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VORTICES IN DILUTE BOSE-EINSTEIN CONDENSATES

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ABSTRACT OF DOCTORAL DISSERTATION

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VORTICES IN DILUTE BOSE-EINSTEIN CONDENSATES

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Opponent(s)	Professor Gordon Baym
Supervisor	Professor Martti M. Salomaa
(Instructor)	Professor Martti M. Salomaa

Abstract

Bose-Einstein condensation, first predicted by Bose and Einstein in 1924, was finally realized in dilute, weakly interacting gases of alkali atoms in 1995. A few years later, quantized vortices---intimately related to the phenomenon of superfluidity---were created and observed in these novel quantum many-body systems.

In this Thesis, vortices in dilute atomic Bose-Einstein condensates are studied theoretically and computationally using microscopic mean-field theory formalisms. Special emphasis is on the structure and the stability of vortices at finite temperatures. The formation of quantized circulation in Bose-Einstein condensates is investigated, as well as multiply quantized vorticity and the adiabaticity of the precessing motion of a vortex.

This research strongly relies on numerically solving the Gross-Pitaevskii equation for the macroscopic condensate wavefunction and the coupled Bogoliubov equations and their variants for the collective quasiparticle excitation eigenmodes. The computed elementary excitation spectra are used, for instance, in determining the local stability of various condensate states. The vortex formation process is studied at finite temperatures in terms of the surface modes of the condensate providing the Landau critical velocities for the breakdown of superfluidity. Free energy calculations are used for determining the thermodynamic equilibrium states.

Singly quantized, axisymmetric vortex states are found to be locally energetically stable even in the zero-temperature limit within the self-consistent finite-temperature approximations. This would imply for the vortex a precession direction opposite to that observed in the experiment. Adiabatic approximation of quantum mechanics is formulated for Bose-Einstein condensed systems and is applied to a case of a moving vortex line. The experimentally observed precessing motion of the vortex is found to be nonadiabatic. A method to create stable multiply quantized vortices using an additional pinning potential is presented. The computed critical trap rotation frequencies for vortex nucleation at finite temperatures are in agreement with experiments and the predictions of zero-temperature field theories.

Keywords Bose-Einstein condensate, vortex, superfluidity, mean-field theory, quasiparticle

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Preface

The research in this Dissertation has been performed in the Materials Physics Laboratory at the Helsinki University of Technology during the years 2000–2002. CSC-Scientific Computing Ltd is acknowledged for providing the supercomputer resources used for obtaining the computational results in this Thesis. Financial support from the Alfred Kordelin Foundation, the Research Council of Helsinki University of Technology and the Magnus Ehrnrooth Foundation is gratefully appreciated. This Thesis was typeset using the LaTeX 2_ε word processing system.

First and foremost, I would like to express my deep gratitude to Sami Virtanen—my mentor and a friend—for his expert guidance during my early steps in the field of Bose-Einstein condensation, and for his professional collaboration all the way to the end of this journey. Thanks are also due to the marvelous times we have enjoyed along the way.

Professor Martti Salomaa, the supervisor of this Dissertation, deserves my unconditional appreciation for his encouragement and trust in this Thesis project during these years. His prompt and invaluable assistance in the literary works and his dynamic leadership are greatly appreciated. He is also responsible for the excellent working facilities in the Materials Physics Laboratory and is warmly acknowledged for having provided me the opportunity to perform this work.

I thank the laboratory personnel for their contribution to the pleasant working environment and for the social aspects of the daily research ranging from company for a lunch through technical discussions on quasicles and other such creatures to the off-duty occasions. I would also like to thank the people I have met in a number of summer schools and conferences for stimulating and inspiring discussions.

Special thanks are due to all my friends for the frequent leisure time activities and the accompanying conversations. These people have kept my feet on the ground when needed and witnessed my take-offs when the landing has seemed secure.

I am deeply indebted to my parents and brothers for their love and support.

"Life lasts relatively longer if one travels
faster and remembers to laugh every
once in a while on the way"

Espoo, August, 2002

Tapio Simula

List of Publications

This Dissertation is a review of the author's work in the field of Bose-Einstein condensates, and in particular, quantized vortices in them. It consists of an overview and the following selection of publications in this field:

I S. M. M. Virtanen, T. P. Simula, and M. M. Salomaa, '*Structure and Stability of Vortices in Dilute Bose-Einstein Condensates*', Physical Review Letters **86**, 2704 (2001).

II S. M. M. Virtanen, T. P. Simula, and M. M. Salomaa, '*Comparison of mean-field theories for vortices in trapped Bose-Einstein condensates*', Journal of Physics A: Condensed Matter **12**, L819 (2001).

III S. M. M. Virtanen, T. P. Simula, and M. M. Salomaa, '*Adiabaticity Criterion for Moving Vortices in Dilute Bose-Einstein Condensates*', Physical Review Letters **87**, 230403 (2001).

IV T. P. Simula, S. M. M. Virtanen, and M. M. Salomaa, '*Stability of multi-quantum vortices in dilute Bose-Einstein condensates*', Physical Review A **65**, 033614 (2002).

V T. P. Simula, S. M. M. Virtanen, and M. M. Salomaa, '*Surface modes and vortex formation in dilute Bose-Einstein condensates at finite temperatures*', Physical Review A, **66**, 035601 (2002).

VI T. P. Simula, S. M. M. Virtanen, and M. M. Salomaa, '*Quantized Circulation in Dilute Bose-Einstein Condensates*', Computer Physics Communications **142**, 396 (2001).

Throughout the overview, these publications are referred to by their Roman numerals©.

Author's Contribution

The research reported in this Thesis has been carried out in the Materials Physics Laboratory at the Helsinki University of Technology. The author has been involved in all aspects of the research reported in Papers I–VI. All the computer programs employed in Papers I–VI have been written by the author and the numerical computations were performed by him; all figures were produced by the author. The author has actively participated in the writing of Papers I–III, and Papers IV–VI were mainly written by him. Results of the research reported in this Thesis have been presented in a number of international conferences by the author[a] and the collaborators[c].

[c] *Workshop on Rotating Bose-Einstein Condensates*, Trento, Italy (2000)
[a] *Conference on Computational Physics 2000*, Gold Coast, Queensland, Australia (2000)
[a,c] *EuroConference on the Physics of Atomic Gases at Low Temperature*, San Feliu de Guixols, Spain (2001)
[a] *International Conference on Theoretical Physics*, Paris, France (2002).

Contents

1 Introduction

"Ich behaupte, daß in diesem Falle eine mit der Gesamtdichte stets wachsende Zahl von Molekülen in den I. Quantenzustand (Zustand ohne kinetische Energie) übergeht, während die übrigen Moleküle sich gemäß dem Parameterwert $\lambda = 1$ verteilen. Die Behauptung geht also dahin, daß etwas Ähnliches eintritt wie beim isothermen Komprimieren eines Dampfes über das Sättigungsvolumen. Es tritt eine Scheidung ein; ein Teil »kondensiert«, der Rest bleibt ein »gesättigtes ideales Gas« ($A = 0, \lambda = 1$)."[1]

These are the words written by Albert Einstein in 1925 [1, 2] to describe the quantum-statistical phenomenon which has later become known as Bose-Einstein condensation. Only few months earlier, Satyendra Bose had derived Planck's law for photons using purely statistical methods. He sent the manuscript to Einstein who translated the paper into German and submitted it for publication [3]. At that time, however, the Bose-Einstein condensation was believed merely to be an anomaly of the ideal-gas approximation and that it would not occur in real, interacting gases.

Owing to the discovery of superfluidity in liquid helium in the late 1930's, the view changed. It has since become understood that the Lambda transition of ^{4}He is an example of Bose-Einstein condensation in a strongly interacting system. The identification of Bose-Einstein condensation in physical systems may be extended even further by identifying the phenomena of superconductivity in metals and the superfluidity of liquid ^{3}He with a Bose-Einstein condensation of the Cooper pairs. However, such an interpretation is more subtle since the ^{3}He atoms in liquid helium and the electrons in superconductors are fermions—not bosons.

Generally speaking, Bose-Einstein condensation occurs when a single quantum state of a many-body system becomes macroscopically occupied by bosonic particles. In practice, the condensation takes place in the lowest energy state, *i.e.*, in the ground-state of the system. Therefore, in order to create such a 'new state of matter'—a Bose-Einstein condensate (BEC)—the system must be cooled down to ultralow temperatures.

Major developments in the 1980's in the areas of laser cooling and trapping of neutral atoms in magnetic fields were crucial steps towards reaching the Bose-Einstein condensation in dilute weakly interacting gases [4–7]. Finally, in 1995 evaporative cooling methods facilitated the required record-low temperatures, leading to the achievement of Bose-Einstein condensation in magnetically trapped alkali-atom gases [8–10]. As a matter of curiosity, even a rigorous mathematical proof for the existence of Bose-Einstein condensation in such systems has later been provided [11].

Superfluidity in various systems is manifested through the occurrence of quantized vorticity. In distinction to normal gases, quantized vortices [12, 13] and vortex lattices [14, 15]

[1] Within the current standard notation $A = -\beta\mu$, where β is the inverse temperature, μ denotes the chemical potential, and $\lambda \equiv e^{-A}$ is the fugacity.

were expectedly found to exist in the trapped atomic BECs. In addition to vortices, other kinds of topological structures, such as solitons [16] and vortex rings [17] have also been observed in dilute BECs. Moreover, purely optical confinement of condensates has enabled one to trap their different internal spin degrees of freedom simultaneously [18]. Such spinor condensates may allow for the existence of even more complicated topological structures, *e.g.* monopoles [19] and skyrmions [20], in the optically trapped dilute Bose-Einstein condensates.

During the past few years, BECs have become a novel test bench for exploring many-body quantum phenomena in interacting systems [21–27]. The strength of the interactions between the atoms can be controlled by Feshbach resonances [28] and even the sense of the interaction can be reversed: a repulsion can be changed into an attraction, leading to the 'bosenova' implosion of the condensate [29]. The transition between the Mott insulator and superfluid states has been observed in BECs confined in optical lattices [30]. The atom lasers [31–33] and condensates in microtraps [34, 35] are expected to open up new avenues for applications. Especially gratifying from the theoretical point of view is the fact that there exist quantitatively accurate approaches yielding predictions in excellent agreement with experimental observations.

The contents of this Thesis is organized as follows. In Chapter 2 we present the general mathematical formalism underlying the research in this Thesis. A quantized vortex line is introduced as a topological defect in the system, arising from the requirement of the irrotationality of the condensate flow field. In the last Section of Chapter 2, the computational methods that have been employed in the numerical work [Paper VI] are outlined.

Answers to the question of how vortices penetrate condensates are provided in Chapter 3. There the experimental methods for creating vortices are described and subsequently discussed theoretically. Especially, the role of surface excitations as the seed for the nonlinear dynamics that leads to vortex formation was the motivation for Paper V and is discussed towards the end of Chapter 3.

Stability properties of vortices and their relation to superfluidity in gaseous BECs was the starting point for this Thesis project. Papers I and II were the first results from that research. The energetic stability of vortices with its connection to the precession of an off-centered vortex line are the topics of Chapter 4. In trying to explain the experimental observations for vortex precession in terms of stationary solutions for a time-independent system, the question on the degree to which the dynamics of a moving vortex line may be considered adiabatic in the quantum-mechanical sense occurred. Paper IV is devoted to studying this problem which is presented in a slightly different perspective in Chapter 4.

The penultimate Chapter 5 considers systems with multiple circulation, and in particular, vortex lattices and multiply quantized vortices. This Chapter is concluded with a discussion on rapidly rotating traps in which interesting phenomena are expected to emerge such as a transition from a vortex lattice to a giant vortex state with associated quantum-Hall physics.

Finally, Chapter 6 summarizes this Thesis.

2 Models

The most rudimentary approach for describing the phenomenon of Bose-Einstein condensation is the analytically soluble ideal-gas approximation described in elementary textbooks on statistical physics. To incorporate effects of weak particle interactions into the description, the celebrated zero-temperature Gross-Pitaevskii (GP) equation [36, 37] for the macroscopic condensate wavefunction is often introduced. In spite of neglecting the noncondensate gas, this nonlinear Schrödinger-type equation has become the standard tool for describing Bose-Einstein condensates due to its relative simplicity and power in predicting both static and dynamic experimentally verifiable phenomena. The collective quasiparticle excitation spectrum of the system may be obtained from the coupled Bogoliubov equations [38, 39] which are also the zero-temperature limit of a more general class of finite-temperature mean-field approximations. Alternatively, the Bogoliubov equations for the elementary excitations may be derived by considering the linear response of the condensate to a driving perturbation [40].

The problem of constructing the appropriate approximating field theory yielding the correct excitation spectrum for the Bose-condensed systems is highly nontrivial. Two crucial requirements for a proper approximation are that it is 'conserving' [41–43], which ensures that the calculated phonon velocity coincides with the compressional speed of sound and 'gapless', meaning that there is no energy gap in the excitation spectrum of the condensate [44, 45]. Put more technically, these requirements state that the poles of the single-particle Green's function and the density autocorrelation function of the system must coincide and that the Hugenholtz-Pines relation [46] must be satisfied, implying the existence of a Goldstone's boson [47].

The first-order Hartree-Fock-Bogoliubov (HFB) approximation and its variants are generically either nonconserving or they contain an energy gap, thus being deficient. Furthermore, they neglect the particle exchange processes and fail to describe the damping of the collective modes. More sophisticated theories filling these gaps have been introduced, for instance within the dielectric formalism [48] and using the quantum kinetic formulation [49–52] taking consistently into account the second-order Beliaev processes in the self-energies [53, 54]. These are, however, computationally more challenging than the static self-consistent approximations, such as the gapless but nonconserving HFB-Popov scheme described in more detail in the following Section. The coupled dynamics of the condensate and the noncondensate as well as the damping of the collective excitations may also be analyzed within the semi-classical approximation in the quantum-hydrodynamic limit [55].

This Chapter outlines the derivation of the model equations used for the numerical computations in Papers I–VI. We discuss how an axisymmetric vortex line is incorporated into the description and finally elucidate the numerical methods used in obtaining the results of Papers I–VI.

2.1 Theoretical formulation

A natural starting point for the microscopic description of a weakly interacting Bose gas is the second-quantized Hamiltonian

$$\begin{aligned}\hat{H} &= \int \hat{\Psi}^\dagger(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{r})\right]\hat{\Psi}(\mathbf{r})\,\mathrm{d}\mathbf{r} \\ &+ \frac{1}{2}\iint \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')V_{\text{int}}(\mathbf{r}-\mathbf{r}')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r})\,\mathrm{d}\mathbf{r}'\,\mathrm{d}\mathbf{r}. \qquad (1)\end{aligned}$$

Above, m is the mass of an atom and the bosonic field operators $\hat{\Psi}^\dagger(\mathbf{r})$ and $\hat{\Psi}(\mathbf{r}')$, respectively, create and annihilate particles at $\mathbf{r}$ and $\mathbf{r}'$; they obey the usual canonical commutation relations

$$[\hat{\Psi}(\mathbf{r}),\hat{\Psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}'); \qquad [\hat{\Psi}(\mathbf{r}),\hat{\Psi}(\mathbf{r}')] = [\hat{\Psi}^\dagger(\mathbf{r}),\hat{\Psi}^\dagger(\mathbf{r}')] = 0. \qquad (2)$$

Working within a particle number conserving formalism, we introduce the grand-canonical Hamiltonian $\hat{K} = \hat{H} - \mu\hat{N}$, where μ is the chemical potential and the particle number operator $\hat{N} = \int \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\,\mathrm{d}\mathbf{r}$. If the system is rotating at an angular velocity $\mathbf{\Omega}$, the proper thermodynamic potential to be minimized at a given temperature T is $\langle \hat{H}_\Omega\rangle - TS$, where S denotes the entropy and $\hat{H}_\Omega = \hat{K} - \mathbf{\Omega}\cdot\hat{\mathbf{L}}$ [56], the angular momentum operator being defined as $\hat{\mathbf{L}} = -i\hbar\int \hat{\Psi}^\dagger(\mathbf{r})(\mathbf{r}\times\nabla)\hat{\Psi}(\mathbf{r})\,\mathrm{d}\mathbf{r}$.

For dilute Bose-Einstein condensates, the usual approximation for the interparticle interaction is a contact potential $V_{\text{int}}(\mathbf{r}-\mathbf{r}') = g\delta(\mathbf{r}-\mathbf{r}')$. The coupling constant $g = 4\pi\hbar^2 a/m$ is given by the Born approximation for the scattering of particles in vacuum with the s-wave scattering length a determining the range of the interactions. This approximation is well justified in the ultra-cold, dilute atomic gases considered [57]. The confining potentials for the atoms in traps have usually been provided by approximately harmonic magnetic fields. Hence, an external trapping potential may be taken to be of the form $V_{\text{ext}}(\mathbf{r}) = \frac{1}{2}m\omega_{\text{tr}}^2\mathbf{r}^2$, where ω_{tr} is the (isotropic) harmonic trapping frequency.

Adopting the concept of spontaneously broken U(1) gauge symmetry[2], the macroscopic ground-state occupation below the critical condensation temperature is manifested by a finite expectation value for the boson field $\langle\hat{\Psi}(\mathbf{r})\rangle \equiv \phi(\mathbf{r})$. This allows one to separate the condensate wavefunction $\phi(\mathbf{r})$ from the rest of the field operator according to $\hat{\Psi}(\mathbf{r}) = \phi(\mathbf{r}) + \hat{\psi}(\mathbf{r})$. Substituting this decomposition into $\hat{H}_\Omega$ and expanding the cubic and quartic operator products according to the self-consistent mean-field approximation as [45]

$$\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \approx 4\tilde{n}(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}) + \Delta^*(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}) + \Delta(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}), \qquad (3a)$$

$$\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \approx 2\tilde{n}(\mathbf{r})\hat{\psi}(\mathbf{r}) + \Delta(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}), \qquad (3b)$$

where $\tilde{n}(\mathbf{r}) \equiv \langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle$ and $\Delta(\mathbf{r}) \equiv \langle\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle$, leaves us with an effective quadratic Hamiltonian $\hat{H}_{\text{eff}}$ that may be diagonalized by a canonical transformation. The anomalous

[2] For a critical discussion on this approach, see for example Ref. [25] and references therein.

average $\Delta(\mathbf{r})$, analogous to the gap function in superconductors, arises from the condensate-induced correlations between the noncondensate atoms, whereas $\tilde{n}(\mathbf{r})$ is the particle density of the atoms not in the condensed state.

Retaining all terms in Eq. (3) yields the full HFB Hamiltonian which predicts an energy gap in the spectrum. The somewhat *ad hoc* Popov approximation (PA) neglects the anomalous correlation function $\Delta(\mathbf{r})$ in order to remove the gap. However, this being the justification for the neglect of the non-negligible $\Delta(\mathbf{r})$ is rather questionable. If both $\tilde{n}(\mathbf{r})$ and $\Delta(\mathbf{r})$ are omitted, we recover the zero-temperature Bogoliubov approximation (BA). Discussion on these approximations in terms of Feynman graphs accounted for when calculating the self-energy diagrams within the Green's function formalism may be found in Ref. [58]. By making the coupling constant position dependent according to $g(\mathbf{r}) = g[1 + \Delta(\mathbf{r})/\phi^2(\mathbf{r})]$, one may keep the pair correlation function and obtain a gapless spectrum as well [59]. This leads to two additional, the so-called G1 and G2, approximations which contain a renormalizable ultraviolet divergence as also the HFB approximation does [60–62]. The modification of the coupling constant g may be justified by noting that the resulting effective interaction yields the correct approximation for the many-body T-matrix in the homogeneous limit [62]. The effects of these gapless approximations on the excitation spectrum and particle densities for vortex states are studied in Paper II. However, none of the above approximations treats the dynamical properties of the noncondensate, thus being inadequate for an accurate modeling of Bose-Einstein condensates at finite temperatures. Above discussed properties of the mean-field approximations are summarized in Tab. I below.

Table I: Properties of the various mean-field approximations employed in the numerical computations. Bullets denote an inclusion of the property within the corresponding approximation. In order to partially take into account effects of the momentum dependence of the collision processes, the condensate-condensate interactions are treated differently from the other collision processes within the G1 approximation, see for example Ref. [62].

	BA	PA	HFB	G1	G2
gapless	•	•		•	•
conserving			•		
noncondensate		•	•	•	•
anomalous average			•	•	•
interaction strength	g	g	g	$g, g(\mathbf{r})$	$g(\mathbf{r})$

The expectation value of the Heisenberg equation of motion for the field operator $i\hbar\partial_t\hat{\Psi}(\mathbf{r},t) = [\hat{\Psi}(\mathbf{r},t), \hat{H}_\Omega]$, yields in the rotating frame of reference the stationary Gross-Pitaevskii equation within the Popov approximation

$$\mu\phi(\mathbf{r}) = \left[\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r})\right) + g|\phi(\mathbf{r})|^2 + 2g\tilde{n}(\mathbf{r}) - \Omega L_z\right]\phi(\mathbf{r}), \tag{4}$$

where μ stands for the chemical potential[3], and the condensate wavefunction is normalized to the particle number N according to $\int[|\phi(\mathbf{r})|^2 + \tilde{n}(\mathbf{r})]\,\mathrm{d}\mathbf{r} = N$. Furthermore, L_z denotes the total orbital angular momentum along the rotation axis. In the limit of large particle number, the quantum pressure, the first term on the rhs of Eq. (4), may be neglected. This corresponds to the so-called Thomas-Fermi approximation allowing an approximate analytic solution for the condensate wavefunction and the chemical potential at zero temperature.

Taking Eq. (4) into account, the effective quadratic Hamiltonian may be diagonalized using the Bogoliubov transformation, $\hat{\Psi}(\mathbf{r}) = \sum_q[u_q(\mathbf{r})\hat{\alpha}_q + v_q^*(\mathbf{r})\hat{\alpha}_q^\dagger]$, and requiring the quasiparticle eigenmodes $u_q(\mathbf{r}), v_q(\mathbf{r})$ and the energy eigenvalues E_q to satisfy the coupled HFB-Popov equations

$$\begin{aligned} \mathcal{L}u_q(\mathbf{r}) + g\phi^2(\mathbf{r})v_q(\mathbf{r}) &= (E_q + \Omega L_z)u_q(\mathbf{r}), && \text{(5a)}\\ \mathcal{L}v_q(\mathbf{r}) + g\phi^{*2}(\mathbf{r})u_q(\mathbf{r}) &= -(E_q + \Omega L_z)v_q(\mathbf{r}). && \text{(5b)} \end{aligned}$$

Above, $\mathcal{L} \equiv -\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathbf{r}) - \mu + 2g[|\phi(\mathbf{r})|^2 + \tilde{n}(\mathbf{r})]$ and an expansion of $\tilde{n}(\mathbf{r})$ in terms of the quasiparticle basis yields the equilibrium noncondensate density

$$\tilde{n}(\mathbf{r}) = \sum_q \left[\left(|u_q(\mathbf{r})|^2 + |v_q(\mathbf{r})|^2\right)\frac{1}{e^{E_q/k_BT} - 1} + |v_q(\mathbf{r})|^2\right], \tag{6}$$

where the last term is a contribution of the quantum depletion $\propto \sqrt{na^3}$ which for these weakly interacting systems is in general less than one per cent. In the first-order mean-field approximations, the quasiparticles are assumed to be noninteracting, thus obeying the Bose-Einstein distribution. Requiring the Bogoliubov transformation to obey the bosonic commutation rules, Eq. (2), sets the normalization condition $\int[|u_q(\mathbf{r})|^2 - |v_{q'}(\mathbf{r})|^2]\,\mathrm{d}\mathbf{r} = \delta_{qq'}$ for the quasiparticle amplitudes. Negative-energy ($E_q < 0$) quasiparticle excitations with positive norm are referred to as 'anomalous modes'.

The self-consistent set of Eqs. (4), (5), and (6) with the appropriate normalization conditions needs to be solved iteratively. It is worth noting that temperature only occurs explicitly in the Bose-Einstein distribution function generating all the temperature-dependent effects via the density of the noncondensate gas. It is also the distribution function that causes

[3] However, due to the interactions there is in general a slight difference between the eigenvalue μ of the Gross-Pitaevskii equation and the true thermodynamic chemical potential $\mu' \equiv \partial E/\partial N$. Effects due to this discrepancy are studied for example in Ref. [63].

numerical difficulties in the convergence of the self-consistent sums when there exist quasiparticle modes close to the condensate energy ($E_q \to 0$). Given a self-consistent solution for the system, the free energy may be evaluated from the expression [64]

$$
\begin{aligned}
F &= \langle \hat{H}_{\text{eff}} \rangle + \mu N - TS & (7)\\
&= \mu N - \frac{g}{2} \int |\phi(\mathbf{r})|^4 \, \mathrm{d}\mathbf{r} - 2g \int |\phi(\mathbf{r})|^2 \tilde{n}(\mathbf{r}) \, \mathrm{d}\mathbf{r} \\
&+ \sum_i n_i E_i - \sum_i E_i \int |v_i(\mathbf{r})|^2 \, \mathrm{d}\mathbf{r} \\
&- T k_{\mathrm{B}} \sum_i [(1+n_i) \ln(1+n_i) - n_i \ln n_i], & (8)
\end{aligned}
$$

where n_i denotes the Bose-Einstein distribution function.

Part of a typical Bogoliubov quasiparticle excitation spectrum for the Bose-Einstein condensate is shown on the lhs of Fig. (1) as a function of the angular momentum quantum number, l. The presence of a quantized vortex line breaks the time-reversal symmetry, removing the degeneracy between the energies of the quasiparticles with opposite angular momenta [65]. This fact has been deployed in the experiments to detect the presence of a vortex by measuring the difference in the oscillation frequency between the quadrupole modes ($l = \pm 2$), thus obtaining the expectation value for the angular momentum of the condensate [66]. Some of the lowest collective modes have been identified on the rhs of Fig. (1). The Goldstone mode at zero energy ($E_q = 0$) and with the relative angular momentum ($l = 0$) corresponds to the condensate itself and the excitation energies and angular momenta are measured relative to it. The breathing mode ($l = 0$) describes the out-of-phase oscillations of the condensate whereas the Kohn (or dipole) mode ($l = 1$) determines the center-of-mass frequency. In this Bogoliubov spectrum, also one anomalous mode ($l = -1$) whose density is localized in the vortex core is present. The corresponding frequency may be associated with that of the off-center precessing motion of the vortex line [67]. The angular momentum states ($l = 1, 2 \ldots$) having the lowest energies are called surface modes; they may be related to the critical trap rotation frequency for vortex nucleation, see Paper IV and Chapter 3 below. For higher energies $|u_q(\mathbf{r})| \gg |v_q(\mathbf{r})|$, such that the Bogoliubov equations decouple and the corresponding quasiparticle excitation modes approach those of single-particle states. This property allows for an accurate description of the high-lying states within the semiclassical approximations.

2.2 Quantized vortex line

The idea of quantized vortices [68] was originally put forward by Onsager [69] and Feynman [70] when considering the superfluid flow properties of liquid helium. In nature, whirlwinds of various kinds, *e.g.*, tornadoes, waterspouts, dust devils, and swirls in the water serve as classical analogs to the vortices in the quantum realm.

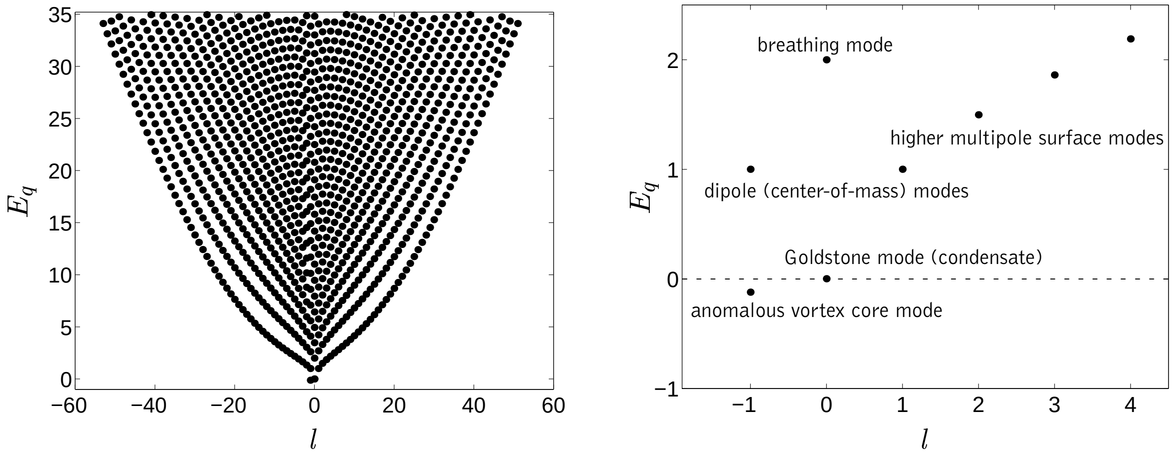

Figure 1: Part of the quasiparticle excitation spectrum for a vortex state. (lhs) Energies of the lowest quasiparticle modes as functions of the angular momentum quantum number l. Due to the presence of the vortex line, the time-reversal symmetry is broken which lifts the degeneracy between the angular momentum states with opposite signs. (rhs) few of the lowest collective modes individualized. Energies are measured with respect to the condensate state, for which $E_q = 0$, $l = 0$.

Starting from the expression for the quantum-mechanical particle current density

$$\mathbf{j} = |\phi(\mathbf{r})|^2\mathbf{v} = -\frac{i\hbar}{2m}[\phi^*(\mathbf{r})\nabla\phi(\mathbf{r}) - \phi(\mathbf{r})\nabla\phi^*(\mathbf{r})], \tag{9}$$

and separating the amplitude $|\phi(\mathbf{r})|$ and the phase $S(\mathbf{r})$ of the condensate wavefunction as $\phi(\mathbf{r}) = |\phi(\mathbf{r})|e^{iS(\mathbf{r})}$, we may identify the velocity field $\mathbf{v}$ of the condensate as the gradient of its phase

$$\mathbf{v} = \frac{\hbar}{m}\nabla S(\mathbf{r}). \tag{10}$$

From this expression, it immediately follows for the purely potential flow of the condensate that

$$\nabla \times \mathbf{v} = \frac{\hbar}{m}\nabla \times \nabla S(\mathbf{r}) = 0 \tag{11}$$

implying that the condensate flow must be irrotational unless there is a singularity in the phase of the condensate wavefunction. An integral of the velocity field around a closed loop is called circulation

$$\Gamma = \oint \mathbf{v} \cdot \mathrm{d}\mathbf{l} = \frac{\hbar}{m}2\pi\mathsf{m} \tag{12}$$

where m is an integer winding number. The condensate wavefunction must be single-valued and its phase may only change through a multiple of 2π around a closed path—hence the factor of $2\pi\mathsf{m}$ in the above equation.

It is thus inferred that if one tries to rotate the condensate it stays at rest until a certain critical threshold rotation velocity is reached, beyond which it becomes energetically favorable for the condensate to deform in such a way that a node in its macroscopic wavefunction develops. The line of vanishing condensate density is called (the core of) a vortex line and the circulation around it is quantized in units of h/m. These topological defects are often interpreted as being the signature of superfluidity in the system. Vortices may also be considered as being the quantized response of the irrotational condensate to an irresistible rotation. In addition to the revolving surface excitations, vortices are the most natural way a condensate may acquire angular momentum.

By comparing the kinetic and potential energy terms in the Gross-Pitaevskii equation, one may define a characteristic length scale over which density perturbations can occur in the condensate [71]. This length is called the healing length and it is given by the expression $\xi = 1/8\pi n_0 a$, where $n_0 = \max[|\phi(\mathbf{r})|^2]$ is the peak density of the condensate. The healing length describes the distance scale, such as the radius of a vortex core, over which the condensate wavefunction 'heals' if locally perturbed from its equilibrium value. Figure 2 shows the computed spatial structure of a singly quantized vortex line for an axisymmetric system. For a similar plot including the noncondensate present at finite temperatures see, for example, Paper I.

In the case of cylindrical symmetry, Eq. (10) implies the radial velocity field $v = \hbar\mathsf{m}/mr$ for the vortex state. Thus the velocity field would become supersonic at distances below the vortex core radius ξ, unless the condensate density vanishes there, thus ensuring that the kinetic energy density remains finite for $r \to 0$.

2.3 Numerical implementation

The work reported in Papers I–VI has strongly relied on the detailed numerical solutions for the stationary vortex states computed using the Gross-Pitaevskii and Bogoliubov equations. The computational details of our numerical methods are documented in Paper VI; in the following we concentrate on the relevant physics involved.

In the computational work we have thus far restricted our considerations to axisymmetric vortex states of the form $\phi(\mathbf{r}) = \phi(r)e^{i\mathsf{m}\theta}$, where m is the winding number determining the number of circulation quanta in the vortex. The equations are solved in a cylindrical coordinate system, $\mathbf{r} = (r, \theta, z)$ where the condensate is harmonically trapped in the radial direction. Periodic boundary conditions are imposed in the axial direction implying the condensate to have the shape of an infinitely long cylinder. However, the physics described by this system closest resembles that of a spherical or oblate condensate geometries in which, for instance, vortex bending is negligible.

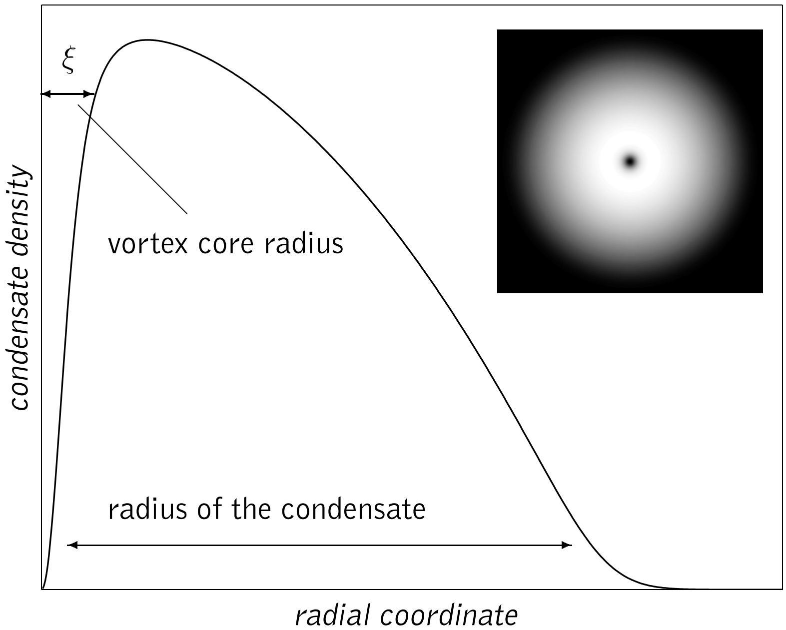

Figure 2: Radial distribution of the condensate density for an axisymmetric vortex line. A density plot from the top is shown in the inset where the black dot corresponds to a vortex core.

The basic computational mean-field approximation scheme is the following:

i) solve the Gross-Pitaevskii Eq. (4) for the condensate wavefunction $\phi(\mathbf{r})$ and the chemical potential μ self-consistently with the normalization condition $\int [|\phi(\mathbf{r})|^2 + \tilde{n}(\mathbf{r})]\, \mathrm{d}\mathbf{r} = N$, using suitable initialization;

ii) calculate the quasiparticle amplitudes $u_q(\mathbf{r}), v_q(\mathbf{r})$ and the excitation eigenenergies E_q using the coupled Bogoliubov Eqs. (5);

iii) compute the noncondensate density $\tilde{n}(\mathbf{r})$ and the anomalous correlation function $\Delta(\mathbf{r})$ by summing over the quasiparticle eigensolutions; see Eq. (6).

The above steps (i-iii) are repeated until convergence for the computed quantities to preassigned accuracy. At the end of the iteration, the desired thermodynamic quantities, such as the free energy, may be computed. It is the requirement of self-consistency in the equations that forbids analytic solutions and also makes the problem computationally challenging.

All equations are discretized on a spatial grid and the differential operators are handled within a finite-difference scheme. The generalized stationary Gross-Pitaevskii equation for the condensate wavefunction is solved iteratively using the relaxation method. The chemical potential for a fixed number of particles is determined by imposing the normalization condition for the condensate density. The coupled equations for the quasiparticle eigenmodes are turned into a matrix eigenvalue problem for a narrow band matrix. This is solved using the implicitly restarted Arnoldi method implemented in the ARPACK subroutine libraries [72]. The direct lattice discretization method is preferred owing to the resulting sparse structure for the eigenvalue problem which would also allow for taking into account nonlocal interactions with little additional computational cost. In comparison, an eigenfunction expansion method also used for computing Bogoliubov excitations for vortex states [73] yields a full matrix in the eigenproblem resulting in a worse computational scaling with the system size. Moreover, within the method used here, the different parts of the spectrum may be computed independently of each other facilitating more efficient computation.

To reduce the computational effort, we employ the semi-classical local density approximation for the high-lying quasiparticle states [74, 75]. In practice, this corresponds to assuming the quasiparticle amplitudes to be smooth functions of the coordinates, such that the kinetic energy operators may be replaced with their corresponding classical values. As a consequence, the Bogoliubov equations reduce to a pair of algebraic equations which are readily solved for the quasiparticle energies and amplitudes. The noncondensate density, for instance, may then be obtained from a simple integration over the momenta. This method yields an excellent approximation if the necessary cutoff is chosen at high enough energies, for which $|u_q(\mathbf{r})| \gg |v_q(\mathbf{r})|$, causing the Bogoliubov equations to decouple and the quasiparticles to become single-particle like. In order to further boost the computational efficiency, over(under)relaxation methods are employed when iteratively solving the condensate wavefunction (noncondensate density) [Paper VI].

3 Vortex formation

The evolution of a vortex-free condensate to a state containing quantized circulation is in general a complicated nonlinear dynamical problem. Nevertheless, using the simple underlying physical principles, it is possible to understand, both qualitatively and quantitatively, the circumstances leading to the onset of vortex formation. In this Chapter, the experimental methods used to create vortices in Bose-Einstein condensates are presented. The Landau criterion for the breakdown of superfluidity is expressed in a form suitable for studying the critical velocity for vortex generation in rotating condensates. The crucial role of the surface modes for the vortex nucleation process, studied in Paper V in greater detail at finite temperatures, is discussed.

3.1 Creation of vortices

Vortices were first created in a two-component Bose-Einstein condensate [12] using a coherent interconversion between the two internal states [76]. The condensate was first prepared in one hyperfine state and a part of the particles was then continuously transferred using microwave field induced transitions into another Zeeman substate, while rotating a laser beam around the initial condensate. This created a singly quantized vortex into the other component with the characteristic 2π phase winding around it.

Another early method to produce quantized vorticity in Bose-Einstein condensates was to use a stirring laser beam to rotate the condensate confined in a prolate trap geometry [13]. In effect, the vortices were created rather via thermal equilibration than by imprinting the vortex phase directly into the condensate. Later, similar methods, analogous to the rotating bucket experiments for the helium superfluids[4], were used to produce large regular lattices with over one hundred vortices in them [15, 77–79]. In addition to such extrinsic rotation, vortices have been generated intrinsically by the rotating thermal cloud [80]. In the latter case, the thermal gas is first rotated and only then cooled below the transition temperature of the Bose-Einstein condensation. Thus the rotating noncondensate component serves to act as the wall of a vessel defining the rotating environment for the newborn condensate. Vortices are then nucleated after the condensate has grown large enough to support quantized vorticity.

The physical principle underlying these measurements was to create a time-dependent rotating anisotropy in the harmonic trapping potential. Such a deformation acts as a revolving perturbation, allowing one to determine a rotating frame of reference in which the Hamiltonian becomes time-independent and the usual thermodynamic arguments apply. Specifically, for a given rotation velocity of the trap, the condensate tends to minimize the free energy by 'adjusting' its angular velocity to the value which closest matches that of the

[4] However, since gaseous condensates are trapped by smooth magnetic fields, there is no intrinsic surface roughness associated with the walls of the bucket that could be responsible for vortex nucleation as for the helium superfluids.

trap [25]. Thus, due to the quantum-mechanical nature of the vortices, there exists a finite threshold frequency of the trap needed to set the condensate into rotation. In a number of numerical computer simulations, the vortices in the rotating condensates have been verified to enter the system from the boundary of the condensate [81–84].

Moreover, vortices have been created through the 'snake' instability of decaying solitons [85] and in the turbulent wake of a moving object [78, 86]. Dark solitons have been observed to decay into vortex rings [17]. Most recently, vortices with topological charges $\mathsf{m} = 2$ and $\mathsf{m} = 4$ have been created [87] by exploiting the spin degrees of freedom of the condensate by continuously changing the direction of the magnetic field confining the atoms in the z direction [88, 89].

3.2 Landau criterion

According to a principle proposed by Landau, superfluidity may be destroyed through the creation of excitations in the system. Considering energy and momentum conservation for a massive object moving in a superfluid, Landau obtained the minimum velocity for the perturbation to create excitations in the condensate [90]. This Landau critical velocity is given by $v_c = \min_p[\epsilon(p)/p]$, where ϵ is the energy of an excitation carrying the momentum p. Specializing to a rotationally invariant system, the critical angular frequency for a circulating perturbation to create (quasiparticle) excitations into a Bose-Einstein condensate is obtained from the expression

$$\Omega_\ell = \min_l \left\{ \frac{\omega_l}{l} \right\}. \tag{13}$$

Here, $\hbar\omega_l$ is the quasiparticle excitation energy corresponding to the angular momentum $\hbar l$. Above Ω_ℓ, the energy of some excitation mode decreases below that of the condensate itself, see Figs. 3 and 4. This means that the condensate may lower its energy by transferring particles into that mode. Hence, the higher angular momentum quasiparticle states become populated and the associated density perturbation may evolve into a quantized vortex.

Comparing the free energies F_m between the singly quantized axisymmetric vortex state ($\mathsf{m} = 1$) and a vortex-free condensate ($\mathsf{m} = 0$), one may estimate the thermodynamic critical frequency

$$\Omega_c = \left. \frac{F_1 - F_0}{\hbar N} \right|_{\Omega=0} \equiv \frac{\Delta E}{L} \tag{14}$$

for vortex stability. Above Ω_c, F_1 becomes lower than F_0 in the rotating frame of reference and hence the state with a vortex is thermodynamically favorable. Another interpretation for Ω_c is to consider it as the Landau critical angular frequency for creating a topological vortex excitation in the condensate. However, the interpretations of Ω_ℓ and Ω_c are quite different, the former determining the threshold for generating quasiparticle excitations in the system by the rotating perturbation, the latter assuming that all the particles would be simultaneously excited into an angular momentum state $l = 1$. In principle, both Ω_c and Ω_ℓ should be determined in the rotating frame of reference through the conditions $F_1 = F_0$ and $\min \omega_l = 0$. In the zero-temperature limit, however, these critical frequencies may be determined in the laboratory frame since the energies of the quasiparticles and that of the vortex state transform under rotation, respectively, as $\omega_l^{\mathrm{rot}} \to \omega_l^{\mathrm{lab}} - \Omega l$ and $F_{\mathsf{m}}^{\mathrm{rot}} \to F_{\mathsf{m}}^{\mathrm{lab}} - \mathsf{m}\hbar\Omega N$.

3.3 Surface modes

In a number of recent experiments, the critical rotation frequency for the creation of vortices has been measured [13–15, 66, 78, 80, 91, 92]. Excluding one exception [78], all of these papers have reported nucleation thresholds for the entry of the first vortex much higher than the appropriate thermodynamic value, Ω_c. The explanation is that at rotation velocities for which the axisymmetric vortex state becomes energetically favorable, there still exists an energy barrier on the surface of the condensate, hindering vortices from entering the system. The implication is that vortices penetrate the condensate as a consequence of a dynamical process outbalancing the surface barrier, thus allowing thermal equilibration to the lower free energy state. Consequently, hysteretic behavior is expected when the trap rotation frequency is ramped above the nucleation threshold and back again [93].

In the hydrodynamic limit, it has been shown that the surface energy barrier vanish-

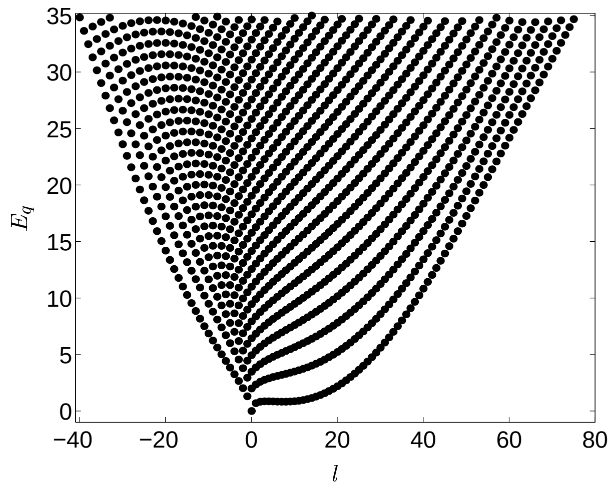

Figure 3: Quasiparticle excitation energies calculated in the rotating frame of reference for $\Omega = 0.3\ \omega_\perp$ as functions of the angular momentum quantum number l. The anomalous mode ($l = -1$) has gained enough in energy to become positive, whereas a further increase in the rotation frequency would suppress the lowest surface modes to energies below that of the condensate state. For a further discussion on the surface instability of a rotating Bose-Einstein condensate, see for example Refs. [94, 95], and Paper V.

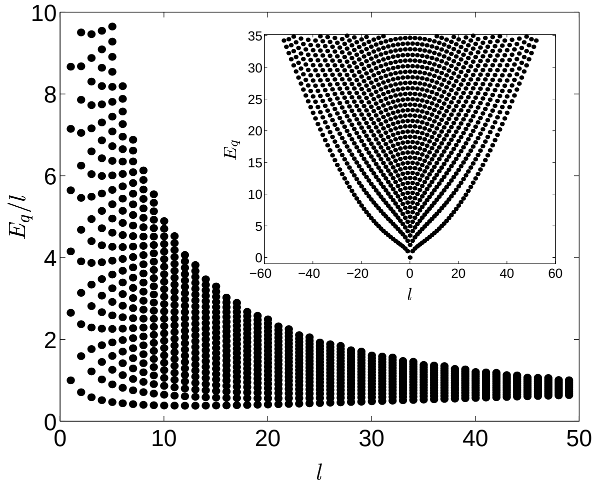

Figure 4: Quasiparticle energies for the nonvortex state scaled by their corresponding angular momentum quantum numbers, l. States up to energies $E_q = 50\,\hbar\omega_\perp$ have been plotted. The inset shows a part of the corresponding symmetric spectrum. The minimum of E_q/l defines the Landau critical frequency, see Eq. (13), for the generation of excitations in the system.

es at the Landau critical velocity for the generation of surface modes in the condensate [96]. These quasiparticle excitations are density perturbations localized in the vicinity of the condensate surface, allowing for continuous transfer of energy and angular momentum to the condensate[5]. The vortices are thus expected to be generated via nonlinear dynamical evolution from the surface modes propagating around the exterior of the condensate.

The theoretical predictions for the vortex nucleation threshold in terms of the Landau critical frequency, Ω_ℓ, are in reasonable agreement with many of the available observations. However, in highly prolate condensate geometries [13, 14, 66, 91] or when the stirring potential has effectively a quadrupolar shape [92], vortices are seen only at very high rotation frequencies $\Omega/\omega_\perp \approx 0.7$, where $\omega_\perp$ is the trapping frequency in the plane perpendicular to the trap rotation axis. This is likely to be explained by the excitation of quadrupolar surface modes, for which ω_l/l yields the value $\approx 0.7\,\omega_\perp$ under quite general circumstances.

In Ref. [97], the dispersion relation was obtained for harmonically trapped BECs in the Thomas-Fermi limit. For the surface modes, the dispersion relation reduces to $\omega_l = \omega_\perp\sqrt{l}$, which yields for low angular momentum states a fair estimate. Especially, the quadrupole mode ($l = 2$) resonance is obtained when the trap rotates at the frequency $\approx 0.7\,\omega_\perp$.

However, for high angular momentum states, the hydrodynamic prediction fails and yields a divergence in Ω_ℓ. Contrary to this, there exists a minimum in ω_l/l calculated using the Bogoliubov equations. This minimum defines the Landau critical velocity for the nucleation of vortices and is found to be in reasonable agreement with the experimen-

[5]Generically, the rotating states of Bose-Einstein condensates are a superposition of different occupied surface modes and quantized vortices [27].

tal observations [98], see also Paper V. In one of the experiments, however, vortices were observed already at lower rotation velocities, coinciding with the corresponding thermodynamic equilibrium value Ω_c [78]. A possible explanation for such a low threshold value is that the vortices were created in the wake of the turbulent flow of the small stirrer for which the local fluid velocity may exceed the effective rotation velocity of the stirrer [99]. The motivation for Paper V was to study the temperature dependencies of Ω_c and Ω_ℓ in order to find out the role of the noncondensate in the vortex nucleation process.

Finally, it is worth noting that in the presence of attractive interactions ($g < 0$), the free energy of the rotating system is minimized by placing the angular momentum into the dipole surface mode ($l = 1$), corresponding to the center-of-mass motion of the condensate [100]. The implication thus is that no vortices are expected to be created in rotating Bose-Einstein condensates with attractive interactions [27]. Moreover, in the noninteracting limit ($g = 0$), any small perturbation, *e.g.*, an asymmetry in the trap potential has been shown to lead to the inversion of the topological charge of the vortex thus implying a structural instability in the vortex state [101].

4 Stability of vortices

This Chapter is devoted to a discussion on the stability of quantized vortices in trapped Bose-Einstein condensates. On a general level, the different stability criteria may be divided into conditions of dynamical and thermodynamical stability. Usually, instabilities in the dynamical sense are accompanied by complex eigenvalues, whereas negative (excitation) energies are a signature of thermodynamic instability. These concepts and their implications for the existence and stability of quantized vortices in BECs are the subject of this Chapter.

We focus to consider stationary states and hence restrict to study the energetic stability in terms of a state being a global[6] or a local minimum of the free energy functional. Besides the different stability criteria, the problem of a precessing off-axis vortex line is presented and its connection to the stability issues is discussed. At the end of the present Chapter, we raise the issue of adiabaticity in the context of quantum mechanics and apply it to a moving vortex line.

4.1 Thermodynamic stability

A convenient way to determine the thermodynamic stability in the BEC systems under consideration is in terms of the free energy $F = \langle \hat{H}_{\text{eff}} \rangle - TS$, see Eq. (8). The state which has the lowest free energy under the given external circumstances, such as temperature and rotation frequency of the trap, defines the globally stable state. The metastable states, *i.e.*, states which are only local minima of the free energy, are thus eventually expected to decay. Nevertheless, under suitable circumstances, *e.g.*, when there is negligible dissipation in the system or a potential barrier, the metastable states may have lifetimes comparable to that of the condensate itself; hence such states may be observable in experiments. However, rigorously speaking, even the condensate itself exists only in a metastable state, its lifetime being determined by the three-body recombination rate.

In nonrotating systems, the vortex-free state has the lowest free energy. If the condensate possesses angular momentum, for example in the form of vortices, the energy of the system is lowered by the amount $\mathbf{\Omega} \cdot \hat{\mathbf{L}}$. Hence there exists a thermodynamic critical rotation velocity Ω_c, defined by the condition $F_1 = F_0$, at which the singly quantized vortex state becomes globally stable (at a given spatial point). At zero temperature, this frequency for a singly quantized axisymmetric vortex line is given by Eq. (14). For a schematic illustration of the stability of a vortex in a rotating trap, see Fig. 5.

In the general case, considering multiply quantized vortices and vortex lattices, the free energy landscape becomes more complicated as there exists a large number of different configurations that have to be taken into account when searching for the minima of the free energy functional. Also, interactions between the vortices complicate the analysis.

[6] Here we only consider axisymmetric configurations, although the true ground-state corresponds to a bent vortex [102, 103]. However, in the oblate and spherical trap geometries, vortex bending is negligible.

4.2 Local stability

A state of the condensate is said to be locally energetically stable if it is a local minimum of the energy functional. In terms of the elementary excitation energies, local energetic stability requires the spectrum of the condensate to be positive definite. If there exist negative quasiparticle excitation energies (with respect to the condensate state) with positive norm, called anomalous modes, the condensate may lower its energy by transferring atoms into these modes. When sufficiently populated, such a mode may lift to positive energies or become the new macroscopic ground-state.

Considering an axisymmetric singly quantized vortex line in a nonrotating trap, one finds that the free energy of a condensate with a vortex is larger than that of a state without the vortex. Moreover, the zero-temperature Bogoliubov quasiparticle spectrum for the vortex state contains one or more anomalous modes that are localized in the vortex core and possesses the relative angular momentum $-\mathsf{m}\hbar$ with respect to the condensate. Thus we conclude that the singly quantized vortex is both locally and globally unstable in the nonrotating trap. Physically, if dissipation is nonnegligible, this energetic instability would imply that an infinitesimal displacement of the vortex from the symmetry axis would cause it to spiral outwards—ultimately causing the vortex to annihilate at the edge of the condensate [104].

When the system is rotated, an anomalous mode with the energy $\hbar\omega_{\mathrm{a}}$ and the angular momentum $-\mathsf{m}\hbar$ will gain in energy the amount $\mathsf{m}\hbar\Omega$ due to the rotation. Hence, the singly quantized vortex line will become locally energetically stable at $\Omega_{\mathrm{a}} = \max|\omega_{\mathrm{a}}|$, in the sense that then the spectrum of the condensate will contain only positive-energy quasiparticle excitations. Similarly, the singly quantized axisymmetric vortex state becomes globally stable at the critical rotation frequency, Ω_{c}. In prolate condensate geometries in which the true stationary configuration above Ω_{c} corresponds to a bent vortex [102, 103], the frequency threshold for the local stability of a straight vortex line may even exceed Ω_{c} [67].

However, the situation is quite different if the noncondensate particles, relevant at finite temperatures, are included in the theoretical description. Then the thermal gas component accumulating in the vortex core can effectively act as a stabilizing potential and lift the anomalous mode to positive energies [73], see also Paper I. In fact, all the self-consistent finite-temperature approximations studied in Papers I and II predict no anomalous modes even in the $T = 0$ limit, suggesting that the axisymmetric vortex line could be locally energetically stable even in nonrotating traps. This apparent contradiction between the zero-temperature Bogoliubov approximation and the finite-temperature theories in the low-temperature limit seems surprising in light of their close agreement for the collective modes in irrotational systems [105].

Besides the local energetic instabilities implied by the anomalous modes, complex eigenvalues may emerge in the spectra of BECs. Such imaginary frequencies occur, for instance, in the case of multiquantum vortices or when the condensate is perturbed by the

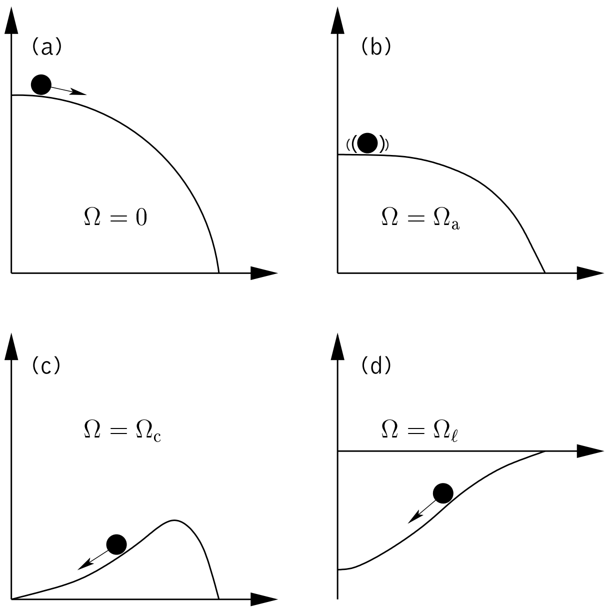

Figure 5: Schematic for the stability of a vortex as a function of the trap rotation frequency. (a) In a nonrotating trap, dissipation would cause the vortex slightly displaced from the center of the trap to spiral out of the condensate. (b) At the metastability frequency Ω_{a}, the anomalous core mode turns positive and the axisymmetric vortex state becomes metastable. (c) At Ω_{c}, the singly quantized vortex becomes thermodynamically favorable at the center of the trap. However, there exists an energy barrier on the condensate surface preventing the vortex from entering the condensate. (d) Finally, at the Landau critical frequency Ω_{ℓ}, the surface barrier vanishes and vortices may spontaneously penetrate the system. For a quantitative discussion on the energy landscape as a function of the vortex position in a rotating trap, see for example Refs. [108, 109] and [26].

presence of a soliton. They signal a dynamical instability in the system, thus being more severe from the point of view of the subsequent time-development of the condensate than the local energetic instabilities; for further discussion, see for example Refs. [106, 107] and references therein.

4.3 Vortex precession

If a vortex line is displaced from the center of a stationary trap, the vortex starts to precess around its equilibrium position. In general, the vortex would exhibit spiraling motion but if the dissipation in the system is weak, the vortex can merely precess around the symmetry axis. Such precession of the vortex has been experimentally observed and the relevant precession frequency has been measured [110]. Moreover, excluding the so-called rogue vortices, the direction of the precession was found to be in the positive direction, *i.e.*, in the same sense as that of the condensate flow. In addition to the precession, tilting motion of the vortex line, induced by anisotropy in the trap potential, has been measured [111].

The precessing motion of the vortex may be understood in terms of the Magnus effect which induces deviation in the trajectory of rotating objects of various kinds due to the anisotropy in the flow field around them [68, 112]. Phenomenologically, the vortex core may be considered as a bubble in a viscous fluid. The density and pressure gradients due to the inhomogeneity in the particle density and the asymmetry in the velocity field, respectively, result in an effective buoyancy force generally towards the outward direction in nonrotating traps, see Fig. 6. In a dissipationless system, energy and angular momentum conservation together with the Magnus effect are then responsible for the precessing motion of the vortex. However, a delicate balance between the various forces, such as the Magnus force and the drag force due to the thermal excitations, determines the direction of the resultant buoyancy force, $\mathbf{F}_{\mathrm{b}}$, and thus the direction of precession according to $\mathbf{v}_{\nu} = -\mathbf{F}_{\mathrm{b}} \times \hat{e}_z / |\phi(\mathbf{r})|^2 h\mathsf{m}$. In particular, sufficient external rotation of the system modifies the flow field around the vortex core in such a way that the vortex would end up spiraling inwards to the center of the trap, thus becoming stable in the rotating trap.

Interestingly enough, the frequency of the anomalous mode may be associated with the precession frequency of the slightly displaced vortex line and the sign of the excitation with the sense of the precession [67, 113]. The interpretation of the anomalous mode with energy $\hbar\omega_{\mathrm{a}}$ and relative angular momentum $-\mathsf{m}\hbar$ is that the condensate would tend to populate that state, thus facilitating a transition back into the nonrotating ground-state. The density perturbation associated with the anomalous mode $\propto e^{i(l\theta+|\omega_{\mathrm{a}}|t)}$ is then viewed as a revolving perturbation with the frequency $\omega_{\mathrm{a}}(\Omega)$ in the positive sense [114]. Especially, due to the linear dependence between ω_{a} and Ω, this implies that if the trap rotation is swept through ω_{a}, the vortex should slow down and eventually change its direction of precession.

For a vortex in two-component condensates, it has been shown [115] that the precession direction can also be opposite to the direction of the condensate flow for $\Omega = 0$. In general, to change the precession direction it is sufficient to generate a local minimum in the free energy since the precession direction depends on its gradient. This may be achieved simply by rotating the system but also suitable engineering of the density distribution would allow counter-precessing vortices.

Finite-temperature calculations reported in [73] and in Papers I and II and also discussed in more length in [116] suggest that the noncondensate gas in the vortex core could cause sufficient density modification to allow stable vortices even in nonrotating traps. However, the Popov approximation employed neglects dynamical effects of the noncondensate and may thus be liable in its predictions in this sense. To settle the precession problem, more experimental investigations in addition to the available data [110] would be needed. Also an implementation of the quantum kinetic equations, taking into account the full coupled dynamics of the condensate and noncondensate, would merit further studies.

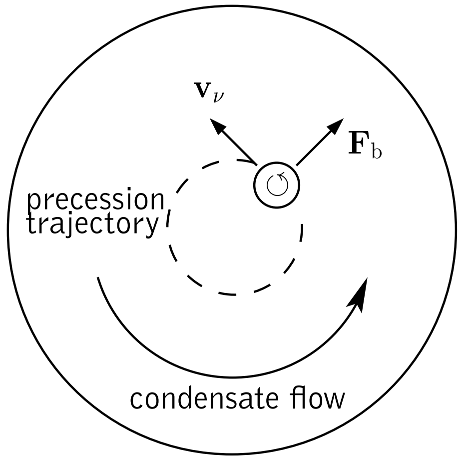

Figure 6: Diagram illustrating the precession of a vortex line. Due to the Magnus effect, an off-centered vortex line starts to precess around its equilibrium position. The direction of the vortex velocity $\mathbf{v}_\nu$ is perpendicular to both the axis of circulation and the effective buoyancy force $\mathbf{F}_\mathrm{b}$ exerted on the vortex. Thus the sense of the precessing motion is determined by the pressure and density gradients, respectively, due to the flow field asymmetry around the vortex core and the inhomogeneity of the condensate density. Moreover, drag forces due to the thermal excitations may affect the vortex motion. If the direction of the resultant buoyancy force is outwards (inwards) with respect to the center of the condensate, the vortex precesses in the clockwise (counter-clockwise) direction with respect to the condensate flow. In the absence of dissipation, the path of the vortex will follow a circular trajectory depicted by a dashed line in the figure.

4.4 Adiabaticity

The difference between theory and experiment raises the question as to what extent can one successfully model dynamic phenomena such as the precession of a vortex line within the stationary formalism? An answer to this question is facilitated by the adiabatic approximation of quantum mechanics [117], and its application to dilute Bose-Einstein condensates is studied in Paper III.

In systems for which the time evolution of the Hamiltonian is slow enough, the eigenstates of the system change continuously in time and the exact time-dependent eigenstates may be approximated by the eigenfunctions of the instantaneous Hamiltonian. The adiabatic approximation of quantum mechanics yields a measure for determining the extent to which such an approximation is valid. Formally, the criterion of adiabaticity for time-dependent Bogoliubov equations may be derived by expanding the solutions of the time-dependent equations in the basis of the corresponding instantaneous quasistationary eigensolutions. Requiring slow time evolution of the physical quantities results in the adiabatic approximation in terms of the quasistationary eigenstates. The adiabatic approximation may also be applied to more general dynamical problems than the moving vortices considered here.

In particular, we are interested to find out whether the difference between the predictions of the Popov and Bogoliubov approximations for the sign of the anomalous mode and thence that of the vortex precession direction observed in the experiment might be due to the nonadiabaticity of the precessing vortex. The opposite sign for the lowest vortex core mode is essentially due to the partial filling of the vortex core by the noncondensate gas within the stationary PA. If it were absent, the results of the BA would apply in this regard even at $T \neq 0$. If the velocity of the vortex is too high, the quasiparticles localized in the vortex core cannot follow the core rigidly, *i.e.*, adiabatically.

Qualitatively, the criterion of the adiabatic approximation for the situation studied may be discussed in terms of a variant of the Heisenberg uncertainty principle $\delta E \delta t \approx \hbar$. The Hamiltonian describing the vortex line and the quasiparticles moving with it at the velocity v changes over the time scale ξ/v, where ξ is the radius of the vortex core. Requiring this time lapse to be much longer than the intrinsic quantum-mechanical oscillation periods of the system, *i.e.*, $\xi/v \gg \delta t$, we obtain a criterion for the vortex velocity, $v \ll \xi\omega_{\mathrm{a}}$, where we have used for the 'energy uncertainty' δE the difference between the energies of the anomalous mode and that of the condensate ground-state. Inserting the values appropriate for the experiment we obtain $v \ll 10\ \mu$m/s, in comparison to the experimental observation $v_{\mathrm{exp}} \approx 100\ \mu$m/s [110]. The conclusion is that owing to the relatively high velocity of the vortex, the quasiparticle cloud may not be able to adiabatically follow the motion of the vortex core [Paper III].

5 Multiple circulation

In addition to an isolated singly quantized vortex, Bose-Einstein condensates can support a lattice of single-quantum vortices when the rotation frequency of the trap is high enough. In principle, also vortices with multiply quantized circulation can be formed but such structures are energetically disfavored and are expected to decay into a set of singly quantized vortices. Recently, however, vortices with two and four circulation quanta have been topologically created in BECs [87], but the lifetime of such structures remains unknown.

In this Chapter, we discuss the rotational properties and the structure of vortex lattices. A stabilization method is presented for multiply quantized vortices by an additional pinning potential. The richness in the vortex phase diagram is further explored by considering traps that are rotated at nearly the frequency of the harmonic trapping potential.

5.1 Vortex lattices

When the harmonic trap rotation frequency exceeds the threshold for vortex nucleation, single-quantum vortices penetrate the condensate. Due to the repulsive interaction between them, they tend to arrange themselves into a triangular Abrikosov lattice. Such structures have been investigated computationally early on [81] and observed experimentally [15, 77–79]. Characteristically, these lattices extend and remain highly oriented all the way to the edge of the condensate. Also different lattice structures have been observed and structural defects, such as dislocations and grain boundaries, have been reported [15]. The nonequilibrium properties of vortex lattices have been studied by disturbing the lattice with quadrupole oscillations [79]. As a result, the lattice planes of an undisturbed hexagonal lattice were seen to shift to a nearly orthorhombic shape and sheet-like structures were observed in which rows of individual vortices appear to have merged. Also the formation and decay of vortex lattices at finite temperatures has been studied experimentally [77].

According to the correspondence principle, vortex lattices mimic solid-body rotation, for which $\nabla \times \mathbf{v} = \nabla \times \Omega \times \mathbf{r} = 2\Omega$, by distributing the vortices over the condensate area in such a way that when coarse grained over the individual vortices, the average vorticity is the same as that of a rigidly rotating liquid. This is achieved if the areal density of the vortices in a lattice is given by $n_\nu = 2\Omega m/h$ which may be used to estimate the number of the vortices in a condensate as a function of the rotation frequency. However, the behavior of the condensate corresponds to that of a classical rigid-body rotator only on average as the flow field of the condensate must vanish in the vortex cores.

With increasing rotation frequency of the trap, the condensate cloud expands and becomes thinner while accommodating more vortices. In the limit of extreme rotation frequency $\Omega = \omega_\perp$, the outward centrifugal force due to the rotation balances the confining trapping force and the motion of the condensate particles become ballistic.

5.2 Multiquantum vortices

The well-known argument against the existence of multiquantum vortices is obtained by considering the energy of a vortex line per unit length $E(\mathsf{m}) \propto \mathsf{m}^2$. It is thus inferred that a collection of a single-quantum vortices with the same vorticity has a lower energy than that of an $\mathsf{m}-$fold quantized vortex. This means that the multiquantum vortex is unstable against dissociation into a lattice of singly quantized vortices. The inclusion of the effects of harmonic trapping and the repulsion between the vortices does not change this conclusion [27].

There are, however, ways of avoiding the dissociation instability problem. In a system having sufficiently weak interactions between the particles, singly quantized vortices may be 'squeezed' together by applying a stronger than harmonic, *e.g.*, a quartic confining potential [118]. Such strongly confining potentials could possibly be realized with the use of Laguerre-Gaussian beams [119]. In addition, a topological method for creating multiply quantized vortices—with the winding number a multiple of two—by deploying the spin degrees of freedom of the condensate has been suggested [88, 89]. Recently, using such a method, vortices with two and four circulation quanta have been experimentally created and observed [87]. These experiments could be used to study the lifetime of multiquantum vortices, which is limited by the dissociation instability. They also yield information on the mutual vortex interactions.

In Paper IV, we investigate yet another method for producing multiply quantized circulation in rotating Bose-Einstein condensates. This scheme relies on the stabilizing effect of an additional pinning potential repelling atoms from its volume. In practice, such a potential could be created by focusing a blue detuned laser beam in the vicinity of the trap center[7]. Another advantage of using the pinning potential is that it renders the multiquantum vortex states also locally stable, which cannot be achieved by a mere rotation of the trap. If created, it would be interesting to study the dissociation dynamics of the decaying multiquantum vortex when the pinning potential would be turned off.

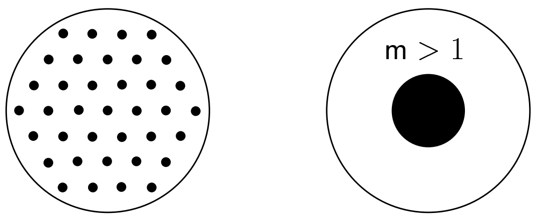

Figure 7: Illustration of a lattice of singly quantized vortices (lhs) and a multiquantum vortex (rhs).

[7] In a strict sense, a multiquantum vortex state should contain only a single point where the condensate density and its phase vanish, in distinction to a genuinely toroidal geometry with a quantized superflow around the torus.

5.3 Rapidly rotating traps

In harmonically confined condensates, the maximum velocity for the trap rotation is limited by the trapping frequency $\omega_\perp$ [120]. However, by using confining potentials that rise faster than quadratically, it is possible to surpass beyond that limit and to discover interesting emergent physics [114, 118, 121, 122].

To draw an analogy with type-II superconductors, the vortex-free Bose-Einstein condensate may be associated with the Meissner state of a superconductor. At the critical rotation frequency Ω_{c1}, the condensate is penetrated by vortices. Similarly, the lower critical field, H_{c1}, destroys the Meissner state as the field pierces the superconductor along quantized vortex filaments. As the field strength is further increased, the vortices fill the whole superconducting sample volume as the mean separation between them becomes comparable to their core radii. Thus a transition to the normal state occurs at the upper critical field, H_{c2}. But the scenario of what occurs in dilute BECs when the trap rotation is increased to high rotation frequencies differs from that of superconductors. Moreover, in the helium superfluids the corresponding limit of rapid rotation is unattainably high and therefore can not be studied experimentally.

When the rotation velocity exceeds Ω_{c1}, the Bose-Einstein condensate, while expanding spatially, becomes populated by singly quantized vortices. More vortices penetrate the condensate in proportion to the rotation frequency forming a uniform Abrikosov lattice. Close to the frequency $\omega_\perp$, the system may enter the quantum-Hall regime [123–126]. Ultimately, the mean separation between the vortices becomes comparable with the radius of the vortex cores and a single density minimum—or a giant vortex state—is expected to form. The condensate flow in the remaining toroidal condensate may even become supersonic. Finally, at yet higher rotation velocities, the radii of the vortices—being comparable to the peak density of the condensate—diverge. If the condensate would be confined by hard walls, however, the system could become essentially two-dimensional and a Kosterlitz-Thouless phase transition could possibly occur in such a system [122].

6 Discussion

In this Dissertation, vortices in dilute Bose-Einstein condensates are studied theoretically and computationally. This work has been motivated by the remarkable series of past and expected future experiments unveiling the extraordinary physical properties of these novel many-body quantum systems—Bose-Einstein condensates. Especially, the stability of different vortex structures has been in the focus of the research reported. Also, the problem of a precessing vortex line and the mechanisms for vortex formation have been considered in detail. The main conclusions of the work are briefly stated below:

Paper I: The structure and excitation spectrum of an axial vortex line were computed self-consistently at ultralow temperatures. No anomalous vortex mode was found even in the zero-temperature limit, in contrast to the prediction of the nonself-consistent Bogoliubov approximation. Furthermore, this result would imply a direction for the precessing vortex opposite to that observed in the experiment.

Paper II: The predictions of three different gapless finite-temperature theories were compared. Especially, large differences were found between the approximations in the energies of the lowest vortex core modes. Accordingly, it was argued that such a notable difference could be used to experimentally discriminate the validity of the approximations.

Paper III: The adiabatic approximation for dilute Bose-Einstein condensates was formulated. Specializing to the case of a moving vortex line, it was shown that the adiabaticity criterion was not satisfied in the vortex precession experiment. The nonadiabaticity was suggested to be a possible partial reason for the observed precession direction of the vortex.

Paper IV: A method for creating multiply quantized vortices in harmonically trapped Bose-Einstein condensates by adding an external pinning potential was proposed. Such multiquantum vortices were found to be both locally and globally stable and were argued to be observable using current experimental techniques.

Paper V: The formation processes of vortices were studied at finite temperatures. The critical trap rotation frequencies for the generation of surface modes with different multipolarities were calculated for a range of temperatures. They were found to be in fair agreement with the experimental observations and the predictions of zero-temperature field theories for vortex nucleation.

Paper VI: Efficient numerical methods for computing the structure and the quasiparticle excitation spectra of dilute Bose-Einstein condensates were reported.

The work reported in this Thesis could be further extended to encompass studies of condensates with spin degrees of freedom. For an accurate comparison with the experiments, all the three spatial dimensions should be treated on an equal footing in the numerical computations. Time-dependent, dynamical phenomena would be an interesting subject for further studies. Especially, the problem of the precessing vortex should be explored thoroughly and the true character of the anomalous vortex core mode revealed. For that purpose, a computationally feasible second-order finite-temperature theory, treating consistently the particle exchange processes between the condensate and noncondensate components as well as the damping of the collective modes, should be developed.

The realization of Bose-Einstein condensation in dilute gases has provided the possibility to study topological defects, *e.g.* vortices, in these novel quantum many-body systems. Vortices, vortex lattices, vortex rings, and most recently also multiquantum vortices have thus far been produced in the experiments. In the future more exotic structures, such as skyrmions and monopoles may be created and observed. The possibility of achieving molecular condensates bring the realms of quantum mechanics one step closer to daily macroscopic phenomena. Atom lasers and BECs in microtraps promise enhanced ability to manipulate atoms coherently on the nanoscale. Applications for these Bose-Einstein condensed 'superatoms' are suggested to be found, for instance, in the areas of lithography and precision metrology. And, maybe, the study of vortices and their formation processes in these idealized quantum laboratories—Bose-Einstein condensates—could one day provide new insight even into our understanding of turbulence in classical fluid dynamics. These being only the early guesses of what BECs could be good for, the physicists of the new millennium are guaranteed to have a plethora of interesting physics to be explored. Fortunately ironic is that, for the time being, a major dilemma for researchers working in the field of Bose-Einstein condensation seems to be an embarrassment of riches of choosing the next theoretical or experimental project.

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Errata

- √ In Paper I, the word Lanczos should be replaced by Arnoldi.

- √ In Paper IV, equation (2.7b) should read

$$\mathcal{L}^* v_q(\mathbf{r}) + g\phi^{*^2}(\mathbf{r}) u_q(\mathbf{r}) = -E_q v_q(\mathbf{r})$$

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Abstracts of Publications I–VI

I We compute the structure of a quantized vortex line in a harmonically trapped dilute atomic Bose-Einstein condensate using the Popov version of the Hartree-Fock-Bogoliubov mean-field theory. The vortex is shown to be (meta)stable in a nonrotating trap even in the zero-temperature limit, thus confirming that weak particle interactions induce for the condensed gas a fundamental property characterizing “classical” superfluids. We present the structure of the vortex at ultralow temperatures and discuss the crucial effect of the thermal gas component to its energetic stability.

II We compute structures of vortex configurations in a harmonically trapped Bose-Einstein condensed atom gas within three different gapless self-consistent mean-field theories. Outside the vortex core region, the density profiles for the condensate and the thermal gas derived from the Hartree-Fock-Bogoliubov-Popov theory are found to differ by only a few per cent from those derived from two of its recently proposed gapless extensions. In the core region, however, the differences between the density profiles are substantial. The structural differences are reflected in the energies of the quasiparticle states localized near the vortex core. In particular, the predictions for the energy of the lowest quasiparticle excitation derived from the theoretical models investigated differ considerably.

III Considering a moving vortex line in a dilute atomic Bose-Einstein condensate within time-dependent Hartree-Fock-Bogoliubov-Popov theory, we derive a criterion for the quasiparticle excitations to follow the vortex core rigidly. The assumption of adiabaticity, which is crucial for the validity of the stationary self-consistent theories in describing such time-dependent phenomena, is shown to imply a stringent criterion for the velocity of the vortex line. Furthermore, this condition is shown to be violated in the recent vortex precession experiments.

IV Multiply quantized vortices in trapped Bose-Einstein condensates are studied using the Bogoliubov theory. Suitable combinations of a localized pinning potential and an external rotation of the system are found to energetically stabilize, both locally and globally, vortices with multiple circulation quanta. We present a phase diagram for stable multiply quantized vortices in terms of the angular rotation frequency of the system and the width of the pinning potential. We argue that multiquantum vortices could be experimentally created using a suitable choice of these two parameters.

V The surface mode spectrum is computed self-consistently for dilute Bose-Einstein condensates, providing the temperature dependence of the surface mode induced vortex nucleation frequency. Both the thermodynamic critical frequency for vortex stability and the nucleation frequency implied by the surface excitations increase as the critical condensation temperature is approached from below. The multipolarity of the destabilizing surface excitation decreases with increasing temperature. The computed finite-temperature critical frequencies support the experimental observations and the zero-temperature calculations for vortex nucleation.

VI We compute using a microscopic mean-field theory the structure and the quasiparticle excitation spectrum of a dilute, trapped Bose-Einstein condensate penetrated by an axisymmetric vortex line. The Gross-Pitaevskii equation for the condensate and the coupled Hartree-Fock-Bogoliubov-Popov equations describing the elementary excitations are solved self-consistently using finite-difference methods. We find locally stable vortex configurations at all temperatures below T_c.

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