2}\frac{\partial^2}{\partial x^2} + (1 + \Delta a)\tanh^2 x - 1 + \frac{k^2}{2} \right] f_{-1,k\nu} + \Delta a \tanh^2 x f_{1,-k\nu}^* \quad (39)$$

By defining functions  $g_{k\nu}(x) = [f_{1,k\nu}(x) - f_{-1,-k\nu}^*(x)] \exp(-i\varepsilon_{k,\nu}t)$  and  $h_{k\nu}(x) = [f_{1,k\nu}(x) + f_{-1,-k\nu}^*(x)] \exp(-i\varepsilon_{k,\nu}t)$  we get the Bogoliubov-de Gennes equations

$$\varepsilon_{k,\nu} \begin{pmatrix} g_{k\nu} \\ h_{k\nu} \end{pmatrix} = \begin{pmatrix} 0 & \widehat{K}_x + V_2(x) \\ \widehat{K}_x + V_2(x) & 0 \end{pmatrix} \begin{pmatrix} g_{k\nu} \\ h_{k\nu} \end{pmatrix} \quad (40)$$

where  $V_1(x) = \tanh^2 x - 1 + k^2/2$ ,  $V_2(x) = V_1(x) + 2\Delta a \tanh^2 x$ , and  $\widehat{K}_x = -\frac{1}{2}\frac{\partial^2}{\partial x^2}$ . The solutions of these equations give the energies  $\varepsilon_{k,\nu}$  of the excitations. If the energy of an excitation is imaginary with a negative imaginary part, one expects a dynamical instability and consequently a decay of the soliton even in the absence of dissipation. It is simple to show that if  $\varepsilon_{k,\nu}$  is a solution then also  $-\varepsilon_{k,\nu}$  is a solution. Therefore the existence of an excitation with positive imaginary part implies the existence of an excitation with a negative imaginary part (and vice versa). This property is often convenient when doing numerical analysis.

In Fig. 3 I show the imaginary part of the numerically calculated spectra (for the solution with lowest magnitude) for a sodium condensate. It is clear that the “snake” instability of the  $m = 0$  component is the dominant process. Nevertheless, it is interesting to observe the dynamical instability of the  $m = \pm 1$  atoms as well. This instability is strongest when  $k \approx 0.975$  whereas the snake instability peaks at  $k \approx 0.69$ . If  $\Delta a$  is increased (in sodium  $\Delta a = 0.04$ ) the dynamical instability due to the  $m = \pm 1$  atoms becomes stronger, but it seems that the snake instability always has a larger imaginary part in its spectra and consequently it dominates.

Similarly we can study a soliton in a spin-1 condensate with ferromagnetic interactions ( $^{87}\text{Rb}$  for example). In this case a soliton in the ground state will be

$$\bar{\psi}(\mathbf{r}) = \psi_s(x) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \quad (41)$$

In the homogeneous case one expects three kinds of excitations [6]: the density mode with a Bogoliubov spectrum and two free-particle-like excitations, one of which has a gap. Linearizing the GP-equations around the

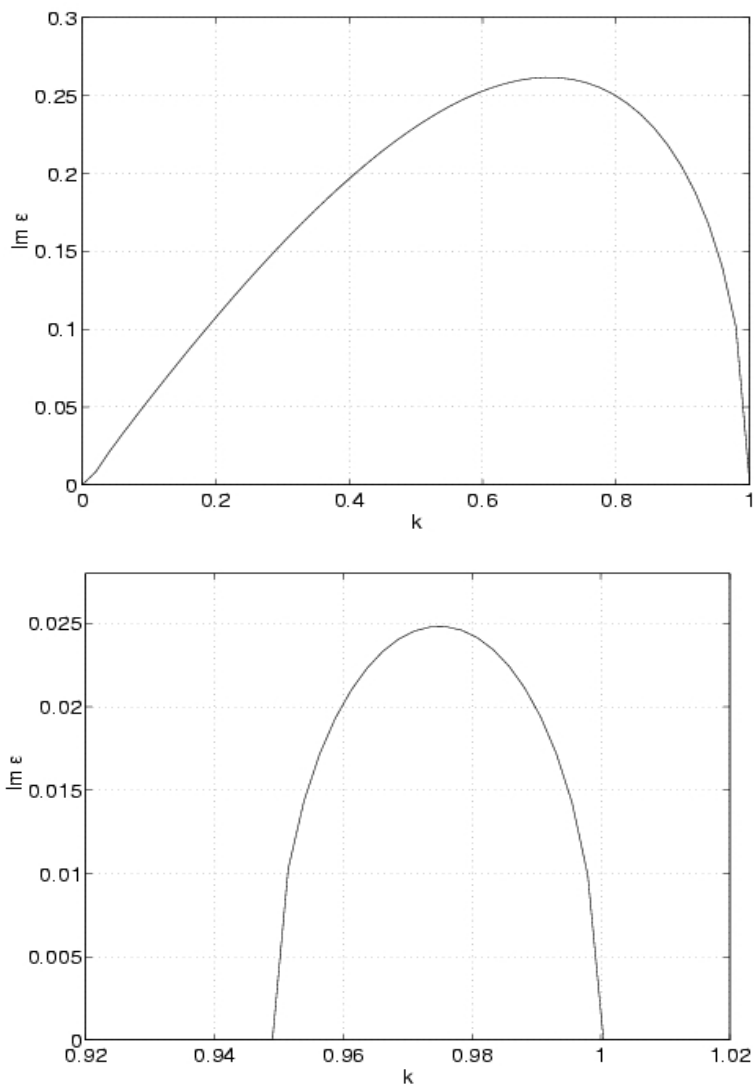


Figure 3: Imaginary parts of the excitation energies for a soliton in sodium spinor condensate (sodium has a polar ground-state) as a function of transverse wavenumber. The top figure is for the  $m = 0$  component and represents the well known snake instability [70]. The bottom figure is for the  $m = \pm 1$  components and is the result of a numerical solution of Eq. (40).

ferromagnetic soliton solution leads to three equations, one for each component. The equation for the  $m = 1$  component is, as expected, similar to the one studied in a scalar condensate [70] and the equations for the  $m = 0, -1$  components are:

$$i \frac{\partial}{\partial t} f_{0,k\nu} = \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \tanh^2 x - 1 + \frac{k^2}{2} \right] f_{0,k\nu} \quad (42)$$

$$i \frac{\partial}{\partial t} f_{-1,k\nu} = \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{k^2}{2} - \frac{2\lambda_a}{g_2} \tanh^2 x \right] f_{-1,k\nu}, \quad (43)$$

where the disturbance  $\delta\psi_m$  was expanded as in Eq. (37). Obviously, these equations are just ordinary single particle Schrödinger equations with trapping potentials determined by the density of the  $m = 1$  component. It is interesting to note that in the homogeneous gas these equations are responsible for the two free-particle-like excitations mentioned above. In inhomogeneous gas these free-particle-like excitations can be simply interpreted as particle-like excitations.

By inspecting Eq. (42), it is clear that for the  $m = 0$  component one can have some bound states indicating that  $m = 0$  atoms would gather into the “core” of the soliton. For the  $m = -1$  component (Eq. (43)) bound states can exist if  $\lambda_a < 0$  (*i.e.* if ferromagnetic state is the ground state), otherwise  $m = -1$  atoms are repelled from the soliton core. All eigenvalues for both components are real so no additional dynamical instability is expected for a soliton in a ferromagnetic state.

As demonstrated above, the Bogoliubov theory for the elementary excitations can be applied to the spinor condensates. For a homogeneous spin-1 condensate this was done in Ref. [6]. There it was shown that all three excitations (density, spin and “quadrupolar spin” excitations) have either the Bogoliubov form (*i.e.*  $E = \sqrt{K(K + 2E_0)}$ , where  $K$  is the kinetic energy) or the free particle form (*i.e.*  $E = K + \Delta E_{gap}$ ). In paper IV we generalized these results to a homogeneous spin-2 condensate and observed that, again, all excitations have either the Bogoliubov or the free particle form. This indicates that excitations in a spinor condensate have a rather universal character. It can be further conjectured that the functional form of the excitations for arbitrary spin is fixed by the symmetries of the interaction Hamiltonian.

### 3.4 Spin-gauge symmetry and superfluid velocity of a spinor condensate

The spinor condensates can exhibit a “spin-gauge” symmetry, meaning equivalence between phase change and spin rotation [6, 72]. In an ordinary magnetic trap effects due to the hyperfine degree of freedom are normally small and usually the condensate is described by a fixed spinor in an adiabatic basis. This means assuming that all atoms are in one  $m$  state and that their spins are everywhere aligned along the direction of the local magnetic field. Ignoring the hyperfine degree of freedom is sensible only if the magnetic field is sufficiently slowly varying.

In an ordinary condensate the superfluid velocity is simply proportional to the gradient of the phase, but in a spinor condensate things are different due to the “spin-gauge” symmetry. If the spin rotation is local, i.e. the rotation is a some function of position, the superfluid velocity does, in general, depend on the rotation as well. A quantity that transforms like a velocity and results in an intuitively obvious particle current ( $\mathbf{j} = n\mathbf{v}_s$ ) is [72]

$$\mathbf{v}_s = -i\frac{\hbar}{m}\zeta^\dagger\nabla\zeta, \quad (44)$$

where  $\zeta$  is the spinor normalized to one. This equation generalizes the superfluid velocity to spinor condensates. By applying a global rotation  $\mathcal{U}$ , defined in terms of Euler angles and spin matrices  $F_\alpha$  as

$$\mathcal{U}(\alpha, \beta, \gamma) = e^{-iF_z\alpha}e^{-iF_y\beta}e^{-iF_z\gamma} \quad (45)$$

together with a gauge transformation  $e^{i\theta}$  to the spinor  $\hat{\zeta}$  we get a new spinor

$$\hat{\zeta}' = e^{i\theta}\mathcal{U}\hat{\zeta} \quad (46)$$

which is physically identical to the original spinor. As the global rotation does not cost energy there will be a collective excitation with energy  $\hbar\omega_0 = 0$  and wavenumber  $k = 0$ . This excitation is the so called spin wave, which simply rotates all the spins. Such a mode is also called a “Goldstone mode” that is connected with the spontaneously broken rotational symmetry.

If the rotation is local, *i.e.* angles  $\alpha$ ,  $\beta$  and  $\gamma$  are functions of position, the superfluid velocity of a spin-1 condensate in a polar state is simply proportional to the phase gradient (as usual). For a ferromagnetic state, on the other hand, the superfluid velocity is more interesting

$$(\mathbf{v}_s)_{ferro} = \frac{\hbar}{m} [\nabla(\theta - \gamma) - \cos\beta\nabla\alpha]. \quad (47)$$

This formula is similar to that of superfluid  ${}^3\text{He} - A$  [72] and indicates a close connection between these two fields of research. These results can be also calculated for condensates with larger spin. In paper IV we noticed that in a spin-2 spinor condensate the superfluid velocities of various states are qualitatively similar to those of spin-1 condensates. In particular, the velocity field of the ferromagnetic ( $F$ ) state is the only one that depends on the spin-rotations.

A ferromagnetic spinor condensate can have remarkable properties. Consider, for example, setting  $\gamma = 0$ ,  $\theta = \tan^{-1}(y/x)$ , and  $\alpha = \theta$  in equation (47). In this case the superfluid velocity is

$$(\mathbf{v}_s)_{ferro} = \frac{\hbar}{mr} [1 - \cos \beta] \hat{e}_\phi, \quad (48)$$

where  $r = \sqrt{x^2 + y^2}$ . Now if  $\beta$  is an increasing function that starts from 0 at  $r = 0$  and approaches  $\pi/2$ , one can have a vortex-like velocity pattern at larger  $r$  and still avoid a vortex core (*i.e.* diverging superfluid flow) at the origin. Even though these coreless vortices [73] are possible they are not topologically stable, but can be continuously transformed into a ground state. One can also show the absence of an energy barrier that would suppress this transformation and make a coreless vortex metastable. (This result is to my knowledge unpublished, but it is a fairly trivial consequence of the Hamiltonian. The proof is identical to that for vortices with even or odd circulation in a spin-1 condensate [6]. See also the paper by Khawaja and Stoof [11], for a topological argument.)

### 3.5 Stability of the superfluid flow in a ferromagnetic spinor condensate

A very important consequence of the spin-gauge symmetry in the ferromagnetic state is that the circulation does not have to be quantized. In a normal scalar condensate the circulation

$$\kappa = \oint \mathbf{v}_s \cdot d\mathbf{l} = \int (\nabla \times \mathbf{v}_s) \cdot d\mathbf{S} \quad (49)$$

can only take values  $N\kappa_0$ , where  $\kappa_0 = \frac{\hbar}{m}$  and  $N$  is an integer. The quantization implies that the flow is stable, and thus represents persistent currents. In a ferromagnetic spinor condensate the flow does not have to be irrotational (*i.e.*  $\nabla \times \mathbf{v}_s = 0$ ). Instead, we have

$$\nabla \times \mathbf{v}_s = \frac{\hbar}{m} \sin \beta \nabla \beta \times \nabla \alpha. \quad (50)$$

This is one expression for the “Mermin-Ho” relation [72,74]. Since the flow is no longer irrotational, circulation is not quantized and, consequently, stability of the flow is not ensured. Only when  $\alpha$  and  $\beta$  are fixed quantization is guaranteed. How the possible instability of the flow is manifested in a spinor condensate is not known. For a scalar condensate dissipation of a superfluid flow is accompanied by the creation of vortices and it has been suggested [72, 73] that in  $^3\text{He} - A$  dissipation proceeds by the creation of coreless vortices. One can suspect that coreless vortices are also involved in the dissipation of a superfluid flow in a ferromagnetic spinor condensate.

Let us assume that we are dealing with an effectively two dimensional system and we choose our rotation angles as  $\alpha = -\frac{mv}{\hbar}x$ ,  $\beta = \pi y/y_{max}$ , and  $\gamma = 0$ . In appropriate units (unit of length is the coherence length and unit of energy is the chemical potential) the superfluid velocity is

$$\mathbf{v}_s(x, y) = v \cos \beta \mathbf{e}_x. \quad (51)$$

This superfluid velocity is always along the  $x$ -axis, but changes sign when  $y$  approaches  $y_{max}$ . Even the fact that this kind of flow is possible is quite remarkable. For a scalar condensate a phase pattern  $\phi(x, y) = vx \cos(\pi y/y_{max})$  results in a superfluid velocity that is similar to Eq. (51) when  $y = 0$  or  $y = y_{max}$ , otherwise it always has also a  $y$ -component in it. For a scalar condensate the kind of flow represented by Eq. (51) is not possible. The circulation of the velocity field in Eq. (51) when the integration is done in the upper half plane ( $y > 0$ ) is  $\kappa = 4vx_{max}$ .

In practice the velocity field in Eq. (51) can be created by putting the ferromagnetic condensate in inhomogeneous magnetic fields. At first the magnetic field, that depends linearly on  $x$ , should be along the  $x$ -axis. This rotates the spinor around the  $x$ -axis with a rotation angle  $\alpha$  that depends on the magnetic dipole  $\mu$ , interaction time  $\tau$ , and the magnetic field gradient  $B'_1$ :

$$\alpha = \frac{\mu \tau B'_1}{\hbar} x. \quad (52)$$

This should be followed by a magnetic field along the  $y$ -axis to rotate the spinor around the  $y$ -axis with an angle

$$\beta = \frac{\mu \tau B'_2}{\hbar} y. \quad (53)$$

As a numerical example, let us assume that the dipole constant is one Bohr magneton and  $v = 1 \text{ mm/s}$ . These parameters imply that  $B'_1 \tau \approx 10^{-8} \text{ Gs/cm}$ . A small, but still realistic value for the field gradient is  $B'_1 =$

0.01 G/cm [53], indicating that the field should be applied to the condensate for about  $1 \mu\text{s}$ . Achieving such a precision in real experiments poses a difficult challenge.

While the velocity field in Eq. (51) is not possible for a scalar condensate, we can easily construct a velocity field that has the same circulation when the integration is taken over the whole two-dimensional condensate, namely

$$v(x, y) = v \text{sign}(y). \quad (54)$$

This velocity field leads to a  $\pi$  phase discontinuity at  $y = 0$  and  $y = \pm y_{max}$  and the wavefunction must be forced to zero at these locations.

We can map the rotation angles  $\alpha$ ,  $\beta$ , and  $\gamma$  into an order parameter for the ferromagnetic spinor condensate and then study the dynamics of the spinor condensate using the Gross-Pitaevskii equations. While direct comparison to scalar condensates is not possible, we can get a feeling for the qualitatively different superfluid properties of the spinor condensates by comparing these results to the results with a scalar condensate with velocity field given by Eq. (54). We start with a homogeneous two-dimensional condensate in a box with periodic boundary conditions and then imprint the desired velocity pattern. If the velocity  $v$  is  $1.5c_s$  the system is unstable. Examples of the resulting transient behavior, for both the spinor condensate and the scalar condensate, are given in figures (4) and (5).

In the spinor case the density of the system is strongly modulated, but it does not vanish at any point. Even though the system would have enough circulation to create tens of (singular) vortices, none are created. Even at  $t = 45$  the maximum superfluid velocity in the system is only about  $3c_s$ . Whether the structures created due to the instability are coreless vortices, is unclear. Their spinor texture is not the same as the spinor texture for the coreless vortices that we discussed before, but the background flow complicates the direct comparison. Also the large number of excitations makes the interpretation of the data difficult.

At lower values of  $v$ , namely  $v = 0.6c_s$ , the system is still unstable, but the timescale for the instability is more than twice longer than when  $v = 1.5c_s$  indicating that the timescale for the instability depends approximately linearly on the velocity  $v$ . In this case the number of excitations is much lower and the creation coreless vortices can be seen very clearly. An example of a small section of the velocity field is shown in figure (6) and the corresponding density is shown in figure (7).

The behavior above is in marked contrast to the scalar condensate. As can be seen from figure (5), in the scalar condensate the dynamical

instability of the system is reflected in the formation of vortices and at vortex cores the density (naturally) vanishes.

These results are as yet unpublished and are to my knowledge the first exact indications of the dramatically different flow properties of a spinor condensate. Obviously this is only the first step, but it is clear that this line of research is worth pursuing. For example, it is unclear how the drag force on an object depends on its velocity through a spinor condensate and also, it is not known when the breakdown of superfluidity in a spinor condensate involves the creation of singular vortices.

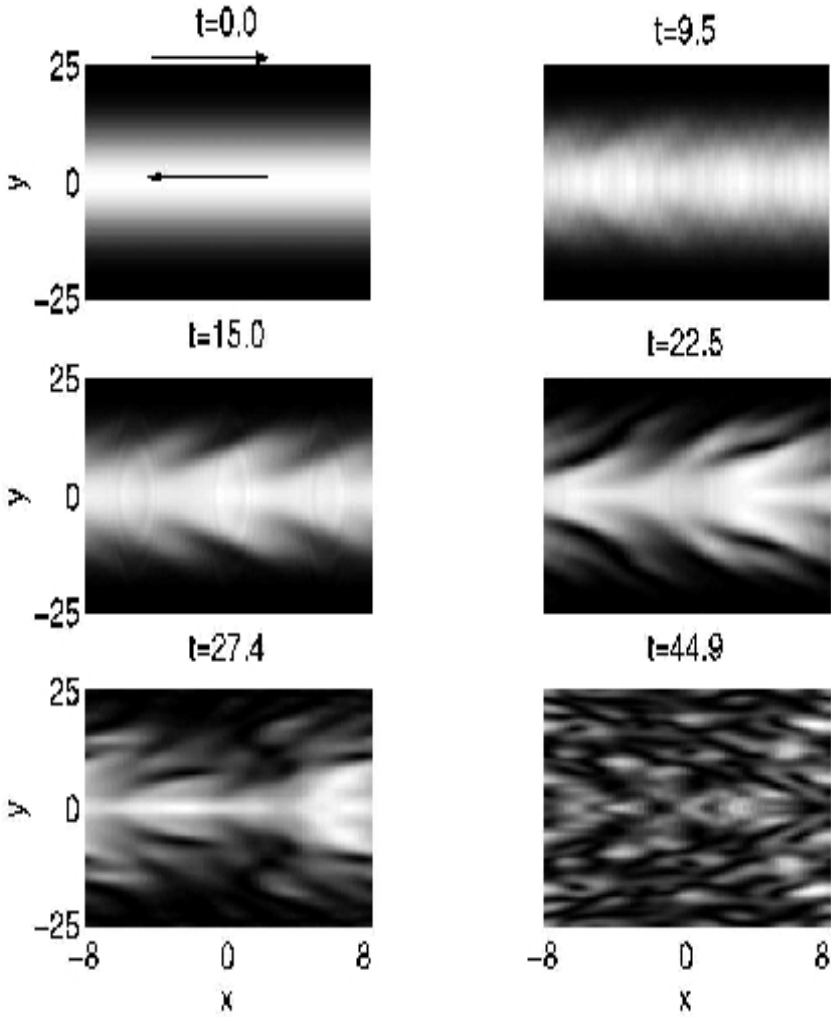


Figure 4: Density of the  $m = 1$  component when the total density of this two-dimensional rubidium  $F = 1$  spinor condensate was initially  $10^{14}$  atoms/cm<sup>3</sup> and the thickness in the  $z$ -direction was one coherence length. At  $t = 0$  the velocity field of Eq. (51) with  $v = 1.5 c_s$  was imprinted into the spinor. With this choice of parameters  $\kappa \approx 50$  when integration is done over upper half plane. Arrows indicate the direction of the flow and bright regions correspond to high density.

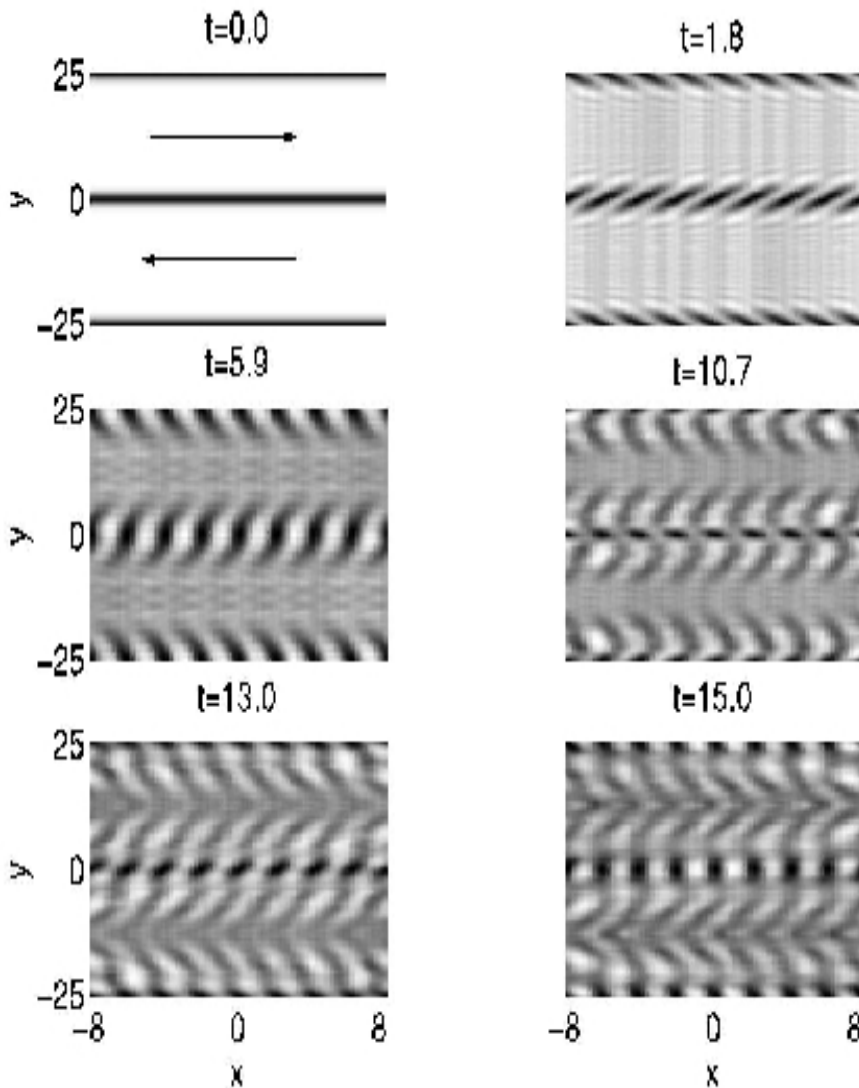


Figure 5: Instability of the superfluid flow in a two-dimensional rubidium scalar condensate at  $F = 1, m = 1$  state. The density was initially  $10^{14}$  atoms/cm<sup>3</sup> and the thickness in the  $z$ -direction was one coherence length. At  $t = 0$  the velocity field of Eq. (54) with  $v = 1.5 c_s$  is imprinted into the wavefunction. Bright regions correspond to high density.

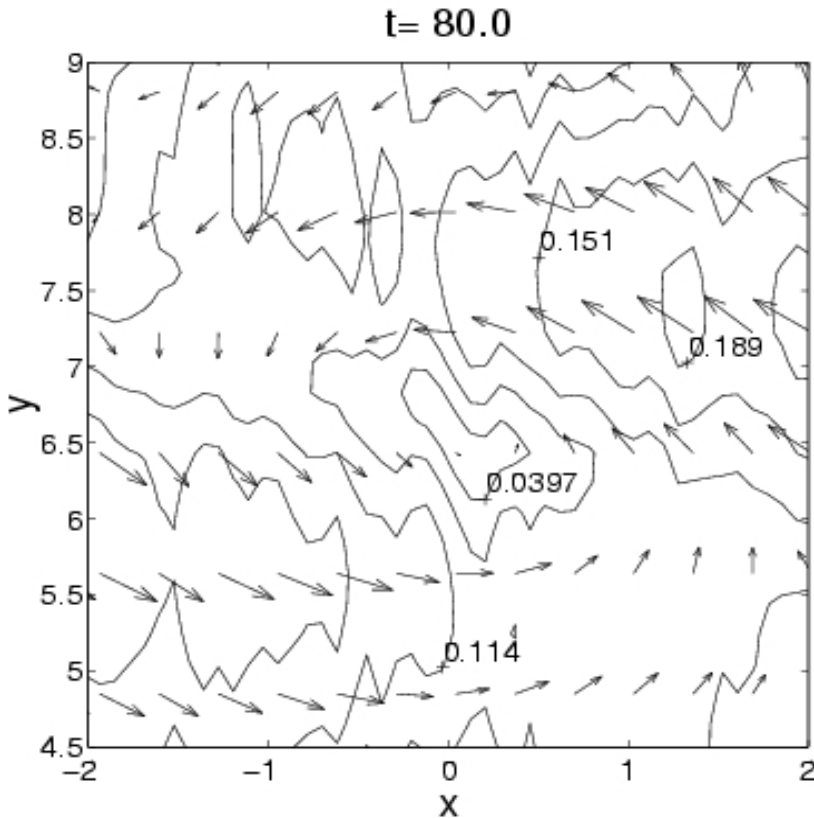


Figure 6: A section of the velocity field of the spinor condensate when, initially,  $v = 0.6 c_s$ . Contour lines are the lines of constant speed and arrows indicate the direction of the flow. The velocity vanishes at the “core” and takes the vortex flow pattern further away. This indicates a presence of a coreless vortex.

### 3.6 Topological excitations in an $f = 1$ spinor condensate

The topological properties of a scalar condensate are fairly trivial. One only has a condensate phase to play with (the order parameter has a  $U(1)$  gauge symmetry) and the only topologically non-trivial excitations are vortices. The order parameter of a spinor condensate has much richer topological properties and allows for different topological excitations. For a spin-1 condensate in the polar state one is free to choose for spinors the overall phase (gauge) and the spin quantization axis (angles  $\alpha$  and  $\beta$ ) without changing the energy. Therefore the parameter space for the antiferromagnetic spinor

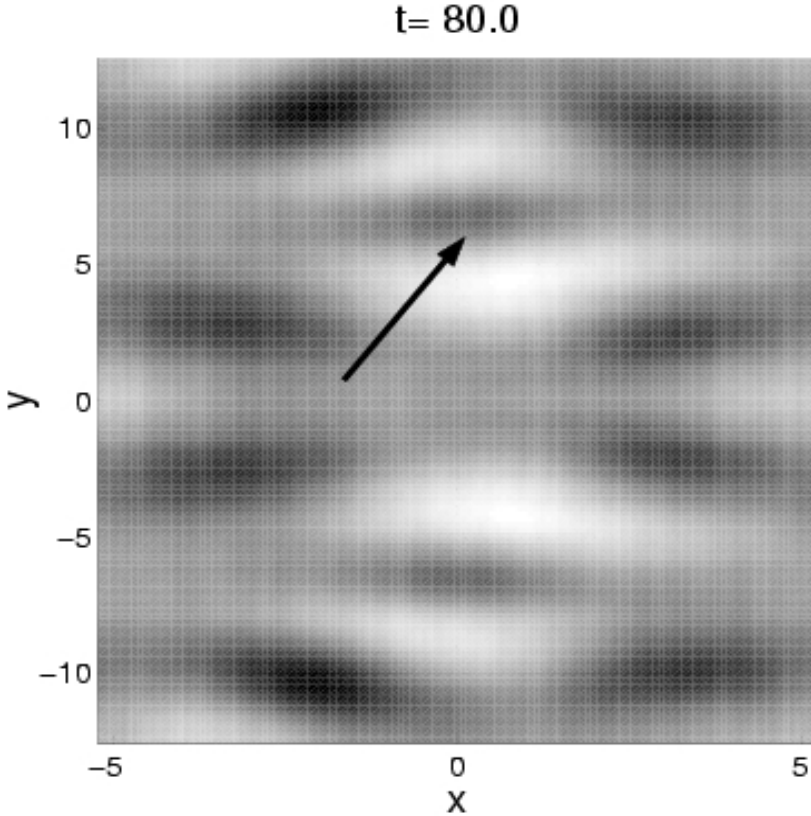


Figure 7: Total density of the spinor condensate when, initially,  $v = 0.6 c_s$ . The figure corresponds to the velocity field seen in figure (6) and the position of the coreless vortex shown in figure (6) is indicated with an arrow.

is  $U(1) \times S^2$ . For the ferromagnetic spinor one is free to choose all Euler angles and the parameter space corresponds to the full rotation group  $SO(3)$ . It is useful to consider the symmetries of the order parameter as local. This means that the order parameter space will not only include minimum energy states, but also those states that can be reached from them with local rotations. Such states resemble ground state locally, but the gradient terms in the Hamiltonian will make their energy higher.

Knowledge of the order parameter space of the ground state has been used to predict the existence of topological excitations [11, 75]. It has been shown that a ferromagnetic condensate can only have vortices with a wind-

ing number equal to 1, whereas an antiferromagnetic condensate can have vortices with arbitrary (integer) winding numbers. For an antiferromagnetic spin-1 condensate one also expects the existence of a singular point-like defect – a monopole [12]. This is characterized by a vector field that is always radial, *i.e.* it is a “hedgehog” excitation. For both ferromagnetic and antiferromagnetic states nonsingular point-like defects should be possible. These are called skyrmions [10].

The skyrmion is a structure where the spin is flipped in a finite region of space. This is done by rotating the ferromagnetic ground state around an axis, that is a radial vector, by an angle  $\omega$  that depends on the distance from the skyrmion core. This angle is  $2\pi$  at the origin and monotonically approaches zero far away from the core. An example of a skyrmion state for spin-1 condensate is presented in figure (8).

The arguments about the possibility of various topological excitations are based on the topological structure of the ground state and have nothing to say about the dynamics of the defect. For example the dynamics will (in general) take the monopole in an anti-ferromagnetic spinor condensate [12, 76] away from the order parameter space of the ground state. Therefore topological arguments should always be checked against the time evolution in real physical systems.

In the literature there has been an unfortunate confusion about the terminology. In his often cited paper [6] Tin-Lun Ho used terms skyrmion and coreless vortex synonymously and some papers claiming to discuss skyrmions are in fact discussing coreless vortices [77, 78]. A coreless vortex is a line-like structure and a skyrmion is a point-like defect.

We studied the properties of monopole in paper V and observed that it does not behave like a particle, *i.e.* it does not preserve its shape and move according to some well defined Newton’s equation of motion. On the contrary, its behavior showed marked similarities with vortex precession in an ordinary condensate. A monopole in an antiferromagnetic spin-1 condensate can be considered as a mixture of a vortex, an anti-vortex, and a soliton that is aligned perpendicular to the vortices. If the monopole core is displaced from the origin, the vortices precess in opposite directions until they meet again and recreate the monopole core. Due to the various disturbing mean fields the precession is not smooth, but qualitatively this description is correct. Also, it should be noted that the spin-1 condensate with a monopole does not stay in the order parameter space of the ground state. The displaced vortex in the  $m = 1$  state will precess opposite to the displaced antivortex in the  $m = -1$  state. Therefore the time-evolution will

take the originally non-magnetized state into a locally magnetized state. In paper V we also discussed a monopole in a binary condensate. Unlike the spin-1 monopole this monopole is stable and is therefore expected to be experimentally more interesting.

Also the skyrmions do not seem to be quite so stable as one would like to think. In figures (9) and (10) I show an unpublished example of the dynamics of the skyrmion solution in spin-1 condensate. The initial state is qualitatively similar to those in Ref. [11] with the exception of a trapping potential, but the dynamical behavior seems to be quite different from what was expected [10, 11]. In particular the skyrmion decays at the time-scale set by the inverse of the trapping frequency. This is considerably faster than the previous estimates [11]. The instability is due to the velocity fields induced by the boundary conditions. If we model the system as homogeneous, the normal component of the velocity must vanish at the boundary. This boundary condition can be imposed with an appropriate image velocity field. A similar method is commonly used for vortices, but its application in this context is more complicated and is a good topic for further research.

The transformation shown in figures (9) and (10) is a continuous transformation so the topology of the order parameter is not changed. Nevertheless, it is mapped into a form that is considerably harder to interpret than the original.

It is interesting to notice that the decay of the skyrmion is anisotropic. This anisotropy has its roots in the spinor texture gradients. Approximating the scattering lengths as equal we can write a Gross-Pitaevskii equation for the total density. The kinetic energy of the spin texture gives rise to the potential term

$$V_S = \frac{\hbar^2}{2m} |\nabla\zeta|^2, \quad (55)$$

where  $\zeta$  is the spinor. In spin-1/2 case the resulting potential is spherically symmetric, but for spin-1 ferromagnetic condensate the potential is anisotropic

$$V_S = \frac{\hbar^2}{2m} \left[ \frac{1}{2} (1 + \cos^2 \theta) \left( \frac{\partial\omega}{\partial r} \right)^2 + (3 - \cos^2 \theta) \frac{1 - \cos\omega}{r^2} \right], \quad (56)$$

where  $\theta$  is the polar angle. This anisotropy is reflected in the anisotropic decay of the skyrmion.

In the Skyrme model of nuclear physics the skyrmions are stabilized with higher order derivative terms [79]. In Bose-Einstein condensates such terms

cannot be justified. It remains to be seen whether the external potential or some nonlinear effect caused by the mean field can be used to stabilize skyrmions in Bose-Einstein condensates.

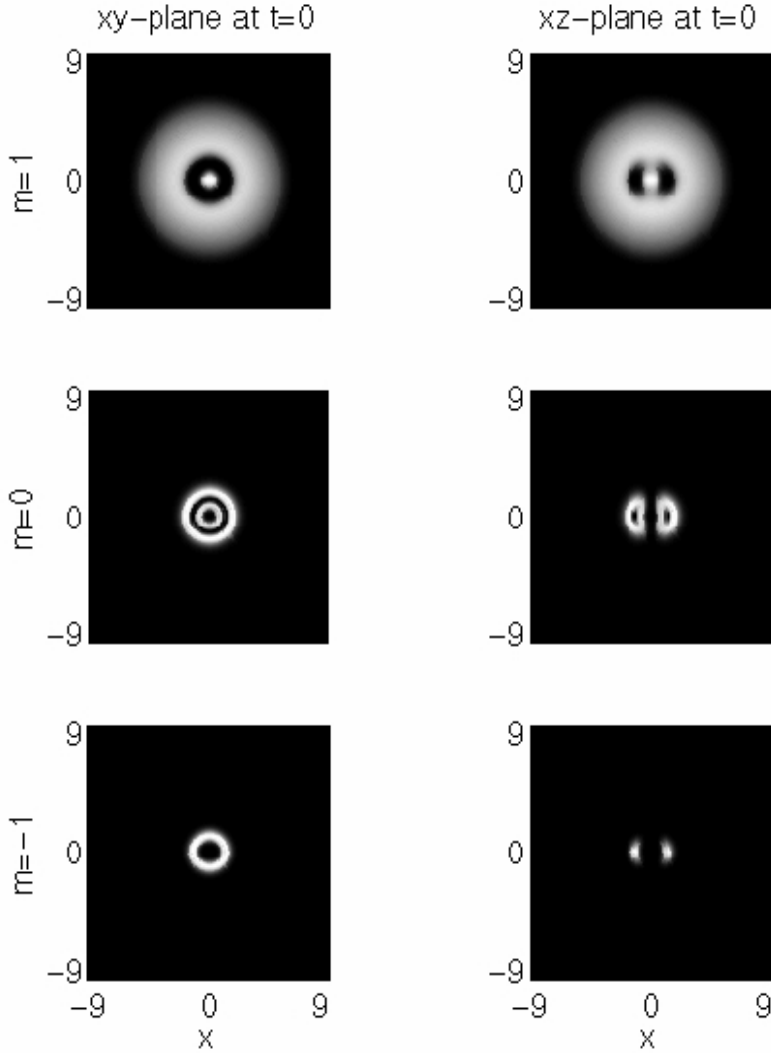


Figure 8: Density of a skyrmion of size  $5\xi$  in a  $^{87}\text{Rb}$  condensate with 200 000 atoms.  $\xi$  is the coherence length at the center of the condensate and the trapping frequency is  $2\pi 50$  Hz.

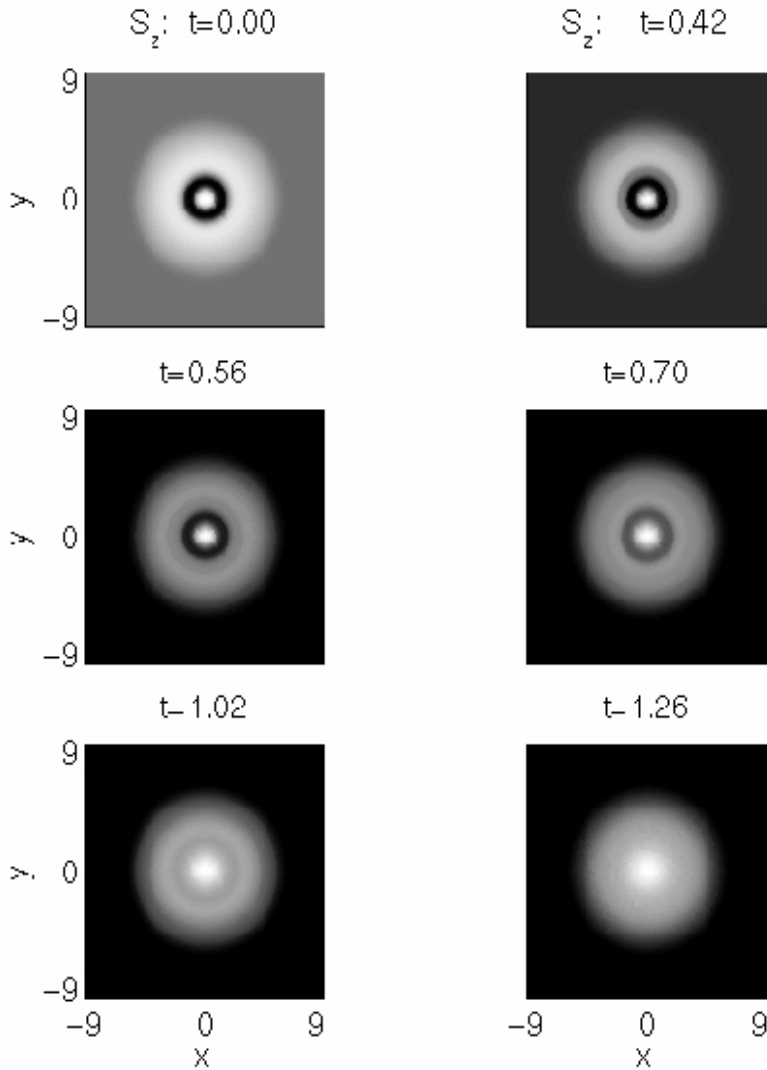


Figure 9: Skyrmion dynamics in a  $^{87}\text{Rb}$  condensate. The initial state and the parameters are the same as in Fig. (8) and the figure shows the  $z$ -component of the spin in the  $xy$ -plane.

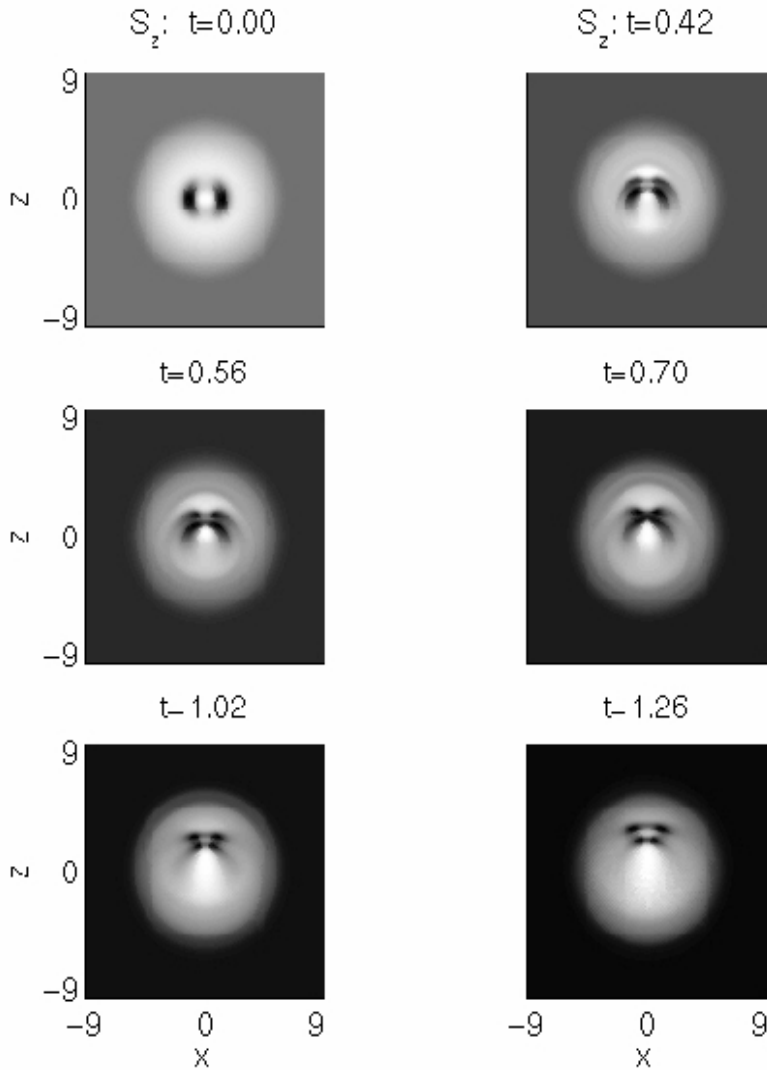


Figure 10: Skyrmion dynamics in a  $^{87}\text{Rb}$  condensate. The initial state and the parameters are the same as in Fig. (8) and the figure shows the  $z$ -component of the spin in the  $xz$ -plane.

## 4 Conclusion

I have studied dynamics and excitations of Bose-Einstein condensates under many different circumstances. Most of the studies use the mean field theory and the accompanying GP-equations. We have learned how vortices behave in restricted geometries and how Bogoliubov theory can be applied to spinor condensates. I have clarified the role played by the shallow optical dipole traps in Bose-Einstein condensates by going beyond the parabolic approximation. These results may prove useful when studying condensation in shallow traps (or optical lattices).

Spinor condensates support new topological excitations such as monopoles and skyrmions. Their dynamics has not been studied before and therefore results presented in this Thesis are relevant. One hoped that skyrmion excitations would have been more stable, but nevertheless they are out there and one can now seek some methods to stabilize them. We have also suggested a fairly robust method to create a monopole in a spinor condensate, presenting a challenge to daring experimentalists who are willing to create monopoles in practice.

Compared to scalar condensates, very little work has been done on spinor condensates. I can see many interesting questions and problems awaiting to be solved. These include, for example, phase decoherence, fragmentation, and the concept of a relative phase in spinor condensates. Also, it would be very useful to generalize the Bogoliubov theory to inhomogeneous systems at non-zero temperatures. Some work in this direction has already been made [80], but the problem is still essentially unsolved.

Quantum stochastic equations have been used to study decoherence in quantum optics and they have also been applied to study scalar condensates [81]. Generalizing this approach to spinor condensates might prove rewarding. Vortex nucleation is currently a hot topic and it is (probably) just a matter of time before vortices in spinor condensates are created. Therefore, investigating superfluid properties of spinor condensates is of great importance. In conclusion, so much interesting work remains to be done that no individual could hope to do everything by himself. Nature is an infinite source of new discoveries. And isn't that just great!

## A Numerical methods

Most of this thesis is about solving the Gross-Pitaevskii equation

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V_{trap}(\mathbf{r})\Psi(\mathbf{r},t) + g|\Psi|^2\Psi(\mathbf{r},t) \quad (57)$$

in various disguises. For a single component condensate Eq. (57) works as it is, but a number of complications arise in the real world. The complications that I have encountered while working on this thesis (to name but a few) include multicomponent condensates with coupling fields, spinor condensates with elastic spin exchange collisions, spinor condensates with spin texture gradients, atomic condensate mixed with molecular condensate and condensates with long-range dipole-dipole interactions. All these special cases require modifications to the programs used to solve the ordinary single component GP-equation.

In the following I approach the numerical problem starting from the bottom, namely from the numerical solution of the time dependent Schrödinger equation. From there I continue to explain the complications caused by adding a mean field, couplings, and various other cases mentioned above.

### A.1 Time dependent Schrödinger equation

The time dependent Schrödinger equation (TSE)

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \hat{H}\Psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r},t) + V_{trap}(\mathbf{r})\Psi(\mathbf{r},t) \quad (58)$$

lies at the heart of non-relativistic quantum physics. Formally it resembles a diffusion equation with a source term. The crucial difference is the imaginary unit in front of the time derivative. This imaginary term causes the numerical methods that might work in solving the diffusion equation to fail miserably in the quantum case. On the other hand, if one is able to solve the time dependent Schrödinger equation numerically, it will be easy to apply essentially the same numerics to a classical diffusion equation.

There are several methods to solve the TSE numerically. The most widely used are the Crank-Nicolson method and the split-operator technique with FFT [82,83]. Both methods are based on approximations to the unitary propagator

$$\hat{U} = \exp\left(-i\Delta t\hat{H}/\hbar\right) \quad (59)$$

which gives the evolution of the wavefunction over a timestep  $\Delta t$  i.e.

$$\Psi(\Delta t) = U\Psi(0). \quad (60)$$

In the Crank-Nicolson method  $\hat{U}$  is approximated to second order in  $\Delta t$  as

$$\hat{U} \approx \frac{1 + \frac{\Delta t}{2\hbar} \hat{H}}{1 - \frac{\Delta t}{2\hbar} \hat{H}}. \quad (61)$$

The method has the advantage of simplicity and robustness for normal TSE. When in a one-dimensional problem the kinetic energy term is approximated with a second order finite difference formula, the problem is reduced to inverting a tridiagonal matrix and can be solved quickly. In the a multidimensional case the resulting problem is sparse and can be solved, even though the programming effort can be considerable. In a multidimensional case also methods like alternating direction implicit [84] might be considered. In these methods the wavefunction is propagated in each direction individually, reducing the problem to a series of one-dimensional problems.

The main disadvantages of the Crank-Nicolson method are, firstly, the inability of the programmer to reuse old code when moving to higher dimensional problems and, secondly, the more serious instability problems with the nonlinear Schrödinger equation, compared to the split-operator technique with FFT.

In the split-operator technique the propagator is approximated as

$$\hat{U} \approx \exp\left(-i\frac{\Delta t}{2\hbar} \hat{K}\right) \exp\left(-i\frac{\Delta t}{\hbar} \hat{V}_{trap}\right) \exp\left(-i\frac{\Delta t}{2\hbar} \hat{K}\right) \quad (62)$$

where the Hamiltonian has been split into the kinetic energy term  $\hat{K} = -\frac{\hbar^2}{2m} \nabla^2$  and the potential term  $\hat{V} = V_{trap}(\mathbf{r})$  so that  $\hat{H} = \hat{K} + \hat{V}$ . (Equation (62) is an approximation since in general  $\hat{K}$  and  $\hat{V}$  do not commute.) Equation (62) is second order in  $\Delta t$  and preserves the norm of the wavefunction by construction since it corresponds to multiplication with complex numbers of unit length. Usually in the simulation we perform a large number of time steps and the kinetic energy operators at the beginning and the end of Eq. (62) can be grouped into one operator namely,

$$\exp\left(-i\frac{\Delta t}{2\hbar} \hat{K}\right) \cdot \exp\left(-i\frac{\Delta t}{2\hbar} \hat{K}\right) = \exp\left(-i\frac{\Delta t}{\hbar} \hat{K}\right). \quad (63)$$

Then the propagator can be approximated as

$$\hat{U} \approx \exp\left(-i\frac{\Delta t}{\hbar} \hat{K}\right) \exp\left(-i\frac{\Delta t}{\hbar} \hat{V}\right). \quad (64)$$

The split-operator technique with FFT consists of the approximation (64) and the application of the fast Fourier-transform when performing the kinetic energy part of the propagation. In practice the algorithm over one time step is:

- I Multiply the wave function with the complex number  $\exp\left(-i\frac{\Delta t}{\hbar}\hat{V}\right)$ .
- II Fourier-transform the wavefunction with FFT.
- III Multiply the Fourier-transform of the wavefunction with the complex number  $\exp\left(-i\frac{\hbar\Delta t}{2m}k^2\right)$ .
- IV Take an inverse Fourier-transform.

In this technique the time step should scale with the square of the grid size *i.e.*  $\Delta t \sim \Delta x^2$ . Typically we have used  $\Delta t = \Delta x^2/6$ . It should be noted, that the use of the FFT is not required. The kinetic energy propagator can be dealt with using other methods as well. Nevertheless, the FFT is often very convenient since it makes the non-local derivative terms local in the Fourier-space and consequently removes the need to solve systems of linear equations.

Cartesian coordinate systems are particularly useful for two important reasons. Firstly they are intuitively the most obvious and transparent coordinate system. In general all different coordinates are treated in the same way and in particular the  $\nabla^2$  operator has the simple form

$$\nabla^2 = \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2}. \quad (65)$$

Since all coordinates are treated similarly, programming is easy and less prone to error. Also, it will be very easy to generalize the code to higher dimensions. The second important reason for the use of the Cartesian coordinates is the availability of the fast Fourier transform (FFT). Solution of partial differential equations is quite easy with the help of FFT, since by Fourier-transforming the function we can turn nonlocal derivative operations into local operations in the Fourier space. This is precisely the reason why we have used the split-operator technique with FFT for solving the GP equation in a Cartesian coordinate system.

In some rare cases one might be interested in solving the TSE in more exotic coordinate systems. In such cases a particularly simple algorithm was given in Ref. [85]. In this method the time-derivative in the TSE is

approximated with second order finite difference formula and the wavefunction over one time step is given by

$$\Psi(t + \Delta t) = \Psi(t - \Delta t) - 2i\Delta t \frac{\hat{H}}{\hbar} \Psi(t). \quad (66)$$

This algorithm is exceedingly simple to program and can be ported to a parallel computer quite easily, but it has two major drawbacks. First, it requires more memory since the wavefunction has to be stored at two different times, not only at the present time. Second, the initialization might be non-trivial. The TSE has to be integrated over a small time step to get the simulation running correctly. In the presence of couplings and other complicating factors the algorithm given by Eq. (66) becomes more and more cumbersome to apply.

### A.1.1 Ground state of the Schrödinger equation

The ground state of the Schrödinger equation can be calculated with the same routine as the real time dependence by making the time step  $\Delta t$  imaginary

$$\Delta t \rightarrow -i\Delta t \quad (67)$$

and remembering to normalize the wavefunction during the iteration. This method of imaginary time propagation is well known [86] and is also used extensively in statistical physics. It is based on an idea that one expands some state  $\psi(x, t)$ , in the basis of eigenstates  $\phi_k(x)$  with energies  $E_k$ :

$$\psi(x, t) = \sum_k c_k \phi_k(x) \exp(-iE_k t/\hbar). \quad (68)$$

If one replaces time  $t$  with imaginary time, then the exponential factors decay rapidly. The ground state has the lowest energy and its decay rate is smallest. Therefore it will “sieved” by the imaginary time propagation from the (in principle) arbitrary initial state.

There are of course many other methods to solve the time independent Schrödinger equation, but we focus only on the imaginary time propagation since it also works for the nonlinear Gross-Pitaevskii equation.

When the time-evolution is the most time consuming part of the simulation, simply making the time step imaginary and renormalizing properly gives an algorithm that usually converges to the ground state well enough. But in some cases this is an overkill since essentially the same results can be achieved with lower order methods. In particular an iteration

$$\Psi_{new} = \Psi_{old} - \frac{\Delta t}{\hbar} \hat{H} \Psi_{old} \quad (69)$$

in combination with renormalization works well enough. It is obvious that Eq. (69) is based on a first order (in  $\Delta t$ ) approximation to the imaginary time propagation operator

$$U_{im} = \exp\left(-\Delta t \hat{H}/\hbar\right). \quad (70)$$

## A.2 From Schrödinger equation to Gross-Pitaevskii equation

The GP equation is a nonlinear Schrödinger equation. This nonlinearity is due to the extra meanfield term

$$g|\Psi|^2\Psi \quad (71)$$

added into the linear Schrödinger equation and makes many methods used to solve the time independent Schrödinger equation impractical. The most widely used method to calculate the ground state of the GP equation is the method of imaginary time propagation. Fortunately the nonlinearity does not cause any particular problems for the time dependent problem, and the same split-operator technique used to solve TSE can be used to solve the GP equation as well. The nonlinear term can simply be incorporated as an extra potential for the wavefunction.

## A.3 Cylindrical coordinates

Often in experiments the Bose-Einstein condensate is trapped in a cylindrically symmetric trap. When this is the case, a fully three-dimensional study is not needed for the calculation of the groundstate properties and one should take advantage of the symmetry of the problem. In cylindrical coordinates  $(r, z)$  it is useful to make the transformation [87]

$$\Psi_{old} = \frac{1}{\sqrt{r}}\Psi. \quad (72)$$

With this transformation the time independent GP equation becomes

$$\mu\Psi(r, z) = -\frac{\hbar^2}{2m} \left[ \frac{\partial^2\Psi}{\partial r^2} + \frac{\partial^2\Psi}{\partial z^2} \right] + \left[ V_{trap}(r, z) - \frac{\hbar^2}{8mr^2} + g\frac{|\Psi|^2}{r} \right] \Psi. \quad (73)$$

This equation can again be solved by imaginary time propagation either by the split-operator technique discussed before or by the simple iteration given in Eq. (69). An alternative method using alternating-direction implicit method is discussed in [88]. In Eq. (73) there is a possible source of

trouble at the  $z$ -axis due to the singularity. This problem can be avoided by imposing a  $\sqrt{r}$  ( $a_1 + a_2 r^2$ ) dependence for the wavefunction for small values of  $r$  and choosing the parameters  $a_1$  and  $a_2$  so that the wavefunction is continuous across the cutoff radius  $r_{cutoff}$ . The appropriate cutoff radius is problem specific and it is necessary to check the results with different cutoff radii. Often the simple  $\sqrt{r}$  dependence is sufficient for convergence.

#### A.4 Spin dynamics in a spinor condensate

The mean field theory of a spinor condensate results in nonlinearly coupled GP equations. These couplings can lead to complex spin-mixing dynamics [55]. When splitting the time-evolution operator we are left with essentially an ordinary time-evolution operator of the GP equation, which we already know how to solve, and the spin-exchange terms. The spin-exchange part of the GP-equations for the spin-1 spinor condensate is

$$\begin{aligned} i\hbar \frac{\partial \Psi_1}{\partial t} &= \lambda_a \Psi_0^2 \Psi_{-1}^* \\ i\hbar \frac{\partial \Psi_0}{\partial t} &= 2\lambda_a \Psi_1 \Psi_{-1} \Psi_0^* \\ i\hbar \frac{\partial \Psi_{-1}}{\partial t} &= \lambda_a \Psi_0^2 \Psi_1^*. \end{aligned} \tag{74}$$

These equations can be solved using the Runge-Kutta method [55]. While this method works quite well, in some cases a more efficient method, developed by the author (unpublished), can be used. In the spirit of split operator methods we can define one part of the total Hamiltonian as

$$H' = \lambda_a \begin{pmatrix} 0 & \Psi_0 \Psi_{-1}^* & 0 \\ \Psi_0^* \Psi_{-1} & 0 & \Psi_0^* \Psi_1 \\ 0 & \Psi_0 \Psi_1^* & 0 \end{pmatrix}. \tag{75}$$

Then the spin-dynamics part of the propagation over a time step  $\Delta t$  is equivalent to propagation with the operator

$$U_{SM} = \exp(-iH'\Delta t/\hbar). \tag{76}$$

This expression can be solved explicitly by using the definition of the exponential operator

$$\exp \hat{M} = I + \frac{\hat{M}}{1!} + \frac{\hat{M}^2}{2!} + \frac{\hat{M}^3}{3!} + \dots \tag{77}$$

In terms of variables  $A = \frac{\lambda_a \Delta t}{\hbar} \Psi_0 \Psi_{-1}^*$ ,  $B = \frac{\lambda_a \Delta t}{\hbar} \Psi_0 \Psi_1^*$ , and  $\Omega = \sqrt{|A|^2 + |B|^2}$  the result of this calculation is

$$U_{SM} = I + \frac{(\cos \Omega - 1)}{\Omega^2} \hat{O}^2 - i \frac{\sin \Omega}{\Omega} \hat{O}, \quad (78)$$

where  $\hat{O}$  is

$$\hat{O} = \begin{pmatrix} 0 & A & 0 \\ A^* & 0 & B^* \\ 0 & B & 0 \end{pmatrix}. \quad (79)$$

This method works quite well in practice. Compared to the adaptive Runge-Kutta routine [84], it can be up to three times faster and it also preserves the norm by construction. When using this method some care must be used in choosing the time step.

In Fig. 11 we compare the results calculated using the adaptive Runge-Kutta method and the method based on Eq. (78) for some typical one-dimensional problems. The simulations were done on a LINUX PC with 256 megabytes of memory and a processor with clock speed of 500MHz.

In Fig. 11 we present the comparison of simulations with 10000 and 100000 sodium atoms, for a certain quasi one-dimensional problem with realistic values for the trap parameters. The initial state was such that 98% of the population was at the  $m = 0$  state and rest was divided evenly between  $m = \pm 1$  states. The phase difference of the  $m = \pm 1$  components to  $m = 0$  component was  $\pi/4$ . The wavefunction was sampled at the grid of 1024 points.

Both methods preserve the norm to a good accuracy and with 10000 atoms are seen to give the same results. Only essential difference in this case is that the method based on Eq. (78) took roughly 3000 seconds to execute whereas the Runge-Kutta method took about 15600 seconds. In Fig. 11 one can also see that if number of atoms is increased to 100000, at long times the results do not agree. A more careful investigation shows that the method based on Eq. (78) has not converged. The method only works if the changes in the wavefunction over one time step are small and when it fails is not well defined, since the wavefunction does not always start to behave erratically.

## A.5 Collective excitations

In the paper I I solved rather complex coupled differential equations for the collective excitations of the condensate in a spherically symmetric trap.

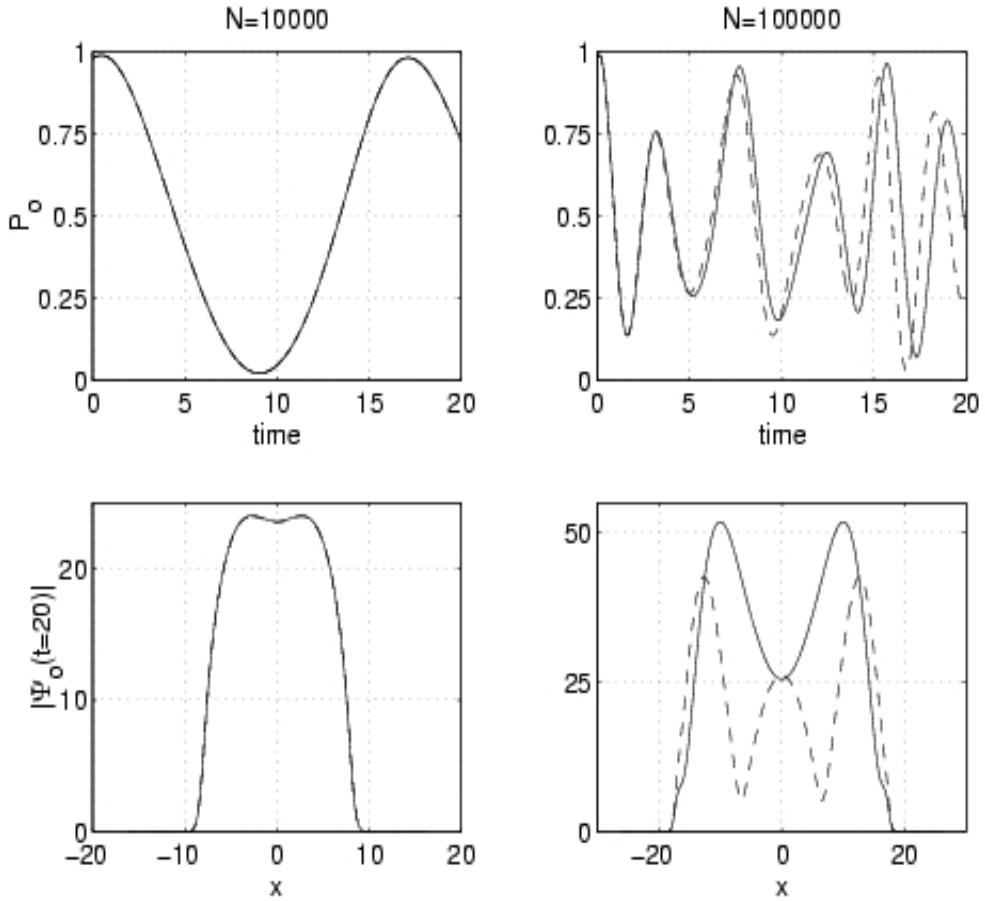


Figure 11: Comparison of results with methods based on Eq. (78) (solid line) and adaptive Runge-Kutta integration (dashed line). With 10000 atoms the results are essentially the same, but some discrepancy can be observed for larger particle numbers.

These equations are the famous Bogoliubov-de Gennes equations in the Popov approximation and look like [38]

$$\begin{aligned} [L + 2gn(\mathbf{r})] u_k(\mathbf{r}) + g|\Psi|^2 v_k(\mathbf{r}) &= \hbar\omega_k u_k(\mathbf{r}), \\ [L + 2gn(\mathbf{r})] v_k(\mathbf{r}) + g|\Psi|^2 u_k(\mathbf{r}) &= -\hbar\omega_k v_k(\mathbf{r}), \end{aligned} \quad (80)$$

where  $L = -\frac{\hbar^2}{2m}\nabla^2 + V_{trap}(\mathbf{r}) - \mu$  and  $u_k$  and  $v_k$  are quasiparticle amplitudes.  $n = |\Psi|^2 + n_T$  is the total density and the non-condensate density  $n_T$  can be calculated from the knowledge of quasiparticle amplitudes. The condensate wavefunction now obeys the generalized GP-equation (see Section 2.3)

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V_{trap}(\mathbf{r})\Psi + g[2n_T + |\Psi|^2]\Psi. \quad (81)$$

In [89, 90] the amplitudes  $u_k$  and  $v_k$  were expanded in the harmonic-oscillator basis. This method transforms the Eq. (80) to an eigenvalue problem for the expansion coefficients. While this method works, we have employed a slightly different method of using the basis of eigenfunctions of the Schrödinger equation

$$[L + 2gn(\mathbf{r})] \phi_i = \epsilon_i \phi_i. \quad (82)$$

The eigenfunctions have to be calculated numerically, but that is not a major problem. This basis has the advantage that the resulting matrix for the eigenvalue problem has a simpler form. The obvious disadvantage is the necessity of storing all the eigenfunctions as they are needed when calculating the matrix coefficients and when expressing the final results for the amplitudes  $u_k$  and  $v_k$ .

The algorithm for the calculation of the collective excitations (when the thermal component can be ignored) is therefore

- I Solve the GP equation for the chemical potential  $\mu$  and the condensate wavefunction  $\Psi$ .
- II Solve Eq. (82) for the basis functions and energies.
- III Solve the quasiparticle amplitudes and energies using Eq. (80) in this basis.

This approximation is quite accurate and results in a gapless energy spectra. This means that there is a Goldstone mode with  $\omega_0 = 0$  and  $u_0 = -v_0 = \Psi$ .

The algorithm presented above still works when non-condensed atoms are included provided the solution is self-consistent. This requires an iteration of the algorithm until both the condensate density and the non-condensate density have converged.

## A.6 Numerical integration and minimization

Quite often in the course of this thesis I have had to perform numerical integration or minimization. I have found Monte-Carlo methods to be extremely helpful and for all practical purposes accurate enough.

The numerical integration of multidimensional functions can be quite tedious. In most methods the accuracy of the integration method becomes worse as the number of dimensions is increased. Also the programming effort increases considerably with number of dimensions. A notable exception to this rule is Monte-Carlo integration. In Monte-Carlo integration a function is sampled randomly and the sum over these random samples is used to approximate the integral of the function. The convergence can be made faster by focusing the sampling of the function in areas where the function has largest values. The author has applied this kind of adaptive Monte-Carlo integration [84] extensively. In addition to the simple and less errorprone programming the Monte-Carlo method also has the advantage of robustness in the sense that it is not very sensitive to possible singular values of the function. The likelihood of hitting such a point while randomly sampling the function is very low and usually they do not have to be treated with special care.

For numerical minimization I have often used simulated annealing. In that method one guesses the minimum  $r$  of the function, calculates the value of the function and then changes the guessed minimum randomly by an amount  $\Delta r$ . If the next guess  $r + \Delta r$  has a lower value than the previous guess, the change is accepted. This process is repeated sufficiently many times. To make the convergence faster it is a good idea to use, on the average, larger “jumps”  $\Delta r$  at the beginning and reduce the average when getting close to the minimum. If the “landscape” of the function has many minima, the algorithm may get stuck at some local minima and will not converge to the true minimum. To minimize this problem one should try different initial guesses and confirm that all iterations converge to the same value. Often this problem of local minimum is not a serious one, since the function might have only one minimum.

For minimization there are many different methods and many of them are better (for many problems) than simulated annealing. Especially a method like conjugate gradient [84] is often superior to simulated annealing, both in terms of accuracy and in terms of speed. The author is fully aware of this, but has taken a practical stance. For all practical purposes simulated annealing has been quick and accurate enough. If the need arises for more refined methods, one should not hesitate to use them.

## References

- [1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Science* **269**, 198 (1995).
- [2] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995).
- [3] C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, *Phys. Rev. Lett.* **75**, 1687 (1995).
- [4] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, *Rev. Mod. Phys.* **71**, 463 (1999).
- [5] T.-L. Ho and V. B. Shenoy, *Phys. Rev. Lett.* **77**, 2595 (1996).
- [6] T.-L. Ho, *Phys. Rev. Lett.* **81**, 742 (1998).
- [7] M. R. Matthews, B. P. Anderson, P. C. Haljan, D. S. Hall, C. E. Wieman, and E. A. Cornell, *Phys. Rev. Lett.* **83**, 2498 (1999).
- [8] K.W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard, *Phys. Rev. Lett.* **84**, 806 (2000).
- [9] J. R. Abo-Shaeer, C. Raman, J. M. Vogels, and W. Ketterle, *Science* **292**, 476 (2001).
- [10] U. Al Khawaja and H. Stoof, *Nature* **411**, 918 (2001).
- [11] U. Al Khawaja and H. Stoof, *Phys. Rev. A* **64**, 043612 (2001).
- [12] H. Stoof, E. Vliegen, and U. Al Khawaja, *Phys. Rev. Lett.* **87**, 120407 (2001).
- [13] S. Burger, K. Bongs, S. Dettmer, W. Ertmer, K. Sengstock, A. Sanpera, G. V. Shlyapnikov, and M. Lewenstein, *Phys. Rev. Lett.* **83**, 5198 (1999).
- [14] J. Denschlag, J.E. Simsarian, D. L. Feder, C. W. Clark, L .A. Collins, J. Cubizolles, L. Deng, E. W. Hagley, K. Helmerson, W. P. Reinhardt, S. L. Rolston, B. I. Schneider, and W. D. Phillips, *Science* **287**, 97 (2000).

- [15] D. S. Jin, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E.A. Cornell, Phys. Rev. Lett. **77**, 420 (1996).
- [16] D. S. Jin, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. **78**, 764 (1997).
- [17] O. M. Maragó, S. A. Hopkins, J. Arlt, E. Hodby, G. Heckenblaikner, and C. J. Foot, Phys. Rev. Lett. **84**, 2056 (2000).
- [18] L. Deng, E. W. Hagley, J. Wen, M. Trippenbach, Y. Band, P. S. Julienne, J. E. Simsarian, K. Helmerson, S. L. Rolston, and W. D. Phillips, Nature **398**, 218 (1999).
- [19] K. Rzążewski, M. Trippenbach, S. J. Singer, and Y. B. Band, Phys. Rev. A **61**, 013606 (1999).
- [20] M. Trippenbach, Y. B. Band, and P. S. Julienne, Phys. Rev. A **62**, 023608 (2000).
- [21] J. Heurich, H. Pu, M. G. Moore, and P. Meystre, Phys. Rev. A **63**, 033605 (2001).
- [22] E. V. Goldstein, K. Plättner, and P. Meystre, J. Res. Natl. Inst. Stand. Tech. **101**, 583 (1996).
- [23] E. P. Gross, Nuovo Cimento **20**, 454 (1961).
- [24] E. P. Gross, J. Math. Phys. **4**, 195 (1963).
- [25] L. P. Pitaevskii, Zh. Eksp. Teor. Fiz **40**, 646 (1961).
- [26] P. Öhberg, Phys. Rev. A **59**, 634 (1999).
- [27] P. Öhberg, Phys. Rev. A **61**, 013601 (2000).
- [28] S. M. M. Virtanen, T. P. Simula, and M. M. Salomaa, Phys. Rev. Lett. **86**, 2704 (2001).
- [29] N. Bogoliubov, J. Phys. USSR **11**, 23 (1947).
- [30] D. M. Stamper-Kurn, M. R. Andrews, A. P. Chikkatur, S. Inouye, H.-J. Miesner, J. Stenger, and W. Ketterle, Phys. Rev. Lett. **80**, 2027 (1998).
- [31] S. N. Bose, Z. Phys. **26**, 178 (1924).

- [32] A. Einstein, Sitzungber. Preuss. Akad. Wiss. **1925**, 3 (1925).
- [33] C. J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (CUP, Cambridge, 2001).
- [34] J. Javanainen and S. M. Yoo, Phys. Rev. Lett. **76**, 161 (1996).
- [35] J. I. Cirac, C. W. Gardiner, M. Naraschewski, and P. Zoller, Phys. Rev. A **54**, R3714 (1996).
- [36] A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).
- [37] Y. Castin and R. Dum, Phys. Rev. A **57**, 3008 (1998).
- [38] T. Bergeman, D. L. Feder, N. L. Balazs, and B. I. Schneider, Phys. Rev. A **61**, 063605 (2000).
- [39] A. Griffin, in *Proceedings of the International School of Physics - Enrico Fermi*, edited by M. Inguscio, S. Stringari, and C. E. Wieman (IOS Press, Amsterdam, 1999), p. 591.
- [40] N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).
- [41] D. A. W. Hutchinson, E. Zaremba, and A. Griffin, Phys. Rev. Lett. **78**, 1842 (1997).
- [42] E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics* (Pergamon Press, Oxford, 1980).
- [43] K. Góral, K. Rzążewski, and T. Pfau, Phys. Rev. A **61**, 051601 (2000).
- [44] S. Yi and L. You, Phys. Rev. A **61**, R041604 (2000).
- [45] S. Yi and L. You, Phys. Rev. A **63**, 053607 (2001).
- [46] L. Santos, G. V. Shlyapnikov, P. Zoller, and M. Lewenstein, Phys. Rev. Lett. **85**, 1791 (2000).
- [47] J.-P. Martikainen, M. Mackie, and K.-A. Suominen, Phys. Rev. A **64**, 037601 (2001).
- [48] P. A. Ruprecht, M. J. Holland, K. Burnett, and M. Edwards, Phys. Rev. A **51**, 4704 (1995).
- [49] R. J. Dodd, M. Edwards, C. J. Williams, C. W. Clark, M. J. Holland, P. A. Ruprecht, and K. Burnett, Phys. Rev. A **54**, 661 (1996).

- [50] B. P. Anderson, P. C. Haljan, C. A. Regal, D. L. Feder, L. A. Collins, C. W. Clark, and E. A. Cornell, *Phys. Rev. Lett.* **86**, 2926 (2001).
- [51] S. Inouye, M. R. Andrews, J. Stenger, H. J. Miesner, D. M. Stamper-Kurn, and W. Ketterle, *Nature* **392**, 151 (1998).
- [52] J. Stenger, S. Inouye, D. M. Stamper-Kurn, H. J. Miesner, A. P. Chikkatur, and W. Ketterle, *Nature* **396**, 345 (1998).
- [53] H. J. Miesner, D. M. Stamper-Kurn, J. Stenger, S. Inouye, A. P. Chikkatur, and W. Ketterle, *Phys. Rev. Lett.* **82**, 2228 (1999).
- [54] M. D. Barrett, J. A. Sauer, and M. S. Chapman, *Phys. Rev. Lett.* **87**, 010404 (2001).
- [55] H. Pu, C. K. Law, S. Raghavan, J. H. Eberly, and N. P. Bigelow, *Phys. Rev. A* **60**, 1463 (1999).
- [56] C. K. Law, H. Pu, and N. P. Bigelow, *Phys. Rev. Lett.* **81**, 5257 (1998).
- [57] C. V. Ciobanu, S.-K. Yip, and T.-L. Ho, *Phys. Rev. A* **61**, 033607 (2000).
- [58] M. Koashi and M. Ueda, *Phys. Rev. Lett.* **84**, 1066 (2000).
- [59] T.-L. Ho and S. K. Yip, *Phys. Rev. Lett.* **84**, 4031 (2000).
- [60] J.-P. Martikainen and K.-A. Suominen, *J. Phys. B* **34**, 4091 (2001).
- [61] P. Nozieres and D. Saint James, *J. Phys.* **43**, 1133 (1982).
- [62] J.-P. Martikainen and K.-A. Suominen, *Phys. Rev. A* **60**, 4175 (1999).
- [63] Y. Castin and J. Dalibard, *Phys. Rev. A* **55**, 4330 (1997).
- [64] T. L. Gustavson, A. P. Chikkatur, A. E. Leanhardt, A. Görlitz, S. Gupta, D. E. Pritchard, and W. Ketterle, *cond-mat/0108496* (2001).
- [65] E. A. Kuznetsov and S. K. Turitsyn, *Sov. Phys. JETP* **67**, 1583 (1988).
- [66] C. Josseland and Y. Pomeau, *Europhys. Lett.* **30**, 43 (1995).
- [67] V. Tikhonenko, J. Christou, B. Luther-Davies, and Y. S. Kivshar, *Opt. Lett.* **21**, 1129 (1996).
- [68] Y. S. Kivshar and B. Luther-Davies, *Phys. Rep.* **298**, 81 (1998).

- [69] J. Brand and W. Reinhardt, *J. Phys. B* **34**, L113 (2001).
- [70] A. E. Muryshev, H. B. van Linden van den Heuvell, and G. V. Shlyapnikov, *Phys. Rev. A* **60**, R2665 (1999).
- [71] J.-P. Martikainen, K.-A. Suominen, L. Santos, T. Schulte, and A. Sanpera, *Phys. Rev. A* **64**, 063602 (2001).
- [72] D. Vollhardt and P. Wölfle, *The Superfluid Phases of Helium 3* (Taylor&Francis, London, 1990).
- [73] T.-L. Ho, *Phys. Rev. B* **18**, 1144 (1978).
- [74] N. D. Mermin and T.-L. Ho, *Phys. Rev. Lett.* **36**, 594 (1978).
- [75] N. D. Mermin, *Rev. Mod. Phys.* **51**, 591 (1979).
- [76] J.-P. Martikainen, A. Collin, and K.-A. Suominen, cond-mat/0106301 (2001).
- [77] K.-P. Matzlin, W. Zhang, and B. C. Sanders, *Phys. Rev. A* **62**, 013602 (2000).
- [78] S. Tuchiya and S. Kurihara, *J. Phys. Soc. Jpn.* **70**, 1182 (2001).
- [79] R. K. Bhaduri, *Models of the Nucleon* (Addison-Wesley, New-York, 1988).
- [80] T. Isoshima, K. Machida, and T. Ohmi, *Phys. Rev. A* **60**, 4857 (1999).
- [81] M. J. Steel, M. K. Olsen, L. I. Plimak, P. D. Drummond, S. M. Tan, M. J. Collett, D. F. Walls, and R. Graham, *Phys. Rev. A* **58**, 4824 (1998).
- [82] K.-A. Suominen, B. M. Garraway, and S. Stenholm, *Phys. Rev. A* **45**, 3060 (1992).
- [83] B. M. Garraway and K.-A. Suominen, *Reports on Progress in Physics* **58**, 365 (1995).
- [84] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C 2nd ed.* (CUP, Cambridge, 1992).
- [85] M. Kira, I. Tittoonen, and S. Stenholm, *Phys. Rev. B* **52**, 10972 (1995).

- [86] H. Gould and J. Tobochnik, *Introduction to Computer Simulation Methods* (Addison Wesley, New-York, 1995).
- [87] N. Nygaard and K. Mølmer, Phys. Rev. A **59**, 2974 (1999).
- [88] M. J. Holland, D. S. Jin, M. L. Chiofalo, and J. Cooper, Phys. Rev. Lett. **78**, 3801 (1997).
- [89] M. Edwards, P. A. Ruprecht, K. Burnett, R. J. Dodd, and C. W. Clark, Phys. Rev. Lett. **77**, 1671 (1996).
- [90] L. You, W. Hoston, and M. Lewenstein, Phys. Rev. A **55**, R1581 (1997).