Classical and Quantum Field Theory of Bose-Einstein Condensates

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Declaration

This thesis is an account of research undertaken between September 2003 and January 2007 at the Department of Physics, Faculty of Science, The Australian National University, Canberra, Australia. I also was affiliated with ACQAO, the Australian Research Council Centre of Excellence for Quantum-Atom Optics. Except where otherwise stated, I present my original results, obtained under the supervision of Dr. Craig M. Savage.

I worked jointly with Beata J. Dąbrowska-Wüster on the truncated Wigner simulations of collapsing condensates and quantum effects in the localisation of matter-waves in optical lattices. The latter project is not included in this thesis. The code for the truncated Wigner simulations of collapsing BECs was written by P. B. Blakie and M. J. Davis. We adapted it to allow dynamical noise terms.

Much of the results regarding Skyrmion stability benefited greatly from work done by T. E. Argue for his honours thesis, which I verified and extended.

Sebastian Wüster
August 1, 2007
For my bright star, Beatka.
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and love. You are the bright shining star, which guides me through my life.
Abstract

We study the application of Bose-Einstein condensates (BECs) to simulations of phenomena across a number of disciplines in physics, using theoretical and computational methods.

Collapsing condensates as created by E. Donley et al. [Nature 415, 39 (2002)] exhibit potentially useful parallels to an inflationary universe. To enable the exploitation of this analogy, we check if current quantum field theories describe collapsing condensates quantitatively, by targeting the discrepancy between experimental and theoretical values for the time to collapse. To this end, we couple the lowest order quantum field correlation functions to the condensate wavefunction, and solve the resulting Hartree-Fock-Bogoliubov equations numerically. Complementarily, we perform stochastic truncated Wigner simulations of the collapse. Both methods also allow us to study finite temperature effects.

We find with neither method that quantum corrections lead to a faster collapse than is predicted by Gross-Pitaevskii theory. We conclude that the discrepancy between the experimental and theoretical values of the collapse time cannot be explained by Gaussian quantum fluctuations or finite temperature effects. Further studies are thus required before the full analogue cosmology potential of collapsing condensates can be utilised.

As the next project, we find experimental parameter regimes in which stable three-dimensional Skyrmions can exist in a condensate. We show that their stability in a harmonic trap depends critically on scattering lengths, atom numbers, trap rotation and trap anisotropy. In particular, for the $^{87}$Rb $|F = 1, m_f = -1\rangle$, $|F = 2, m_f = 1\rangle$ hyperfine states, stability is sensitive to the scattering lengths at the 2% level. We find stable Skyrmions with slightly more than $2 \times 10^6$ atoms, which can be stabilised against drifting out of the trap by laser pinning.

As a stepping stone towards Skyrmions, we propose a method for the stabilisation of a stack of parallel vortex rings in a Bose-Einstein condensate. The method makes use of a “hollow” laser beam containing an optical vortex, which
realises an optical tunnel for the condensate. Using realistic experimental parameters, we demonstrate numerically that our method can stabilise up to 9 vortex rings.

Finally, we focus on analogue gravity, further exploiting the analogy between flowing condensates and general relativistic curved space time. We compare several realistic setups, investigating their suitability for the observation of analogue Hawking radiation. We link our proposal of stable ring flows to analogue gravity, by studying supersonic flows in the optical tunnel. We show that long-living immobile condensate solitons generated in the tunnel exhibit sonic horizons, and discuss whether these could be employed to study extreme cases in analogue gravity.

Beyond these, our survey indicates that for conventional analogue Hawking radiation, simple outflow from a condensate reservoir, in effectively one dimension, has the best properties. We show with three dimensional simulations that stable sonic horizons exist under realistic conditions. However, we highlight that three-body losses impose limitations on the achievable analogue Hawking temperatures. These limitations vary between the atomic species and favour light atoms.

Our results indicate that Bose-Einstein condensates will soon be useful for interdisciplinary studies by analogy, but also show that the experiments will be challenging.
# Notation and Terminology

## Notation

This summary gives an overview of the used symbols. They are grouped alphabetically, first Latin and then Greek.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$\sim$</td>
<td>Signals dimensionless quantities.</td>
</tr>
<tr>
<td>$a_0$</td>
<td>Bohr radius, $a_0 = 5.29177 \times 10^{-11}$ m.</td>
</tr>
<tr>
<td>$a_{\text{coll}}$</td>
<td>Negative scattering length during collapse.</td>
</tr>
<tr>
<td>$a_{ij}$</td>
<td>New values of $^{87}\text{Rb}$ multi-component scattering lengths.</td>
</tr>
<tr>
<td>$\tilde{a}_{ij}$</td>
<td>Old values of $^{87}\text{Rb}$ multi-component scattering lengths.</td>
</tr>
<tr>
<td>$a_{\text{init}}$</td>
<td>Initial scattering length.</td>
</tr>
<tr>
<td>$a_s$</td>
<td>Atomic s-wave scattering length.</td>
</tr>
<tr>
<td>$c$</td>
<td>Single-component condensate speed of sound.</td>
</tr>
<tr>
<td>$c_+, c_-$</td>
<td>Multi-component condensate speeds of sound.</td>
</tr>
<tr>
<td>$E_{\text{cut}}$</td>
<td>Energy cutoff.</td>
</tr>
<tr>
<td>$d\xi$</td>
<td>Dynamical noise term in the TWA due to three-body losses.</td>
</tr>
<tr>
<td>$D$</td>
<td>Rapidity parameter for the horizon. Within $\Delta x = D\xi$ the Mach number is allowed to vary by $\sim 1$.</td>
</tr>
<tr>
<td>$g$</td>
<td>Physical atom-molecule coupling.</td>
</tr>
<tr>
<td>$g_0$</td>
<td>Bare atom-molecule coupling.</td>
</tr>
<tr>
<td>$G_A$</td>
<td>Anomalous correlations, $G_A(x, x') = \langle \chi(x')\chi(x) \rangle$.</td>
</tr>
<tr>
<td>$\tilde{G}_A$</td>
<td>Pairing field, $\tilde{G}_A(x) = G_A(x, x)$.</td>
</tr>
<tr>
<td>$G_N$</td>
<td>Normal correlations, $G_N(x, x') = \langle \chi^i(x')\chi(x) \rangle$.</td>
</tr>
<tr>
<td>$\tilde{G}_N$</td>
<td>Density of uncondensed atoms, $\tilde{G}_N(x) = G_N(x, x)$.</td>
</tr>
<tr>
<td>$\tilde{G}_{N/A}(r, r')$</td>
<td>Rescaled correlation functions, $G_{N/A}(r, r') = \tilde{G}_N(r, r')/r/r'$.</td>
</tr>
<tr>
<td>$\hbar$</td>
<td>Planck’s constant, $\hbar = 1.05457 \times 10^{-34}$ Js.</td>
</tr>
<tr>
<td>$\hat{H}$</td>
<td>Many-body Hamiltonian.</td>
</tr>
<tr>
<td>$\hat{H}_0(x)$</td>
<td>Single-particle Hamiltonian.</td>
</tr>
</tbody>
</table>
NOTATION AND TERMINOLOGY

$J$  
Atom flux.

$k_B$  
Boltzmann’s constant, $k_B = 1.38066 \times 10^{-23}$ J/K.

$K$  
Momentum cutoff.

$K_1, K_2, K_3$  
One, two and three-body loss coefficient.

$\hat{L}$  
Angular momentum operator.

$m$  
Atomic mass.

$M$  
Single component condensate Mach number $M = v/c$.

$n, n_{\text{cond}}$  
Condensate density.

$n_{\text{peak}}$  
Density peak value.

$n_{\text{unc}}$  
Density of uncondensed atoms.

$\dot{n}_1$  
Density fluctuation operator.

$N_1, N_2$  
Condensate atom number in components one and two.

$N_{\text{cond}}$  
Condensate atom number.

$N_{\text{init}}$  
Initial condensate atom number.

$N_r$  
Fraction of atoms in component 2, $N_r = N_2/N_{\text{tot}}$.

$N_{\text{remn}}$  
Remnant atom number.

$N_{\text{tot}}$  
Total atom number. In chapter 3: $N_{\text{tot}} = N_{\text{cond}} + N_{\text{unc}}$. In chapter 4: $N_{\text{tot}} = N_1 + N_2$.

$N_{\text{unc}}$  
Number of uncondensed atoms.

$O(x)$  
Shape of outcoupling region.

$t_{\text{collapse}}$  
Collapse time. Time after initiation of collapse until which only small atom loss occurs.

$T_H$  
Analogue Hawking temperature.

$U$  
Physical interaction strength. To be distinguished from the bare interaction strength $U_0$ when quantum effects are present.

$U_0$  
Interaction strength in the GPE and HFB equations. For quantum theory this is the bare coupling, to be distinguished from the physical coupling $U$. For semi-classical theory there is no distinction and we write $U_0$ or $U$.

$U_{\text{bg}}$  
Background scattering length of atom-molecule resonance theory. This is the physical scattering strength far away from the resonance. Near the resonance this value is modified to $U(B)$, $B$ is the magnetic field.

$U_{ij}$  
Multi-component interaction strengths, $U_{ij} = \frac{4\pi\hbar^2 a_{ij}}{m}$.

$v$  
Single component condensate speed $v = |\mathbf{v}|$.

$\mathbf{v}$  
Single component condensate velocity.

$V$  
External potential for the condensate.

$V_0$  
In chapter 4: Amplitude of laser pinning potential.

In chapter 5: Amplitude of exit nozzle potential.
\( V_{h,i} \)  
Amplitude of hump potentials.

\( V_t, V_v \)  
Trap potential and optical vortex potential for atom-light skyrmions.

\( w_0 \)  
Assorted focal widths of laser beams used for optical manipulation.

\( w_i \)  
Widths of hump potentials.

\( W \)  
In chapter 4: Skyrmion winding number.

In chapter 5: height of the hump potential.

**Greek alphabet**

\( \alpha, \beta, \gamma, \Gamma, \delta, \Delta, \epsilon, \zeta, \eta, \theta, \Theta, \iota, \kappa, \lambda, \Lambda, \mu, \nu, \xi, \Xi, \omicron, \pi, \Pi, \rho, \sigma, \Sigma, \tau, \upsilon, \phi, \Phi, \chi, \psi, \Psi, \omega, \Omega. \)

\( \alpha \)  
Constant related to the momentum cutoff.

\( \alpha_t, \alpha(x) \)  
Stochastic wave function.

\( \gamma \)  
Outcoupling strength.

\( \eta \)  
In chapter 3: Initial state quantum noise.

In chapter 5: Trap anisotropy \( \eta = \omega_x / \omega \perp \).

\( \vartheta \)  
Condensate phase.

\( \hat{\vartheta} \)  
Phase fluctuation operator.

\( \lambda \)  
Assorted wavelengths of laser beams used for optical manipulation.

\( \mu \)  
Chemical potential.

\( \nu \)  
Physical molecular field detuning.

\( \nu_0 \)  
Bare molecular field detuning.

\( \tau_{\text{evolve}} \)  
Evolution time. Time after initiation of collapse that the BEC is left to evolve freely before the atom number is measured.

\( \phi(x) \)  
Condensate wavefunction.

\( \phi_a(x), \phi_m(x) \)  
Atom and molecule wavefunctions.

\( \phi_1(x), \phi_2(x) \)  
Wave functions of different hyperfine components.

\( \hat{\phi}_a(r) \)  
Rescaled wave function, \( \phi_a = \hat{\phi}_a / r \).

\( \hat{\chi}(x) \)  
Fluctuating component of the field operator.

\( \hat{\chi}_a(x), \hat{\chi}_m(x) \)  
Fluctuations of atom and molecule field.

\( \hat{\rho} \)  
The system’s density operator.

\( \xi \)  
Condensate healing length, \( \xi = \hbar / (\sqrt{2}mc) \).

\( \hat{\Psi}(x), \hat{\Psi}_a(x) \)  
Atomic field operator.

\( \hat{\Psi}_m(x) \)  
Molecular field operator.

\( \omega_x, \omega_y, \omega_z \)  
Trap frequencies along the cartesian axes.

\( \omega_\perp \)  
Transverse trap frequency of a cigar shaped trap or a waveguide.

\( \mathbf{\Omega}, \Omega \)  
Angular velocity of trap rotation. \( \Omega = |\mathbf{\Omega}| \).
Glossary

We provide brief definitions of frequently used terms and abbreviations, specified for our context and sorted alphabetically.

“analogy”, the Mathematical equivalence between the equation for BEC excitations in the hydrodynamic regime and that for a scalar quantum field in curved spacetime. Also the operator commutation relations are identical, allowing the study of curved spacetime quantum effects in BECs.

BEC Bose-Einstein condensate.

black hole horizon, BH Surface in the BEC flow where the normal component of the flow turns from subsonic to supersonic. Analogue of the event horizon around an astrophysical black hole.

component Part of the BEC with atoms in one specific hyperfine state.

de-Laval nozzle Constriction of a tube to create supersonic flow in aerodynamics. In a BEC, we can also use a hump potential.

depletion Presence of uncondensed atoms at zero temperature due to interactions.

downstream In the direction of flow.

ergoregion Region in the condensate where the velocity modulus exceeds the speed of sound. Phonons can escape from this region, but they cannot remain motionless as seen in the lab frame.

Feshbach resonance Resonant bound state in atomic collisions. The energy of the resonance can be adjusted with a magnetic field. This allows steering of the interactions in a BEC using a magnetic field.

GPE Gross-Pitaevskii equation.

GR General relativity.

grey soliton Dip in the condensate density to a fraction $f$ of the background value. $f = 0$ would be a dark soliton. For $f > 0$ the dip is moving.

grid Set of discrete points used to represent the spatial domain in numerical computations.

healing length Natural length scale for variations of the condensate wave function.

HFB Hartree-Fock-Bogoliubov.

horizon See “black hole horizon” and “white hole horizon”.
<table>
<thead>
<tr>
<th>Term</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>hump potential</td>
<td>Optically generated potentials, placed in the way of the BEC flow.</td>
</tr>
<tr>
<td>hydrodynamic equations</td>
<td>Bernoulli’s equation (energy conservation) and continuity equation (number conservation). The BEC obeys these in the hydrodynamic regime.</td>
</tr>
<tr>
<td>hydrodynamic regime</td>
<td>A BEC only varies on length scales larger than the healing length. In this regime the condensate behaves like an inviscid, irrotational fluid.</td>
</tr>
<tr>
<td>line singularity</td>
<td>Line with undefined BEC phase due to circulating flow.</td>
</tr>
<tr>
<td>line vortex</td>
<td>Circular condensate flow around the line singularity.</td>
</tr>
<tr>
<td>leaking out</td>
<td>Condensate with just high enough chemical potential to leave a reservoir, streaming over the confining hump potential.</td>
</tr>
<tr>
<td>optical piston</td>
<td>Repulsive optical potential that is moving in time, creating a piston that pushes the condensate.</td>
</tr>
<tr>
<td>optical tunnel</td>
<td>Finite length tunnel formed by the core of a focused optical vortex laser beam.</td>
</tr>
<tr>
<td>optical vortex</td>
<td>Laser beam with a phase singularity on its axis. Because of the singularity, the light intensity of the beam has a hollow profile.</td>
</tr>
<tr>
<td>phase imprinting</td>
<td>Engineering a phase and hence a flow field in the condensate by means of interaction with electromagnetic waves.</td>
</tr>
<tr>
<td>phase separation</td>
<td>Immiscibility of two hyperfine components of the BEC. Under the influence of dissipation, these separate spatially, leaving only a small overlap region at the contact surface.</td>
</tr>
<tr>
<td>phonon</td>
<td>BEC excitation with wavenumber $q$ that fulfills $q\xi \ll 1$.</td>
</tr>
<tr>
<td>pinning potential</td>
<td>Repulsive optical potential, placed on the singularity of a matter wave vortex, to prevents its contraction or drift towards low density regions of the condensate.</td>
</tr>
<tr>
<td>QID</td>
<td>Quasi-one dimensional. A BEC with $\mu \ll h\omega_{\perp}$. Transverse excitations are frozen out.</td>
</tr>
<tr>
<td>resonance theory</td>
<td>Description of a Feshbach resonance in a BEC by coupled atom and molecule fields.</td>
</tr>
<tr>
<td>ring singularity</td>
<td>Ring with undefined BEC phase due to condensate flow.</td>
</tr>
<tr>
<td>ring vortex</td>
<td>Condensate flow around the ring singularity. Imagine flow on the surface of a torus, threading the hole.</td>
</tr>
<tr>
<td>scattering length</td>
<td>Parameter $a_s$, describing the whole scattering behaviour of cold atoms in the s-wave regime.</td>
</tr>
<tr>
<td>SDE</td>
<td>Stochastic differential equation.</td>
</tr>
<tr>
<td>semi-classical theory</td>
<td>BEC mean field theory. Quantum field effects are neglected and the condensate can be described by a single wave function.</td>
</tr>
</tbody>
</table>
NOTATION AND TERMINOLOGY

singularity  See “ring singularity” and “line singularity”.
soliton  Used here synonymously with “solitary wave”. Localised solution of a wave equation that propagates without change of shape.
sonic horizon  See “black hole horizon” and “white hole horizon”.
stochastic wave function  Solution of a stochastic differential equation. For us the Gross-Pitaevskii mean-field with the addition of initial random noise.
three-body loss  Three atoms collide and form a molecule among them. All three atoms are lost from the condensate.
transsonic  A flow that turns from subsonic to supersonic (spatially).
TTF  Transverse Thomas-Fermi. A BEC with $\mu \gg \hbar \omega_{\perp}$. The transverse profile is determined in the Thomas-Fermi approximation.
TWA  Truncated Wigner approximation.
upstream  Against the direction of flow.
vortex charge  Topological invariant. Indicates how often the phase wraps over $U(1)$ on a line around the vortex singularity.
white hole horizon, WH  Surface in the BEC flow where the normal component of the flow returns from supersonic to subsonic. The analogue object exists in astrophysics as the inner horizon around an electrically charged black hole.
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