

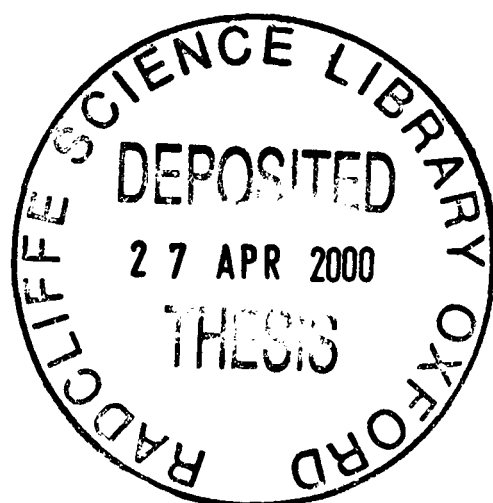
A theoretical study on manipulation of trapped atomic Bose-Einstein Condensates

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Thesis submitted for the degree of Doctor of Philosophy
at the University of Oxford



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In this thesis a number of aspects on possible manipulation of Bose-Einstein condensate in trapped atomic gases is investigated. First, a model for atom optical experiments involving Bose condensates is proposed and numerical simulations are presented to illustrate its characteristics. We demonstrate ways of focusing and splitting the condensate by modifying experimentally adjustable parameters. We show that there are at least two ways of implementing atom optical elements: one may modulate the interatomic scattering length in space, or alternatively, use a sinusoidal, externally applied potential.

The temporal evolution of quasiparticle excitations is studied via the Gross-Pitaevskii Equation. Nonlinear mode mixing of quasiparticles is introduced, and is observed using a quasiparticle projection method. This is used as a basis of time-dependent finite temperature simulations, which we argue to be valid under regimes of high occupation number. An illustration via a closely related evaporative cooling simulation is provided.

A phenomenological damping formalism for superfluidity near the λ point is adopted to describe the damping of excitations in a Bose-Einstein condensate. An estimate for the damping parameter is found. The damping formalism as a numerical tool to calculate the ground eigenstate of the condensate is explored.

A novel, experimentally realisable interferometry for Bose-Einstein condensates using near-field diffraction is proposed. The scheme is based on the phenomenon of intermode traces or quantum carpets; we demonstrate the structured spatio-temporal pattern for the dilute, atomic Bose-Einstein condensate. The pattern is found to change with temperature, which allows us to perform interferometric temperature measurements.

Finally, an output coupler for Bose-Einstein Condensates based on stimulated Raman transition is investigated. The spectrum and coherence are calculated for an atomic beam slowly coupled out of a trap containing a partially condensed Bose gas at finite temperatures. A number conserving Hartree-Fock-Bogliubov formalism has been used to incorporate finite temperature effects. Various different processes are found to become dominant for a suitable choice of the coupling parameters.

Dedication

To my family.

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List of publications

- “Atom optical elements for Bose-Einstein condensates” S. Choi and K. Burnett *Phys. Rev. A*, **56**, 3825 (1997) [Chapter 2]
- “Nonlinear mixing of quasi-particles in an inhomogeneous Bose condensate” S. Morgan, S. Choi, K. Burnett, and M. Edwards *Phys. Rev. A* **57** 3818 (1998) [Chapter 3]
- “Phenomenological damping in trapped atomic Bose-Einstein condensates” S. Choi, S. Morgan, and K. Burnett *Phys. Rev. A* **57** 4057 (1998) [Chapter 4]
- “Comparing alternative mean field theories in trapped Bose gas” N.P. Proukakis, S. Morgan, S. Choi, and K. Burnett *Phys. Rev. A* **58** 2435 (1998) [Chapter 5]
- “Exciting, cooling and vortex trapping in a trapped atomic Bose-Einstein condensate” R.J. Marshall, G.H.C. New, K. Burnett, and S. Choi *Phys. Rev. A* **59** 2085 (1999) [Chapter 5]
- “Quantum carpet interferometry for trapped Bose-Einstein condensates” S. Choi, K. Burnett, O. Friesch, B. Kneer, and W. P. Schleich To be submitted to *Phys. Rev Lett.* (1999) [Chapter 6]

- “Coherent output, stimulated quantum evaporation and pair breaking in a trapped atomic Bose gas” Y. Japha, S. Choi, K. Burnett, and Y.B. Band *Phys. Rev Lett.* **82** 1079 (1999) [Chapter 8]
- “Adiabatic output coupling of finite temperature BEC” S. Choi, Y. Japha, and K. Burnett Accepted for publication *Phys. Rev A* (2000) [Chapter 8]

Chapter 1

Introduction

The experimental realisation in 1995 of Bose-Einstein condensation (BEC) in trapped, atomic gases represents a culmination of enormous recent advances in experimental laser-cooling techniques that enabled us reach temperatures within a billionth of absolute zero; its achievement has been fittingly noted as the “Holy Grail” of atomic physics[1]. To date, the coldest temperature in the universe has been achieved in some 13 laboratories around the world, with BEC being observed in several different species of alkali atoms. More than 900 papers on the study of BEC have been published in the past 4 years alone, reflecting the enormous amount of interest among researchers on this system[2].

Bose-Einstein condensation was first predicted by Einstein in 1924, based on Bose’s study of statistical behaviour of photons[3]. The key idea is that a gas of non-interacting identical bosons would undergo a *phase transition* and “condense” into a single quantum state when their de Broglie wavelengths overlap. More precisely, for the homogeneous boson system, the condition for the phase transition to occur is written as[4]:

$$n\Lambda_{dB}^3 = 2.612 \tag{1.1}$$

where n is the density of the particles and $\Lambda_{dB} = h/\sqrt{2\pi mk_B T}$ is the thermal de Broglie wavelength with h being Planck’s constant, m the mass of a single particle, k_B the Boltzmann constant and T the temperature of the gas. Clearly the lower the temperature, the longer is the corresponding de Broglie wavelength and more likely is the overlap between the particles. A system of identical particles

with the dimensionless “phase space density,” $n\Lambda_{dB}^3$, of order unity is referred to as a quantum degenerate system. Quantum degeneracy is at the heart of the behaviour of superfluid helium and exciton gases in semiconductors.

Just as the advent of laser started an entirely new field of Quantum Optics 40 years ago, BEC marks a start of a new field in the quantum mechanical study of coherent atomic systems. Unlike the laser, however, BEC is a matter wave with no inherent translational motion, and there is currently an urgent need to find ways to manipulate the experimentally produced condensates. Some of the methods to understand and manipulate this new state of matter form the main theme of this thesis.

We start the chapter with a brief description of historical motivation for BEC research in the next section. We then describe the two main perspectives which summarise the background to the current state of BEC research: (1) BEC theories developed since 1950’s, and (2) advances in experimental techniques that finally produced BEC in trapped atomic gases. Lastly, a section on the general organisation of the thesis is provided.

1.1 A Brief History of BEC

Experimental and theoretical research on BEC spans many decades. Despite the fact that the recent experimental milestone has been set up by the atomic and optical physicists, the study of BEC has always involved various different fields of physics. In fact, historically, it was the discovery of superfluidity in liquid Helium that sparked the initial interest in BEC research.

Early works on BEC (1930’s - 1950’s)

As soon as superfluidity was discovered in liquid ^4He Fritz London[5] made the bold conjecture in 1938 that this superfluidity was related to the form of Bose-Einstein condensation, suitably generalised to a liquid. The basis of London’s argument was that if ^4He was treated as an ideal Bose gas, the transition temperature would be 3.15 K, which is remarkably close to the observed superfluid transition temperature of 2.17 K. However, confirmation of these ideas about superfluid ^4He took many years, partly because the very successful Landau theory of superfluid ^4He based on a phenomenological model of phonon-roton interac-

tions made no reference to Bose statistics[6]. Direct evidence of BEC in superfluid emerged only later from neutron scattering measurements[7].

One of the most important early theoretical work on superfluidity is the work of Bogoliubov[8] who showed the connection between a Bose condensate and a phonon-like dispersion relation for long-wavelength elementary excitations. This work captured many general features of BEC and is still an important basis of current BEC research. Other important works include the work of Penrose and Onsager[9] which showed how to formulate in a precise way the concept of Bose-condensation in the interacting Bose system. Meanwhile, Beliaev[10] provided us with a general field theoretical formulation to calculate the properties of a Bose system in the presence of a Bose condensate. Beliaev also emphasised for the first time the key role played by the phase of the Bose order parameter and its relation to superfluid velocity.

More recent period (1950's - 1960's)

The early works by London, Landau, Bogoliubov, Penrose and Beliaev laid the foundation for intensive theoretical work on interacting Bose-condensed system in the period 1958-1965. Some of the best modern theoretical physicists have contributed much to the knowledge of BEC during this period. For instance, R. P. Feynman presented the first microscopic analysis based on quantum mechanics of the roton part of the quasiparticle spectrum[11], and studied how the many-body wave functions $\Psi_N(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ for the ground and the lowest excited states of liquid ^4He are affected by the Bose statistics. He also carried out fundamental work on vortices in superfluid ^4He . On the other hand, Lee, Huang, and Yang made the first finite temperature calculations for an interacting Bose gas by means of a pseudo-potential method on a gas of hard spheres[12]. The motivation of these works was always to understand the excitations and other properties of superfluid ^4He but the hypothetical case of a “dilute, weakly interacting Bose gas” was often considered as an illustrative example.

To a large extent, the study of BEC has been confined to only a small number of many-body theorists. One of the reasons is that characteristic features of the Bose condensate and Bose broken symmetry can not easily be extracted from the complicated dynamics of the superfluid ^4He .

Experimental attempts (1960's -)

In view of the difficulties in dealing with a strongly interacting dense system like superfluid ^4He , it is not surprising that since 1960's there has been an increasing experimental effort to achieve BEC in a *dilute* Bose gas. Efforts to Bose condense atomic hydrogen began more than 15 years ago.

In these experiments, hydrogen atoms were cooled in a dilution refrigerator, trapped by a magnetic field and then further cooled by evaporation. By magnetically aligning the spins of the hydrogen atoms, one obtains a system that remains a gas even at $T = 0$. Moreover, its density could be varied over several orders of magnitude ranging from a weakly to a strongly interacting Bose gas. The study of spin-polarised hydrogen stimulated much theoretical and experimental interest in achieving BEC in a sample of dilute atomic gas over the last decade. BEC was finally created and observed successfully in July 1995 by the group of Wieman and Cornell at JILA in a gas of ^{87}Rb atoms[13]. In the same year, the MIT group of Ketterle and the Rice group of Hulet have observed BEC in Na and ^7Li respectively[14, 15]. BEC was finally produced in Hydrogen at MIT in June 1998, after being plagued for decades by unavoidable losses due to recombinations of individual atoms to form H_2 molecules[16]. In stark contrast to the superfluid ^4He , the experimentally produced condensates are inhomogeneous, finite sized systems with the number of atoms ranging from a few thousands to several millions.

1.2 Overview of BEC Theories

Theoretical work on BEC may be categorised in several different ways depending on the type of approximations and conditions used; for example, homogeneous *vs.* inhomogeneous systems and interacting *vs.* noninteracting (ideal) gases. By inhomogeneous we mean a system with a trapping potential such that the condensate density profile is not constant. The bulk of theories that have been developed in the 50's and 60's were for the homogeneous systems. The recent experimental samples of BEC require theories that correspond to *weakly-interacting* bosons in an *inhomogeneous* system. In this section we go over very briefly outlines of three possible theoretical regimes: non-interacting, weakly interacting, and, in the form of superfluidity, strongly interacting bosons. Both homogeneous

and inhomogeneous systems are considered in each category; not surprisingly, the (in)homogeneity of the system has a rather profound effect on the properties of BEC.

1.2.1 Non-interacting, ideal Bose gas

The ideal gas case contains all the necessary physics that can guide us in our study of the interacting condensates. In this subsection we give a short outline of the physics of ideal bosonic gases. It is apparent especially with ideal gases that the effect of quantum statistics rather than interactions causes the “condensation” of the atoms.

Homogeneous system

The case of *homogeneous* ideal bosonic gases is already a classic textbook material[4]. The criterion for the quantum degeneracy has already been discussed in Eq. (1.1). The main important results to note are the critical temperature of phase transition:

$$N = 2.612V/\lambda_{dB}^3(T_c), \quad (1.2)$$

where N is the total number of particles, V the volume of the system and $\lambda_{dB}(T_c)$ the thermal de Broglie wavelength at the critical temperature; the temperature dependence of the condensate fraction:

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2}, \quad (1.3)$$

with N_0 being the number of atoms in the condensate, and the total energy of the system given by the expression

$$\frac{E}{Nk_B T_c} = \frac{3\zeta(5/2)}{2\zeta(3/2)} \left(\frac{T}{T_c}\right)^{5/2} \quad (1.4)$$

where ζ denotes Riemann-Zeta functions. These and other results can be readily found in many standard texts on Statistical Mechanics.

Inhomogeneous system

Inhomogeneity is one of the important features of the experimentally achieved trapped Bose condensates. One physical consequence is that the effect of the two-body interactions becomes significant, despite the very dilute nature of the trapped gases. By considering an *ideal* inhomogeneous gas we are ignoring the effect of these enhanced interatomic interactions. However, even without the inclusion of interactions, the inhomogeneity of the gas itself brings about several important consequences. For example, the detection of BEC is possible not only in momentum space as in the case of homogeneous superfluid Helium but also in co-ordinate space.

With a confining potential in quadratic form,

$$V_{\text{ext}} = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \quad (1.5)$$

the ground state $\phi(\mathbf{r}_1, \dots, \mathbf{r}_N)$ of N non-interacting bosons may be expressed quantum mechanically as a product state $\phi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \prod_i \varphi_0(\mathbf{r}_i)$ where

$$\varphi_0(\mathbf{r}_i) = \left(\frac{m\omega_{ho}}{\pi\hbar} \right)^{3/4} \exp \left[-\frac{m}{2\hbar} (\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2) \right] \quad (1.6)$$

with $\omega_{ho} = (\omega_x \omega_y \omega_z)^{1/3}$. In ideal, trapped bosons, this product state represents exactly the quantum state of BEC. It follows that the corresponding density distribution is given by

$$n(\mathbf{r}) = N |\varphi_0(\mathbf{r})|^2, \quad (1.7)$$

implying that in harmonic traps the condensate reveals itself with the appearance of a distinct peak in the central region of the density distribution as a result of identical gaussians piling on top of each other. Indeed, BEC was first detected experimentally as an occurrence of a sharp peak over a broader distribution in both the velocity and spatial distributions. The critical temperature for the onset of condensation, T_c , can be shown to be given by

$$N = \left(\frac{k_B T_c}{0.94 \hbar \omega_{ho}} \right)^3 \quad (1.8)$$

where ω_{ho} is a geometric mean of the three trap frequencies as defined above.

The condensate fraction as a function of temperature is given by

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^3 \quad (1.9)$$

while the total energy is given by

$$\frac{E}{Nk_B T_c} = \frac{3\zeta(4)}{\zeta(3)} \left(\frac{T}{T_c}\right)^4. \quad (1.10)$$

Comparing these results with the homogeneous counterpart, we see clearly the dramatic changes in the behaviour of the temperature dependent properties.

1.2.2 Weakly interacting Bose gas

Interactions between atoms is unavoidable in a real gas, and in particular, the effect of interactions is enhanced in an inhomogeneous system. A complete description of real, interacting gases requires a much more complicated theory than the ideal gas counterpart. However, the diluteness of the experimentally produced BEC makes it possible for us to apply the theory of a *weakly interacting* Bose gas. The effects of interactions are then included in a rather simple way – a single parameter, the *s*-wave scattering length is sufficient for an accurate description.

In this subsection we give a short summary of the main theoretical tools used in the description of weakly interacting Bose gases, namely the second quantisation and the mean field approximation. We note that this thesis is essentially based on the mean-field theory.

Second quantisation

The starting point in the description of interacting bosons is the many-body interacting Hamiltonian:

$$\begin{aligned} \hat{H} = & \int d^3\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}, t) \left[-\frac{\hbar^2}{2m} \nabla_r^2 + V_{\text{trap}}(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}, t) \\ & + \frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}^\dagger(\mathbf{r}', t) \hat{V}(\mathbf{r} - \mathbf{r}') \hat{\Psi}(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}', t), \end{aligned} \quad (1.11)$$

where $\hat{\Psi}(\mathbf{r}, t)$ and $\hat{\Psi}^\dagger(\mathbf{r}', t)$ are respectively the boson field operators that annihilate and create a particle at position $\mathbf{r}$, and $V(\mathbf{r} - \mathbf{r}')$ is the two-body interatomic potential. Eq. (1.11) gives the interacting Hamiltonian for the inhomogeneous case; the homogeneous case is treated by setting $V_{\text{trap}}(\mathbf{r}) = 0$.

In general, the field operator can be expanded as

$$\hat{\Psi}(\mathbf{r}) = \sum_i a_i \psi_i(\mathbf{r}) \quad (1.12)$$

where $\psi_i(\mathbf{r})$ are single particle wave functions and a_i are the corresponding annihilation operators. The operators a_i and $a_i^\dagger$ are defined in Fock space through the relations

$$a_i^\dagger |n_0, n_1, \dots, n_i \dots\rangle = \sqrt{n_i + 1} |n_0, n_1, \dots, n_i + 1 \dots\rangle \quad (1.13)$$

$$a_i |n_0, n_1, \dots, n_i \dots\rangle = \sqrt{n_i} |n_0, n_1, \dots, n_i - 1 \dots\rangle \quad (1.14)$$

where n_i are the eigenvalues of the number operator $a_i^\dagger a_i$ for atoms in single particle state. The operators a_i obey the usual boson commutation rules:

$$[a_j, a_k^\dagger] = \delta_{j,k}, \quad [a_j, a_k] = 0, \quad [a_j^\dagger, a_k^\dagger] = 0. \quad (1.15)$$

For the case of *weak* interactions, and low energy scattering, the details of interaction potential becomes unimportant and the interactions can be shown to be described by the *s*-wave scattering process. The interaction potential can then be treated as an effective zero-range contact interaction

$$\hat{V}(\mathbf{r} - \mathbf{r}') = \mathcal{V} \delta(\mathbf{r} - \mathbf{r}') \quad (1.16)$$

with the strength of interaction given by:

$$\mathcal{V} = \frac{4\pi\hbar^2 a}{m}, \quad (1.17)$$

where a is the *s*-wave scattering length. In a hard sphere gas, the scattering length a equals the diameter of the atoms. We note that there are also currently attempts to include the scattering interaction more rigorously than Eq. (1.16), although in such cases the theory rapidly becomes very complicated and the

treatment of the trapped Bose gas becomes far too difficult[17].

Mean field approximation

The basic idea for the mean-field description of dilute Bose gases was formulated by Bogoliubov[8]. It states that, in the limit of macroscopically large occupation of a single particle level, $n_0 = N_0 \gg 1$, the states with N_0 and $N_0 \pm 1$ atoms correspond to the same physical configuration, so that the operators a_0 and $a_0^\dagger$ may be treated like c -numbers: $a_0 = a_0^\dagger = \sqrt{N_0}$.

By generalising the Bogoliubov prescription to the case of non-uniform and time-dependent configuration, one writes the field operator in the mean field approximation as:

$$\hat{\Psi}(\mathbf{r}, t) = \psi(\mathbf{r}, t) + \hat{\delta}(\mathbf{r}, t), \quad (1.18)$$

where $\psi(\mathbf{r}, t)$ is a complex function defined as the expectation value of the field operator: $\psi(\mathbf{r}, t) \equiv \langle \hat{\Psi}(\mathbf{r}, t) \rangle$, and the operator part, $\hat{\delta}$, is taken to be a stochastic quantity such that $\langle \hat{\delta} \rangle = 0$ ¹. The function $\psi(\mathbf{r}, t)$ which acts as an order parameter is a classical field often referred to as the condensate wave function. The decomposition of Eq. (1.18) implies the asymptotic behaviour for the one-particle density matrix $\rho_1(\mathbf{r}', \mathbf{r}, t) = \langle \hat{\Psi}^\dagger(\mathbf{r}') \hat{\Psi}(\mathbf{r}) \rangle$:

$$\lim_{|\mathbf{r}' - \mathbf{r}| \rightarrow \infty} \rho_1(\mathbf{r}', \mathbf{r}, t) = \psi^*(\mathbf{r}', t) \psi(\mathbf{r}, t). \quad (1.19)$$

Equation (1.19) is usually taken to be the technical definition of the Bose-Einstein condensation[9] and denotes what is known as the off-diagonal long range order or ODLRO. We note that the mean field $\psi(\mathbf{r}, t)$ possesses a well-defined phase which corresponds to assuming a broken gauge symmetry in the many-body system. In the Bogoliubov mean-field prescription, the condensate acts like a classical particle reservoir which non-condensate atoms can enter and leave via scattering. The number of atoms is then no longer a constant of motion.

Homogeneous system

One of the key consequences of the interatomic interaction is the depletion of the condensate population even at $T = 0$. A major result of the famous Bogoliubov's

¹The higher correlations such as $\langle \hat{\delta}^\dagger \hat{\delta} \rangle$ and $\langle \hat{\delta}^\dagger \hat{\delta} \hat{\delta} \rangle$ are not necessarily zero; these are discussed further in Chapter 5.

calculation is:

$$\frac{N_0}{N} = \left[1 - \frac{8}{3} \left(\frac{na^3}{\pi} \right)^{1/2} \right], \quad (1.20)$$

where $n = N/V$ is the density, and a is the s -wave scattering length. This is the result for $T = 0$. For dilute Bose gas, we typically have $na^3 \ll 1$. Another important result is the presence of an acoustic (or phonon) excitation spectrum at long wavelengths. For wave vector $k \ll mc/\hbar$ the excitation energy is found to be given by

$$E_k \approx \hbar ck \quad (1.21)$$

with the phonon velocity

$$c = \sqrt{\frac{4N\pi\hbar^2 a}{m^2}}. \quad (1.22)$$

Clearly $c \rightarrow 0$ for $a \rightarrow 0$ implying that the interatomic interaction is responsible for the characteristic phonon spectrum.

An important development for the homogeneous case is the generalised Green's function formalism which has been put forward by Beliaev in 1958[10] and developed further by Hugenholtz and Pines[18]. The complete Green's function approach applied to dilute, homogeneous BEC at finite temperatures was published only very recently by Shi and Griffin[19].

Inhomogeneous system

The theory of weakly-interacting, inhomogeneous Bose gas is indeed the current area of intense research, and is the theme of this thesis. Details of main results from the mean field theory are given in Chapters 2, 3 and 5. The main results are the equation of motion for the condensate wave function (Chapter 2), the quasiparticle excitation spectrum in a trap (Chapters 3 and 5), and the treatment of finite temperature BEC in thermodynamic equilibrium (Chapter 5). We note that the inclusion of a trapping potential results in having to calculate various quantities numerically.

An alternative approach to the description of current experimentally produced BEC is the Quantum Kinetic Theory (QKT). A brief introduction to QKT is also given in the thesis (Chapter 4). The QKT requires the use of the so called number-conserving Bogoliubov approach which avoids the issue of indeterminate number of atoms under the mean field approximation. In Chapter 8, we introduce

a similar number-conserving approach to describe the time evolution of an output coupler for BEC.

1.2.3 Superfluidity

Superfluidity is one of the most spectacular consequences of Bose-Einstein condensation. It presents us with an array of novel phenomena: absence of fluid viscosity, reduction of the moment of inertia, new collective phenomena (eg. second and third sound), and quantised vortices. However, as noted previously, the explicit connection between superfluidity and BEC is nontrivial and has been a subject of vigorous investigation over several decades. It is well-known that superfluid is a difficult system to handle theoretically because of the strong interactions between the atoms.

From the standpoint of trapped, atomic BEC, it is important that a contact is made between the mean field theories discussed earlier and the superfluid equations of motion. Indeed, under the condition $Na/a_{ho} \gg 1$, hydrodynamic theory of superfluids may be derived. Writing the complex order parameter ψ in terms of a modulus and phase,

$$\psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)} e^{iS(\mathbf{r}, t)} \quad (1.23)$$

and noting $\mathbf{v} = (\hbar/m)\nabla S$, it can be shown that the equation of motion for the condensate, the Gross-Pitaevskii Equation, may be written in the form of two coupled equations for the density and velocity field:

$$\frac{\partial}{\partial t} n + \nabla \cdot (\mathbf{v} n) = 0 \quad (1.24)$$

and

$$m \frac{\partial}{\partial t} \mathbf{v} + \nabla \cdot \left(V_{\text{ext}} + U_0 n - \frac{\hbar^2}{2m\sqrt{n}} \nabla^2 \sqrt{n} + \frac{mv^2}{2} \right) \cdot (\mathbf{v} n) = 0 \quad (1.25)$$

The regime of $Na/a_{ho} \gg 1$ is characterised by the fact that strong enough repulsive interaction among atoms results in smooth density profiles. One can then neglect the kinetic pressure term in $\hbar^2$ in the equation for the velocity field to

give

$$m \frac{\partial}{\partial t} \mathbf{v} + \nabla \left(V_{\text{ext}} + U_0 n + \frac{mv^2}{2} \right) \cdot (\mathbf{v} n) = 0. \quad (1.26)$$

Equations (1.24) and (1.26) have so far been used to predict accurately frequencies of collective excitations and other important quantities[20].

1.3 Experimental techniques to achieve BEC

The experiments to create BEC in alkali gases comprises three parts: (a) laser cooling and trapping which are particularly efficient for alkali atoms, (b) increase in the phase space density by transferring the cold atoms to a specialised trap, and finally, (c) evaporative cooling which is a technique originally developed for spin-polarised Hydrogen. In this section, we discuss in more detail these three main experimental steps to Bose condensation.

We note that, in addition to the ingenious integration of the independent cooling techniques, favourable collision parameters and the possibility of easy diagnostics of the atomic samples made experimental realisation possible in the system of alkali atoms.

1.3.1 Laser cooling, and trapping

Starting from the initial proposals from the seventies[21], progressively colder and colder temperatures for the atomic samples were achieved using laser light down to within 10^{-6}K of the absolute zero in the recent years. The significance of these works in cooling and trapping atoms has been recognised in the awarding of Nobel Prizes to C. Cohen-Tannoudji, S. Chu and W. D. Phillips in 1997. In this subsection we discuss the important fundamental concepts of Doppler cooling, Optical molasses, sub-Doppler cooling, and Magneto-optical traps. A more comprehensive review of the field is found in Ref. [22].

Doppler cooling

A typical Doppler cooling scheme is shown in Fig. 1.1. In this scheme, an atom of mass M absorbs a photon of frequency ν and spontaneously emits the photon in an arbitrary direction. Because of conservation of momentum, the atom changes

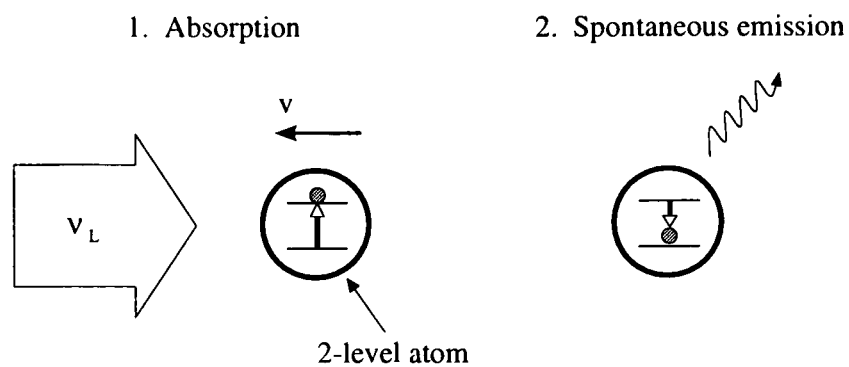


Figure 1.1: Schematic diagram of laser cooling of two level atoms

its velocity by a recoil velocity $v_{\text{recoil}} = h/M\lambda$, where the wavelength of light, $\lambda = 589\text{nm}$ for the D_2 transition of sodium, so that the corresponding recoil velocity is $\approx 3\text{cm s}^{-1}$ per photon absorption. Laser light with a frequency smaller than the atomic resonance frequency is used, so as to compensate for the Doppler shift from the oncoming atoms. The spontaneous emission of light that follows has no preferred direction, so that the net effect of a sequence of such absorption-emission cycles is a reduction of the atomic velocity. In principle, a sodium atom with initial velocity $v_0 \approx 1000\text{m s}^{-1}$ would come to a halt after absorption-emission of $v_0/v_{\text{recoil}} \approx 33000$ photons. Since the rate of scattering is of the order of excited life time τ , with $\tau \approx 20\text{ns}$ for Na, atoms can be stopped in a few milliseconds.

The cooling process stops when the atoms, because of the change in velocity, are no longer in resonance with the laser light. The desired atomic velocity may be achieved by chirping of laser frequency or tuning of atomic frequency by applying magnetic fields to prolong the resonance condition.

Optical molasses

Having lasers detuned by a Doppler shift implies that only atoms which are counter-propagating can “feel” the effect of the incoming laser, which then reduces its speed. For low velocities, the force on the atoms depends linearly on velocity as in a viscous medium. This Doppler cooling scheme, extended to three dimensions using three pairs of counter-propagating laser beams in orthogonal direction is called optical molasses. The first optical molasses was demonstrated in 1985 with sodium atoms[23].

The minimum temperature achievable in optical molasses can be estimated by

finding the balance between two effects: the cooling due to the viscous force and heating due to the spontaneous emission. The minimum temperature achievable in an optical molasses is given by:

$$k_B T_D = \frac{h\Gamma}{2} \quad (1.27)$$

where $\Gamma = 1/2\pi\tau$ is the natural width of atomic resonance. T_D is called the Doppler limit. Typical values of T_D are $240\mu K$ for sodium and $120\mu K$ for cesium.

Sub-Doppler cooling

Measurements of the temperature of the atoms in optical molasses revealed that the temperature was much lower than expected and not far from the recoil temperature which is the theoretical minimum temperature of laser cooling. Recoil temperature T_{recoil} is defined as the temperature corresponding to the recoil energy due to the absorption of a single photon:

$$\frac{1}{2}k_B T_{\text{recoil}} = \frac{1}{2M} \left(\frac{h\nu_L}{c} \right)^2 \quad (1.28)$$

T_{recoil} is $2.4\mu K$ for sodium and 197nK for cesium.

The mechanism for sub-Doppler cooling has been explained by taking into account light induced shifts of the atomic levels and optical pumping effect[24]. A qualitative understanding is provided by considering a two-level atom interacting with two counter-propagating laser beams of orthogonal linear polarisation. The resulting light field has a polarisation which varies with position, rendering position dependent shift of Zeeman sublevels for the atoms within the light field. Any atom moving across the light field therefore sees a series of potential hills. An atom arriving at the top of the potential hill is optically pumped to the bottom of the potential hill, and the potential energy gained at the expense of kinetic energy is dissipated in this process. Just as Sisyphus of Greek mythology, the atom then again has to climb up a potential hill. In this way the atom is cooled down repetitively reaching its sub-Doppler temperature to approximately ten times the recoil temperature.

Magneto-optical trapping

A magneto-optical trap, or MOT, is a method to confine and cool neutral atoms. It is a combination of a set of laser beams and a quadrupole magnetic field; it usually consists of six laser beams which form three orthogonal pairs each made of two counter-propagating beams with opposite circular polarisations, intersecting in the zero point of the magnetic field generated by two parallel coils with currents flowing in opposite directions. Through the position dependent Zeeman splitting induced by the shape of the quadrupole magnetic field and the Doppler cooling effect, atoms are pushed to the centre of the trap where the magnetic field is zero. Atoms displaced from the position of zero magnetic field preferentially absorb photons from the laser beam coming from that direction and feel the force back towards the origin. The resulting motion of the atoms in a MOT is that of damped harmonic oscillator.

First proposed by Dalibard and demonstrated experimentally[25], the MOT plays a crucial role in BEC experiments, since high density atomic samples are required in producing a BEC. The maximum density of atoms that can be achieved in a MOT is limited by two factors: first the collisions between ground state and excited state atoms contributing to the loss of atoms and second, repulsive forces between the trapped atoms due to reabsorption of scattered photons. By optically pumping atoms to a state where they do not interact with the trapping laser, one can improve the density of atoms dramatically. The maximum phase space density obtained with the laser cooling and trapping methods is in the range $10^{-5} - 10^{-4}$.

1.3.2 Increasing the Phase-Space Density

In order to achieve BEC, the phase-space density has to be increased dramatically. The density achieved using MOT is still too small for BEC. The next step in experiments after trapping cold atoms in a MOT is to transfer them to a purely magnetic trap, without the optical field. A magnetic trap was first used by W. Paul to confine neutrons[26]. Compared to MOT, magnetic traps allow confinement of atoms at much lower temperatures because the effects due to radiation are absent e.g. the photon recoil limit. Magnetic traps are conservative traps – atoms trapped in a magnetic trap has to be cooled first using independent means

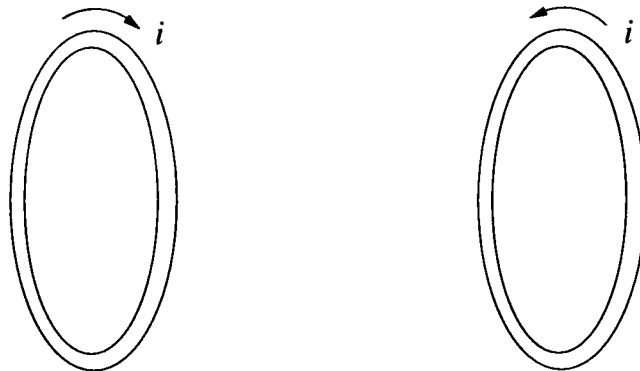
such as evaporative cooling. The simplest magnetic trap is a quadrupole trap (Fig. 1.2) which produces a spherical-quadrupole magnetic field crossing a zero at the centre and a linear field variation around it. This is however unsuitable for BEC since, as the atom density increases, atoms are lost through Majorana flips.

More specialised traps have been developed for the production of BEC, by trying to overcome these spin-flip losses while keeping the advantage of tight confinement of quadrupole trap. They include the time-averaged orbiting potential (TOP) trap[13] which is created by adding a continuously changing bias field that moves the location of the field zero much faster than atoms can follow. An optical-plug trap was used for BEC in sodium[14]. The optical dipole force from a tightly focused Ar laser beam at the point of zero magnetic field gave repulsive push away from the centre, effectively “plugging” the hole in the quadrupole trap. Also a permanent magnet could be used to generate the required field intensity and curvature for the Lithium BEC[15]. More recent developments include variants of Ioffe-Pritchard(IP) traps such as the “baseball” trap[27] and the “cloverleaf” trap[28], where the names denote the shape of the trapping coils. The IP traps[29] consists of two coils plus four straight conductors with current in alternating directions (Fig. 1.2). Unlike quadrupole traps, such a trap has no vanishing magnetic field and the spin-flips can be suppressed.

1.3.3 Evaporative Cooling

Having cooled, trapped and tightly confined the atoms, one needs to lower the temperature further across the critical temperature to achieve a phase space density necessary for BEC. This has been done by the process of evaporative cooling. Evaporative cooling was first proposed[30] and demonstrated[31] for atomic Hydrogen. The technique was extended to alkali atoms[32] becoming a key step in the production of BEC. The evaporative cooling procedure is based on the selective removal of atoms which have an energy higher than the average energy, and subsequent rethermalisation of the sample by collisions. Since the average energy of the atoms remaining in the traps is reduced in this process, the new equilibrium state of the gas corresponds to a lower temperature. With optimised evaporative procedures, it is possible to achieve a dramatic reduction of the gas temperature and an increase of the phase-space density by 5-6 orders of magnitude. In

Quadrupole Trap



Ioffe-Pritchard Trap

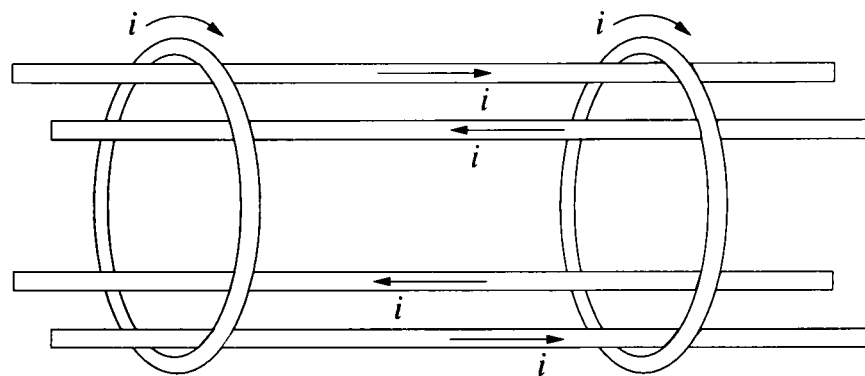


Figure 1.2: Schematic diagram of the Quadrupole and Ioffe-Pritchard Traps

the experiments so far, an RF-field was used to induce spin-flip transitions from trapped to untrapped states.

Optimisation of evaporative cooling involves taking into account the unavoidable loss mechanisms. Losses due to background gas collisions may be reduced by using ultra-high vacuum chambers. On the other hand, loss of atoms through inelastic collisions resulting in dipole relaxation or three body recombination is unavoidable. The success of BEC in alkali atoms owes to the fact that alkali atoms have favourably high elastic scattering cross sections. Comprehensive treatment of evaporative cooling can be found in Ref. [33] and references therein.

1.4 Organisation of this thesis

The thesis is organised as follows:

In **Chapter 2** we introduce the concept of atom optics and immediately apply this to the case of BEC. This gives our first method to manipulate a given condensate. We derive also in this chapter the well-known Gross-Pitaevskii equation

for the condensates.

Chapter 3 introduces the concept of quasiparticles in trapped BEC. With interacting particles, the concept of quasiparticles and pairing become important, and it introduces a whole new aspect into the physics of BEC. We give an illustration of this with examples from the simulation of nonlinear mixing of quasiparticles. These concepts are used in the remainder of the thesis.

In **Chapter 4**, a phenomenological description of damping of quasiparticle excitation is given. Technique of quasiparticle projection developed in Chapter 3 is utilised to discriminate the condensate component from excitations, and the damping time of excitation is estimated. Its possible use as a numerical tool is also discussed in the chapter.

In **Chapter 5**, we present ways to describe a finite temperature BEC. The Hartree-Fock-Bogoliubov formalism is introduced, as well as a way to simulate finite temperature BEC evolved in time. Ideas discussed in this chapter form the basis for results given in Chapters 6 and 8. As an example, simulation of evaporative cooling in 2 dimensions is demonstrated.

Chapter 6 proposes a new type of interferometer using BEC, based on the phenomenon of quantum carpets. This is shown to be a promising method for measuring the temperature of the condensate.

In a short review chapter, **Chapter 7**, we discuss the concept of coherence and also of atom laser. This sets the stage for the study of the output coupler for BEC which are currently the closest realisation of an atom laser.

We study in **Chapter 8** features of an output coupler based on stimulated Raman process. Distinct finite temperature effects are investigated and the coherence of the output atoms are presented.

Finally, we conclude in **Chapter 9** with a summary of main results of the thesis and an outlook on possibilities for future research.

Chapter 2

Atom Optical Elements for Bose-Einstein Condensates

2.1 Introduction

Since the first experimental realisation of BEC in trapped gases, rapid progress has been made in studying their physical properties. One of the exciting prospects for BEC has been the possibility of realising a coherent source of atoms, the atom laser, in analogy with the optical laser[34, 35]. With the experimental demonstration at MIT of highly visible interference fringes formed from two independent condensates coupled out of a trap[36, 37] one could argue that, in a sense, we already have with us a coherent atomic source, a rudimentary atom laser, and that one should be looking for effective ways to control the output beam of such sources. By control we mean focusing and beam splitting of flowing condensates, in analogy with the conventional optics. In fact, there has been tremendous progress made over the last few years in the field of atom optics in which the motion of (uncondensed) atoms is controlled via the light forces[38, 39]. We study in this chapter possible atom optical experiments involving Bose condensates. We begin, therefore, by reviewing briefly some of the concepts of the relatively new field of atom optics. We then discuss in Sec. 2.3 relevant aspects of atom optics for the system of ultracold atoms, and introduce the equation of motion for the condensate wave function, the Gross-Pitaevskii Equation (GPE). In Sec. 2.4 we describe how atom optical experiments involving BEC may be modelled, and in Sec. 2.5 the results of a number of simulations demonstrating the effect of these

atom optical elements are presented. Finally, the results are discussed in view of the available experimental parameters in Sec. 2.6.

2.2 Atom optics

The field of atom optics relies fundamentally upon the founding stone of quantum mechanics, the wave-particle duality. The concept of *matter waves*, introduced by de Broglie in 1923, states that any moving object has associated with it a wavelength λ :

$$\lambda = \frac{h}{p} \quad (2.1)$$

where h is the Planck's constant and p the momentum of the object. Due to their mass, atoms have short de Broglie wavelengths of the order ~ 0.1 nm for the typical case of laser cooled ^{87}Rb travelling at $\sim 45\text{ms}^{-1}$ at temperature $\sim 20\text{K}$ ¹. Atom optics refers to general techniques to exploit this wave property of neutral atoms and manipulate their trajectories. For example, matter wave diffraction from crystals have been used. It is, however, the recent advances in tunable lasers that brought about rapid advances in this field; the lasers are able to alter precisely the motion of neutral atoms through a variety of atom-photon interactions. In this sense, atom optics is a field in which the role of light and matter in conventional optics is exactly reversed.

Motivation

There are several advantages in using neutral atoms in applications such as interferometry. For instance, atoms are less sensitive to static electromagnetic fields than electrons or other charged particles. Owing to the unique atomic properties such as the mass and the presence of the internal energy level structures, atom interferometry promises important applications such as measurement of inertial and gravitational effects, tests of quantum mechanics, and measurements of atomic and scattering properties. Other possible applications of atom optics include atom microscopy (short de Broglie wavelength implying higher resolution when atoms are used as the surface probe) and high resolution atom lithography.

¹At ultracold temperatures $\sim \mu\text{K}$, the de Broglie wavelength becomes much longer, and the system enters the regime of *nonlinear atom optics*. This is discussed below.

Components of atom optics

As in any conventional optical experiment, a typical atom optical experiment involves three essential components:

1. Source: Thermal expansion or launching of laser cooled atoms have traditionally been used as the source of atoms. An ideal atomic source should provide an intense, well-collimated, and monochromatic atomic beam. In this regard, the experimentally produced trapped atomic BEC is already close to an ideal source since it clearly satisfies the conditions of high intensity and monochromaticity.
2. Array of optical elements: Just as in conventional optics, optical elements such as mirrors, lenses, beam splitters, collimators, apertures etc. are needed to control the atomic waves.
3. Detector: A number of schemes are used for detecting atomic beams. The preferred technique depends on atomic species and desired spatial or velocity resolution. Examples include fluorescent detection or resonant ionization. For current experiments involving BEC, techniques suitable for ultracold atoms such as the absorption or phase contrast imaging are required.

2.3 Evolution of ultracold atoms

Recent theoretical development of atom optics deals with single atomic waves described by the Schrödinger equation with a specific atom-photon interaction potential. In progressing to lower and lower temperatures, a quantum field theoretic treatment is required. This is because, at ultra low temperatures, the atomic de Broglie wavelength starts to become comparable with interatomic spacings, and each atom then interacts with $N - 1$ other atoms. The waves eventually overlap one another in BEC at temperatures below the critical temperature. Before the advent of the trapped atomic BEC, there have been a number of studies done on manipulating uncondensed but ultracold atoms using light forces under a subfield known as “nonlinear atom optics.” For a detailed discussion of nonlinear atom optics, readers are referred to papers by Lenz *et al.*[40] and Zhang *et*

al.[41, 42, 43]. In this section, we describe briefly how a nonlinear Schrödinger equation (NLSE) for ultracold atoms may be derived starting with a many-body Hamiltonian in nonlinear atom optics. Then the corresponding NLSE for a system of Bose condensed atoms, the Gross-Pitaevskii Equation, is derived.

2.3.1 NLSE for ultracold, uncondensed atoms

In nonlinear atom optics, the commonly used field-theoretic Hamiltonian has the form:

$$\begin{aligned} \hat{H} = & \sum_{l,m} \int d^3\mathbf{r} \hat{\Psi}_l^\dagger(\mathbf{r}, t) \hat{H}_0 \hat{\Psi}_m(\mathbf{r}, t) \\ & + \frac{1}{2} \sum_{l,m,n,p} \int d^3\mathbf{r} d^3\mathbf{r}' \hat{\Psi}_l^\dagger(\mathbf{r}, t) \hat{\Psi}_m^\dagger(\mathbf{r}', t) \hat{V}(\mathbf{r} - \mathbf{r}') \hat{\Psi}_n(\mathbf{r}, t) \hat{\Psi}_p(\mathbf{r}', t), \end{aligned} \quad (2.2)$$

where $\hat{H}_0$ is the single particle Hamiltonian

$$\hat{H}_0 = -\frac{\hbar^2}{2m} \nabla_r^2 + V(\mathbf{r}), \quad (2.3)$$

and the field operator $\hat{\Psi}$ obeys the standard boson commutation relations. Here, each of the labels l, m, n, p indicates complete description of single atom states i.e. both the centre of mass and internal quantum numbers. We note that the Hamiltonian of Eq. (2.2) is more general than Eq. (1.11) in that it explicitly takes into account transitions between atomic states. For the cases that don't involve state change one may take $l = m = n = p$, and the Hamiltonian reduces to Eq. (1.11). This more general type of Hamiltonian, Eq. (2.2), will be used again in Chapter 8 in which we discuss a Raman output coupler that explicitly couples two distinct atomic states.

Equation of motion

Writing the N -atom wave function as a product of N single-atom wave functions $\phi(\mathbf{r}_i, t)$ (Hartree approximation),

$$\Phi(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N; t) = \prod_{i=1}^N \phi_i(\mathbf{r}_i, t), \quad (2.4)$$

the equation of motion for the effective single-particle wave states $\phi_l(\mathbf{r}, t)$ of non-linear atom optics is found using the variational principle as a system of coupled nonlinear Schrödinger equations[40]:

$$\begin{aligned}
 i\hbar \frac{\partial \phi_l(\mathbf{r}, t)}{\partial t} &= \sum_m \langle l | \hat{H}_0 | m \rangle \phi_m(\mathbf{r}, t) \\
 &+ (N-1) \int d^3\mathbf{r}' \sum_{m,n,p} \langle lm | \hat{V}(\mathbf{r} - \mathbf{r}') | np \rangle \phi_m^*(\mathbf{r}', t) \phi_n(\mathbf{r}', t) \phi_p(\mathbf{r}, t),
 \end{aligned}
 \tag{2.5}$$

Typically, labels l, m, n, o take on values e, g where e and g denotes excited and ground states of the atom respectively. Here we have introduced matrix elements of single particle Hamiltonian $\hat{H}_0$ and the interaction potential $\hat{V}$ in the occupation number basis. Different physical systems are modelled by the choice of $\hat{V}$ and the labels l, m, n, o .

2.3.2 The Gross-Pitaevskii Equation

We derive in this section the NLSE for the condensates using the mean field theory approach of Ginzburg and Landau[44]. We start in this case with the Hamiltonian of Eq. (1.11) since the atoms are assumed to be all in the same internal state, and consequently the summation over indices l, m, n, o is irrelevant. We take, in accordance with the current experimental configurations, the magnetic confining potential $V(\mathbf{r})$ to be harmonic, and approximate the interatomic potential by that of the contact interaction, Eq. (1.16). The Heisenberg equation of motion for the operator $\hat{\Psi}$ is then:

$$\begin{aligned}
 i\hbar \frac{\partial \hat{\Psi}(\mathbf{r}, t)}{\partial t} &= [\hat{\Psi}(\mathbf{r}, t), \hat{H}] \\
 &= \left[-\frac{\hbar^2}{2m} \nabla_r^2 + V_{\text{trap}}(\mathbf{r}) + \mathcal{V} \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \right] \hat{\Psi}(\mathbf{r}, t).
 \end{aligned}
 \tag{2.6}$$

By the mean-field approximation, we take the expectation value of the operator $\hat{\Psi}(\mathbf{r}, t)$ to be a c -number wave function, $\langle \hat{\Psi}(\mathbf{r}, t) \rangle = \psi(\mathbf{r}, t)$; taking the expectation values in Eq. (2.6), and introducing the scattering length a via Eq. (1.17), the

GPE for the condensate wave function, ψ , is finally given by:

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla_r^2 + V_{\text{trap}}(\mathbf{r}) + C_n |\psi|^2 \right] \psi, \quad (2.7)$$

where

$$C_n = N\mathcal{V} = \frac{4\pi N\hbar^2 a}{m}, \quad (2.8)$$

with N being the number of particles in the sample, and m the mass of a single particle. Physically, the GPE describes the dynamics of a single atom moving in the presence of both an external potential $V(\mathbf{r})$ and a mean field induced by N atoms in the system, where N is of the order $\sim 10^6$ in recent experimental samples.

It is noted also that over the last few years, the GPE has been found to provide an excellent description of condensate behaviour over a range of temperatures from near $T = 0$ K to a sizeable fraction of T/T_c where T_c is the critical temperature of phase transition[20, 45, 46, 47]. The GPE has been used to simulate the damping of excitations in surprisingly good agreement with the low temperature experimental results[48].

2.4 Atom Optics with BEC

2.4.1 Configuration

We intend to investigate two types of possible experimental arrangements to manipulate the BEC. As the first possibility, we consider a typical atom optical configuration as shown schematically in Fig. 2.1: Firstly the condensate is prepared in a trap and released so that it freely falls under gravity. Such a situation is described by turning the trap off i.e. setting $V_{\text{trap}} = 0$. The ballistically expanding condensate is then passed through an interaction region in which it is subject to an interaction potential, before it again falls freely in space onto a detector or a surface. As the second possible experimental arrangement, we look at the effect of externally induced interaction *in the presence* of the confining trap. This gives a way of manipulating the condensate while within a trap, unaffected by the forces of the ballistic expansion.

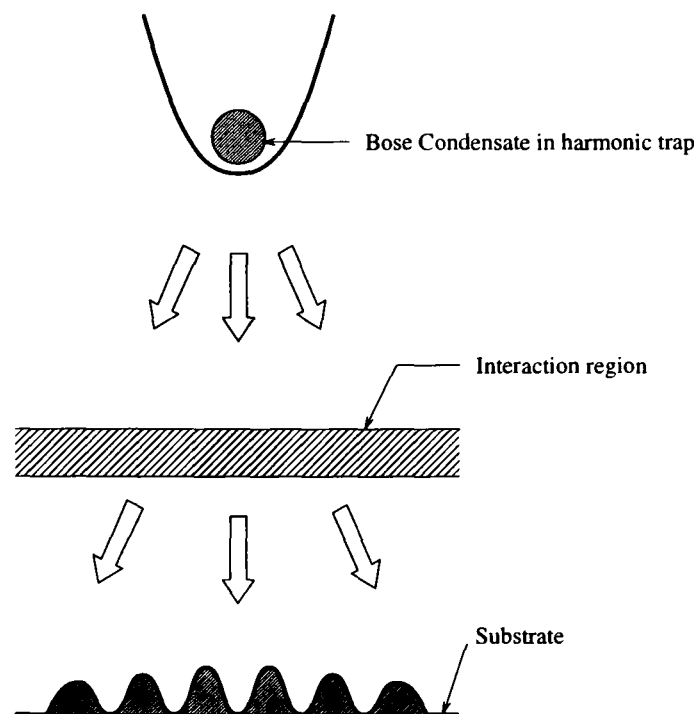


Figure 2.1: Schematic diagram of possible experimental configuration. The condensate prepared in a trap is released so that it passes through an interaction region in which it is subject to a modified potential. It then falls freely in space onto the surface of a substrate or a detector.

2.4.2 Modelling atom optical elements

We wish to model, in the context of the GPE, how the atom optical elements may produce focusing and splitting of a condensate. In the context of a single mode condensate in a trap, coupling between various internal levels as in nonlinear atom optics is not applicable. We therefore apply the general idea of optically generated potentials to model the atom optical elements. An optical potential may be thought of as an effective spatially-dependent “eigenpotential” generated by the atom-photon interactions experienced by the input eigenstate to the Hamiltonian. In order to simulate this effect for the case of the condensate, we propose two ways: one is to transform the shape of the externally applied magnetic potential; the potential may be tailored so that atoms see a “valley” at certain points in space, which then provides a way to atom focusing. The presence of the nonlinear repulsive interatomic interactions is expected to significantly modify the effect of such potentials. Secondly, we suppose that the scattering length can, in general, be decomposed into two parts:

$$a = a_{\text{intrinsic}} + a_{\text{induced}}, \quad (2.9)$$

that is to say, the strength of the overall interatomic interaction may be viewed as the sum of that due to intrinsic interactions and the modification due to an external influence such as that of the laser, magnetic field or RF-induced interaction. $a_{\text{intrinsic}}$ denotes the scattering length in the absence of an external field, and is an experimentally measurable quantity; a_{induced} is that induced by an external electromagnetic field for which there are various theoretical predictions. Such externally induced modification may occur, for example, when pairs of atoms, driven by the external field, have the ground state mixed with an electronically excited quasimolecular state. This quasimolecular state can have much stronger interaction, modifying the scattering amplitude in the process. It is predicted, for example, that the overall scattering length, a , may be varied by the application of a magnetic field for $F = 3$, $m_F = -3$ hyperfine state in Cs[49]. A blue detuned “optical shielding” type laser of variable intensity[50, 51] is also believed to be a good way to achieve control over the effective scattering length. We note therefore that the strength of the mean field interaction, C_n may be made position dependent, since the induced scattering length, a_{induced} , may be varied in space with an application of a laser field with a spatial variation in intensity. This is our second proposed method of implementing the effect of an atom optical element.

We should emphasise that we shall be demonstrating the effect of these arrangements rather than providing detailed descriptions of how such a configuration would be constructed in practice. Direct application of these techniques using dipole forces will not always be possible due to a variety of factors; these include the possible heating of the condensate by the laser field which may destroy the condensation. Ideally one wants to apply light fields to transfer momentum to the atoms in a controlled manner while keeping the atom assembly condensed. This is, of course, a particularly severe task for ultracold BEC’s. We shall, however, discuss later some of what we see as the main limitations of such schemes.

2.4.3 Implementation

In the first configuration i.e. that of Fig. 2.1 we look at two types of interactions: spatial modulation of scattering length in the interaction region, so that the

corresponding evolution is given by:

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla_r^2 + \mathcal{C}(\cos \mathbf{k} \cdot \mathbf{r} + \mathcal{D})|\psi|^2 \right] \psi, \quad (2.10)$$

and use of sinusoidal potential in the interaction region as described by:

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla_r^2 + \mathcal{A} \cos \mathbf{k} \cdot \mathbf{r} + C_n |\psi|^2 \right] \psi, \quad (2.11)$$

where $\mathcal{C}$ and $\mathcal{A}$ are the amplitudes and k the wave number which can be adjusted. We present the results for the case when $\mathcal{D} = 0$, and also the case when the sinusoidal variation is limited to positive scattering lengths, by a suitable adjustment of $\mathcal{D}$.

Using either method, the atomic motion may be modified in a controllable manner. The two methods are qualitatively different since the first involving C_n is of an intrinsic nature, which arises from interaction of atoms in a many body system while the second involves imposing an external potential. We see that unlike conventional atom optics, we now have two avenues to impose potential gradient, which may or may not be applied simultaneously and opens up the possibility of manipulating the relative amplitudes and phases of these two potentials. In this way, it seems possible to generate an effective overall potential gradient, which may even vary over time, to tailor our atom optical component.

As the second possible experimental arrangement, i.e. looking at externally induced interaction in the presence of a trap, we consider the effect of spatially varying the interatomic scattering length in the presence of the confining trap. The condensate is not dropped, and therefore we can only study the case in which one has both types of potentials present simultaneously. This is modelled by an equation with a minor modification to the standard GPE:

$$i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla_r^2 + V_{\text{trap}}(\mathbf{r}) + f(\mathbf{r})|\psi|^2 \right] \psi. \quad (2.12)$$

We consider the case of $f(\mathbf{r}) = \mathcal{G}\mathbf{r}^2$ as well as $f(\mathbf{r}) = \mathcal{C}(\cos \mathbf{k} \cdot \mathbf{r} + \mathcal{D})$, where $\mathcal{G}$, $\mathcal{C}$, $\mathcal{D}$ are constants, in order to test general features of such an arrangement.

We note that the condensate formed using the cloverleaf trap at MIT has an

aspect ratio of 20[28]. This means that a 1D GPE may be expected to provide an adequate qualitative description of the evolution of a cross section of such condensate. The spatial modulation of C_n discussed above would, in this case, be along the long axis. To be more precise, one may allow some Gaussian spreading of C_n in the radial direction of the cigar-shaped condensate. i.e. $C_n(\mathbf{r})_{\text{radial}}$ of the form

$$C_n(\mathbf{r})_{\text{radial}} \propto e^{-\kappa \mathbf{r}_{\text{radial}}^2}. \quad (2.13)$$

We assume the coupling between the $C_n(\mathbf{r})_{\text{axial}}$ and $C_n(\mathbf{r})_{\text{radial}}$ to be weak. The 1D GPE with modified linear and non-linear potentials was integrated using a 4th order Runge-Kutta integration routine (See Appendix A) over various configuration times in order to find the optimal condition for focusing and splitting. In the following we assume that all our atoms originally have positive scattering lengths.

2.5 Results

2.5.1 First configuration

In order to simulate the experiment of type shown in Fig. 2.1, we need to specify how long we let the condensate to free fall, interact with the chosen field and then fall freely again onto a detector or a substrate. It was found from simulations that, once the initial free evolution time is chosen, the final spatial distribution of the condensate that we see at the detector depends, as would be expected, quite sensitively on the duration of interaction and the subsequent free fall. In our simulations, an experimentally reasonable initial free fall time was chosen and then the interaction and the subsequent free fall times have been selected so as to give optimum probability distribution in terms of sharpness and regularity of the peaks on the final detector.

Spatial modulation of C_n in the interaction region

In conventional atom optics, parabolic optical potentials are used to provide a focusing effect. We have, therefore, tried a parabolic modulation of C_n in the interaction region. It was found that, in order to see any noticeable focusing effect by such an arrangement, we need a very steep position dependence, such

that around the tail region of the condensate, C_n of the order of around 20 times the original value is needed. A theoretical treatment by Fedichev *et al.*[52] indicates that although it might be possible to change the scattering length by comparable amounts, the accompanying inelastic scattering rate also undergoes a correspondingly large increase. Since this is not experimentally favourable, we do not pursue the parabolic variation any further and instead concentrate on the sinusoidal modulation of C_n in the interaction region.

We have let our condensate to ballistically expand for $t = \pi/\omega$ to model the initial free fall part of Fig. 2.1. The axial trap frequency of the MIT cloverleaf trap was reported to be $\omega = 2\pi \times 18$ Hz which translates t to time of order 27 ms. Figure 2.2(a) shows in solid line the probability distribution immediately after the interaction region, interacting for duration $t = 0.3\pi/\omega$ with modulation amplitude $\mathcal{C} = C_n$, $\mathcal{D} = 0$ and wave number $k = 2$ in harmonic oscillator units. The dashed line indicates the ballistically expanded condensate just before the interaction. This interaction time, which corresponds to approximately 8 ms in the MIT trap parameters, gave the best result in terms of sharpness, height and regularity of the peaks. The shape of the spatial modulation is shown as the dotted line. We see that the number of peaks and valleys match the number of spikes in the condensate as to be expected from conventional potential gradient idea. Indeed, it was found that in an identical simulation with $k = 1$ i.e. half the wave number, we get 4 prominent spikes in the final distribution instead of 8 as seen here. It is then reasonable to expect that the sharpness of these peaks, as indicated by the ratio of their height to widths would increase if the amplitude of the potential was increased; the results agree with this prediction. The maximum peak height of 0.094 for Fig. 2.2(a) was increased to 0.162 as a result of doubling the amplitude of modulation while keeping the general shape.

After the interaction region, the condensate was let to evolve freely. Figure 2.2(b) shows the final probability distribution after the distribution shown in Fig. 2.2(a) was freely evolved for duration $t = 0.3\pi/\omega$. The time of free evolution was again chosen so as to give the best distribution. The peaks are now broader and have been displaced so that now there is a peak at the origin, as a result of rather complex dynamical motion of various parts of the condensate as it expands. The dotted lines represent the shape of the effective potential that was originally in place in the interaction region. It was found that a regular proba-

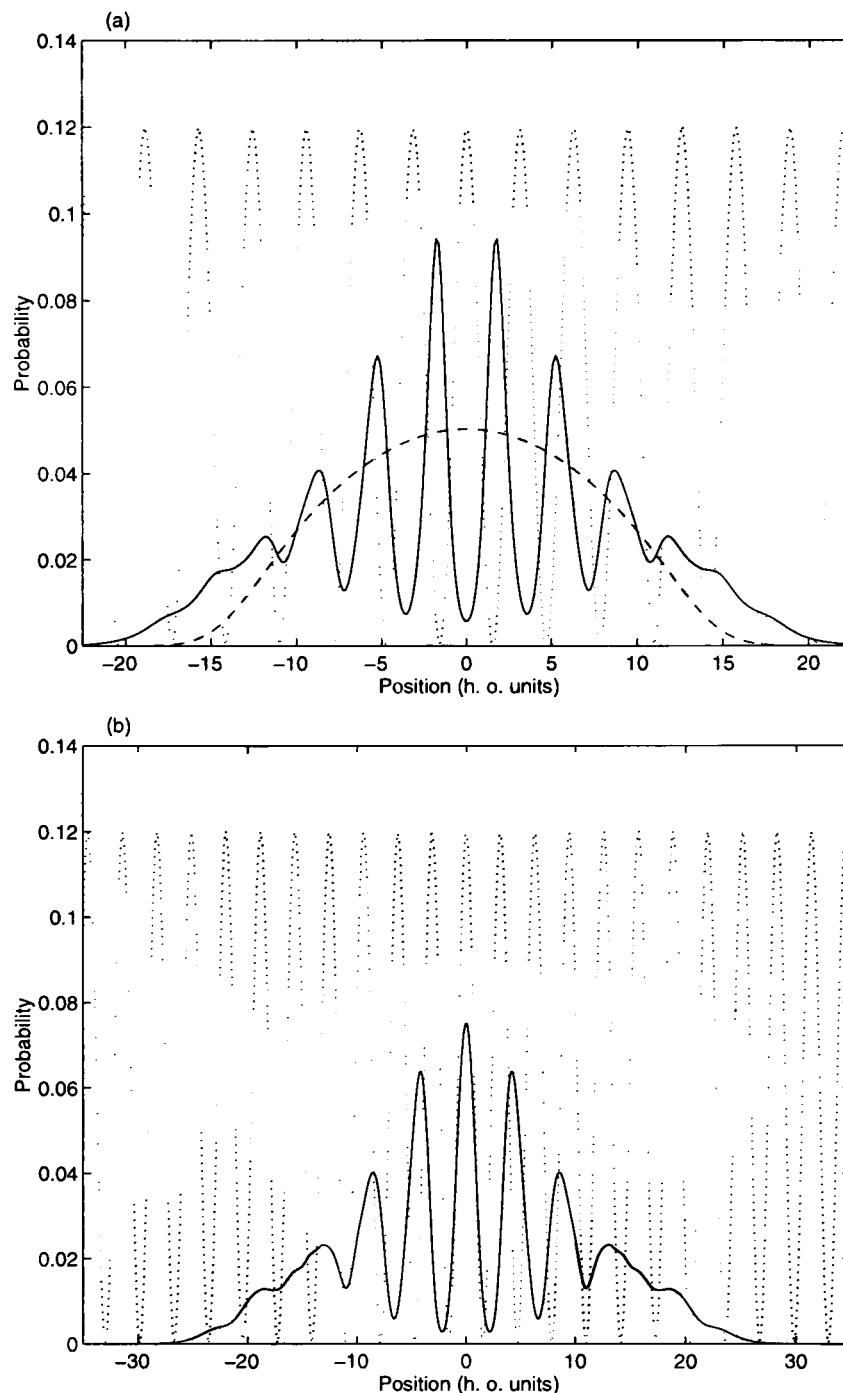


Figure 2.2: (a) Probability distribution immediately after the interaction region of Fig. 2.1 after interacting for the duration $t = 0.3\pi/\omega$ in the interaction region (solid line). $\mathcal{C} = C_n$, $\mathcal{D} = 0$ and $k = 2$. The dashed line is the shape of the condensate just before the interaction. (b) Final probability distribution after further free evolution for duration $t = 0.3\pi/\omega$. In both (a) and (b), the dotted line indicates the shape of the potential that was in place in the interaction region.

bility distribution is again restored after $t = 0.8\pi/\omega$, with shorter and broader peaks.

The case of a sinusoidal variation of the scattering length which remains positive was also investigated. This was simply accomplished by translating the potential vertically so that the minimum value of C_n is now 0 instead of $-C_n$ as

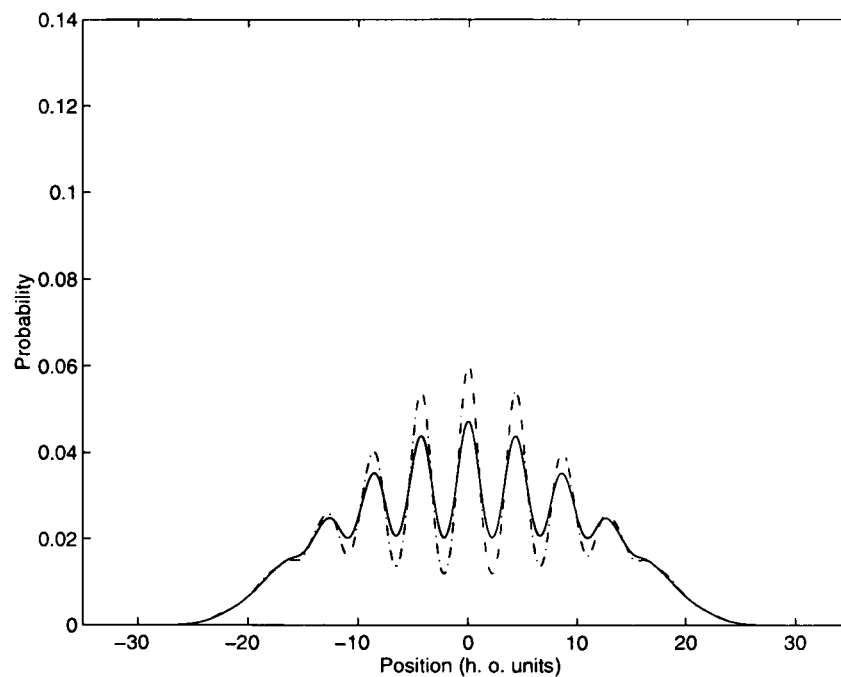


Figure 2.3: Probability distribution when the scattering length remains positive. This was simply accomplished by translating the potential vertically ($\mathcal{D} = 1$). Solid line represents the case of varying the potential between 0 and C_n while the dot-dash curve corresponds to the potential which varies between 0 and $2C_n$.

in the previous case. The final result is shown in Fig. 2.3. The solid line is the case when C_n varies from 0 to C_n . The dot-dashed line indicate the case when C_n varies from 0 to $2C_n$. We see that there is no qualitative difference from the previous case in which negative scattering length was allowed; the amplitude of modulation seems to be the determining factor rather than the sign.

The effect of longer initial free evolution time than π/ω was to give shorter peaks, but with the same general shape and width. This can be explained from the fact that after a longer free fall, the condensate has spread out more and its peak height is consequently shorter when it interacts with fields in the interaction region.

Using a sinusoidal potential in the interaction region

In a direct analogue to the case of spatial modulation of C_n , we simulate the same experiment of Fig. 2.1, but here we employ a sinusoidal potential in the interaction region while leaving C_n spatially invariant i.e. Eq. (2.11). The initial free fall time was again chosen to be π/ω .

The probability distribution immediately after the interaction region of Fig. 2.1 for a sinusoidal potential is shown as solid line in Fig. 2.4(a). In this case, Eq. (2.11) was integrated with $\mathcal{A} = 1$ and $k = 2$ over interaction time $t = 0.2\pi/\omega$.

As before, the shape of the sinusoidal potential is shown in dotted line, and the dashed line indicates the ballistically expanded condensate immediately before the interaction. When the amplitude of modulation was doubled, the maximum peak height of 0.073 shown in Fig. 2.4(a) was found to increase to 0.102 while keeping the same general shape. Again, when an initial free evolution time longer than π/ω was considered, shorter peaks were produced, giving smaller peak height-to-width ratio, as discussed previously.

The final probability distribution after a subsequent free evolution of duration $t = 0.3\pi/\omega$ is shown as solid line in Fig. 2.4(b). It was again found that a regular probability distribution is restored after $t = 0.9\pi/\omega$, with shorter and broader peaks. When one uses $\mathcal{A} = 2$ in the sinusoidal potential, the corresponding probability distribution is as given by the dot-dash line in Fig. 2.4(b). For this case, free evolution time after the interaction of $0.4\pi/\omega$ was used. We see here that the effect of modifying the confining trap potential is qualitatively the same as that of modulating C_n and that their effect in both cases may be understood by simply using the potential gradient idea, as in conventional atom optics.

We note also that parabolic potential over the interaction region is another possible configuration for focusing. It was found, however, that although focusing effect does arise in the sense of counteracting the ballistic expansion, its effectiveness was rather small and broadening took place on a very short time scale after leaving the interaction region. This is possibly because by this stage, repulsive interactions dominate in a dynamically expanding condensate, such that the original trap potential is not sufficient to counteract the expansion. Again a very steep parabolic potential was needed to observe an efficient focusing effect.

2.5.2 Second configuration

In this subsection, we look at the possibility of imposing both the spatial modulation of C_n and a confining trap. We look at the evolution such as that described by Eq. (2.12), which, in addition to the atom optical configuration discussed in the previous subsection, is another possible experimental arrangement. Since, in this case, the confining trap prevents ballistic expansion, a parabolic variation in C_n with more realistic values of the scattering length could be studied.

Figure 2.5(a) displays the probability distribution of the original trapped condensate in solid line while the dot-dash line displays the distribution with a

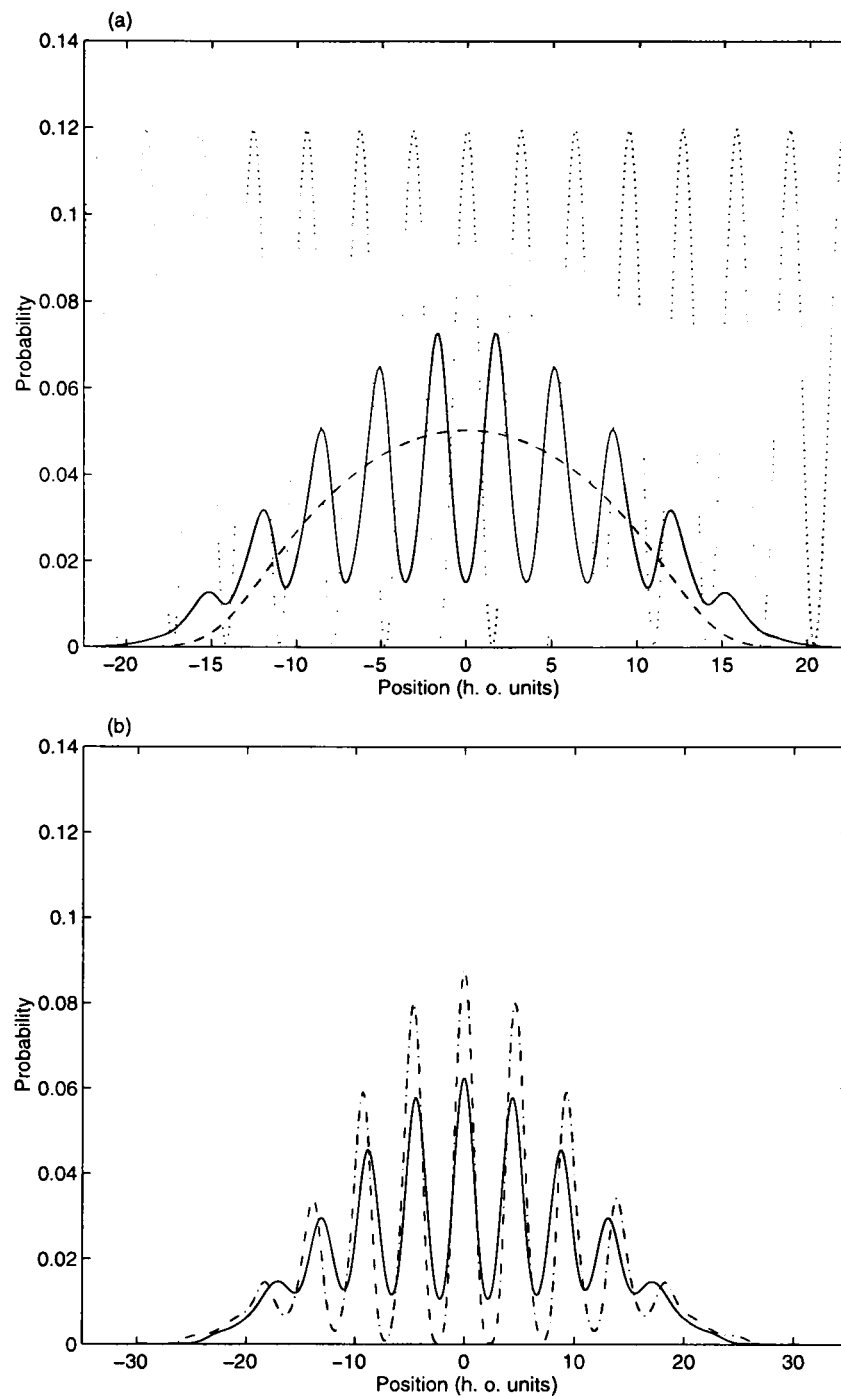


Figure 2.4: (a) Probability distribution immediately after the interaction region for a sinusoidal potential. $\mathcal{A} = 1$ and $k = 2$ with an interaction time $t = 0.2\pi/\omega$ (solid line). The dotted and the dashed curve shown similarly as in Fig. 2.2. (b) Final probability distribution after further free evolution. ($\mathcal{A} = 1, k = 2$) for $t = 0.3\pi/\omega$ (solid line). The dot-dash line represents the corresponding distribution for $\mathcal{A} = 2, k = 2$, and $t = 0.4\pi/\omega$.

parabolic variation on the non linear coefficient in Eq. (2.12). This is the result after time $t = 0.5\pi/\omega$ where ω is the trap frequency. In this simulation we assumed that C_n varies as $C_n x^2/400$ in harmonic oscillator units so that we have $C_n(x) = 0$ at the origin and C_n at $x = \pm 20$. We see here a focusing effect within the trap.

The height, and consequently the width, of the peak was found to vary over

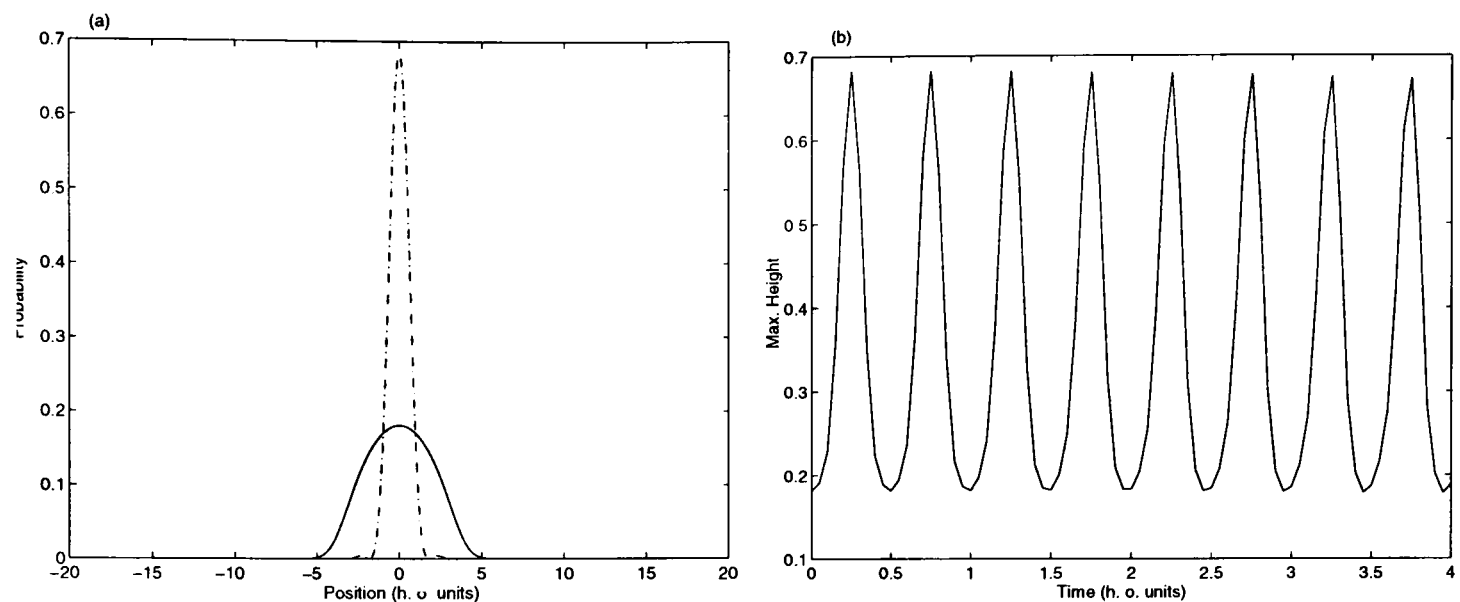


Figure 2.5: (a) Solid line: Probability distribution of the trapped condensate. Dot-dash line: Probability distribution after time $t = 0.5\pi/\omega$ when a parabolic variation on the nonlinear coefficient is imposed. (b) Variation of the maximum peak height over time in the presence of parabolic C_n .

time in an oscillatory fashion. Figure 2.5(b) shows the evolution of the maximum height of the peak over time in the presence of this parabolic potential. The behaviour can be qualitatively understood from the fact that the condensate on the wings of the Gaussian-like initial distribution ‘feels’ a push towards the centre, resulting in the build up of the peak height; the peak height then starts to decrease after a maximum as the condensate pass through each other and results in broadening of the base of the distribution. A slowly-varying beating type envelope appears on the oscillatory curve when a different parabolic distribution is used; for instance when the C_n varies as $C_n x^2/100$ rather than $C_n x^2/400$. This slowly-varying beat pattern is caused by effective phase difference between the potentials acting on the condensate. In this example, the potentials act as two distinct “springs” which are out of phase with one another in time; this effect becomes more pronounced when the tightness of the parabolic potential due to C_n is changed.

The resulting probability distribution when a sinusoidal rather than a parabolic variation of scattering length is imposed is shown in Fig. 2.6(a). We see that an action similar to beam splitting occurs with two prominent peaks. The time of interaction shown is $t = 0.4\pi/\omega$. Again there is a time dependent behaviour as to be expected.

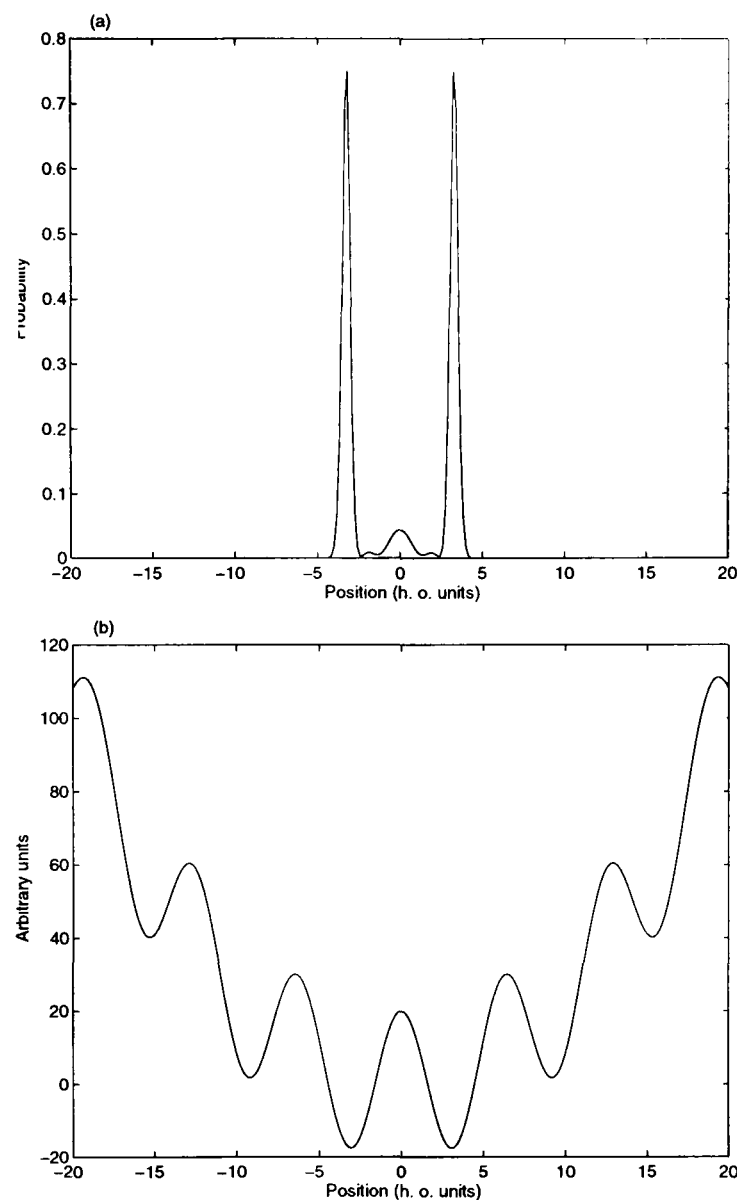


Figure 2.6: (a) Probability distribution after time $t = 0.4\pi/\omega$ with a sinusoidal variation of the non-linear coefficient in the presence of the trap. (b) A qualitative shape of the effective potential obtained by superposing the two independent potentials on the linear and nonlinear terms.

The somewhat unexpected shape of Fig. 2.6(a) can be explained by superposing the two independent potentials; Fig. 2.6(b) shows the shape of the overall potential when the parabolic trapping potential and the sinusoidal one modulating the non-linear constant is superposed. (This is a plot of x vs. $\frac{x^2}{4} + C_n \cos x$.) It is clear from the shape that the most likely probability distribution is that of two peaks, as any further peaks would require additional energy. Again, the time-dependent variation of the probability distribution can be explained by the fact that, as the condensate changes its shape over time, both the trapping potential and the sinusoidal potential from the nonlinearity exert time-varying forces. It is noted that in Fig. 2.6(a), we used $k = 1$ modulation, and the separation between

the two peaks was reduced for higher k , as to be expected. When the trap was turned off, it showed a lot more peaks than the expected number of around 4 (c.f. Figs. 2.3- 2.4). This is readily seen to be the effect of the trapping potential; there is an extra force from the sides toward the centre, resulting in high number of peaks in the main region $x = -10 \dots 10$. What is clear from simulations of this subsection is that we can manipulate the shape of an initially stationary condensate within a trap by modulating the non-linearity constant.

2.6 Discussion

In this section we attempt to estimate possible experimental values. First of all, we note that the interaction times used in simulations of the order of 10 ms are very much within the limits of present technology, since a typical atom lithography set up has the total time taken from a thermal source to substrate of the order $\sim 0.67\text{ms}$ [39]. It is also noted that typical time of flight of the condensate used in recent experiments before imaging is around 40 ms, so the total time taken from source to detector in our numerical simulations matches those of real experiment very closely. The total distance the condensate falls in our example from source to detector is, then, around 1 cm. The width of each peak in simulations is around 2 harmonic oscillator units which, for sodium atoms and the cloverleaf trap, corresponds to approximately $7 \mu\text{m}$. Possible ways to reduce this width even further would be by using the modulating field of higher value of amplitude to k ratio in the interaction region and also by using a trap of higher frequency than $2\pi \times 18 \text{ Hz}$. The effect of increasing k alone would mean the peaks become more closely spaced.

The area under each peak was such that the number of atoms in each peak would be around 10% of total number of atoms. A very important point is whether there is any limit to the number of atoms in each peak due to interactions between the particles. This aspect was investigated by looking at the probability distributions for the case where we employ sinusoidal potential, i.e. Eq. (2.11), but with various values of interatomic interaction strength characterised by C_n . It was indeed found that the “fringe visibility” defined as

$$V = \frac{P_{\max} - P_{\min}}{P_{\max} + P_{\min}}, \quad (2.14)$$

where $P_{\max}$ and $P_{\min}$ represent the maximum and the minimum of the “fringe pattern” decreases quite dramatically when we use a larger value of C_n . As an approximate indication, simulation with $C_n = 150$, as compared to $C_n = 20$ used in Fig. 2.4 gives $V = 0.24$ as compared to original $V = 0.72$. The times used were $0.5\pi/\omega$, $0.2\pi/\omega$, and $0.3\pi/\omega$. The initial free evolution time was chosen to be $t = 0.5\pi/\omega$ rather than π/ω because in this case of large C_n , the cloud spreads out too much by the time $t = \pi/\omega$. Noting that C_n is also proportional to N , the total number of the condensate particles, this brings us to the question of whether production of an *intense* beam of atoms in an atom laser is a requirement when atom optical elements of this kind is used. This aspect seems to be an important limiting factor in the design and implementation of any atom optical experiment using Bose condensates. One may, in principle, use a higher value of $\mathcal{A}$ for high values of C_n to improve the visibility. This implies that to be effective, various parameters have to be adjusted carefully to optimise the set up for each instance.

Modulation of scattering length and use of sinusoidally varying potential raise the issue of experimental feasibility, as these will certainly involve interaction of an electromagnetic field with ultracold atoms. The primary effect of light on cold trapped atoms is to cause loss processes by giving atoms enough energy to escape the trap, through such processes as photon recoil and photo-association. The rate at which an atom heats up as a result of photon recoil is given by

$$\Gamma = \gamma \left(\frac{\Omega}{\delta} \right)^2 \quad (2.15)$$

where γ is the natural atomic linewidth, Ω the Rabi frequency and δ the detuning. It is assumed here that $|\delta| \gg \Omega$ and $|\delta| \gg \gamma$. A recent theoretical study by Fedichev *et al.* shows that it is, in fact, possible to alter the scattering length by as much as 350% for ^7Li and minimise recoil or photo-association losses with a selection of frequency detuning and Rabi frequency[52]. In order to have small recoil losses along with a significant change of a it is necessary that the detuning, δ be large and negative, and chosen to be not too far from a vibrational resonance with one of the bound p states of the electronically excited quasimolecule. All our simulations depend on the assumption that the possible heating of the condensate is either negligible, or has typical time scale which is long compared to the interaction times considered here. We also note that generation of optical

potentials by Raman transition has recently been proposed as a way to reduce the spontaneous emission rate[53]. The atom optical elements discussed in this chapter may be achieved via magnetic as well as optical fields, and it is conceivable that certain arrangement such as, say, an optical shielding laser combined with a magnetic field-induced potential gradient might provide a solution. More study, however, would be required on exactly how one can implement these atom optical elements.

In summary, it was found from numerical simulations involving various configurations that focusing and splitting effects can be achieved within the context of the non-linear Schrödinger equation with modified potentials. It is pointed out that our simulations just show a possible theoretical model, without inclusion of such effects as the spontaneous emission of atoms as might be the case when the external potential involves an optical dipole force. Various possible improvements may be made in order to accommodate such effects into theory. For example the effect of inelastic collisions may be incorporated by letting C_n be complex. However, at present, there is no clear indication of how big such effects will be in practice. Further studies along the lines of atom optics could involve the study of coherence property of the condensate which have been modified in this way. Other possibilities include finding a way to use the two potentials simultaneously to tailor an atom optical element of an arbitrary specification, and eventually finding a way to prepare vortex states in the condensate through such modification. We note that the optical imprint method to generate a vortex is already being used. These studies are of relevance to the investigation of superfluidity in a trapped alkali Bose gas, and in this sense, the atom optical elements for the condensates can be more than just equivalents of conventional optical elements.

Chapter 3

Quasiparticle excitations in trapped BEC

3.1 Introduction

The measurement of the quasiparticle excitation spectrum was one of the earliest experimental achievements in the field of trapped atomic BEC[46, 54]. These measurements have provided surprisingly good agreement with the theoretical predictions based solely on the linear response theory of GPE[20, 45], allowing GPE to be “taken much more seriously” among researchers. In this chapter we give a very brief review of the concept of quasiparticle excitation spectrum of the condensate. We then introduce an orthogonalisation procedure on the quasiparticles with respect to the condensate wave function. We investigate a specific example where the concepts of quasiparticles and their orthogonal projection may be directly applied – the nonlinear mixing of quasiparticle modes. The occurrence of nonlinear mode mixing is a natural corollary of the many-body Hamiltonian[Eq. (1.11)] which has the same structure as that of four-wave mixing or high harmonic generation in Quantum Optics. The results and notations of this chapter are used extensively in the rest of the thesis; we use these concepts in the next chapter on damping of quasiparticle excitations, and in Chapter 5 we use the notations introduced here to describe BEC at finite temperatures.

3.2 Quasiparticle excitations

The concept of quasiparticles in a many body system is perhaps most clearly illustrated in a book by Mattuck[55]. A quasiparticle can be thought of as a set of interacting particles which may collectively be treated as being a fictitious non-interacting body. An example of this is a positively charged particle surrounded by a cloud of negatively charged particles; such quasiparticles are clearly noninteracting at least approximately, and greatly facilitate calculations on the many body system.

These non-interacting quasiparticles naturally possess a range of energies, and another way to view them is as the fundamental excitations, or in the context of BEC, the normal modes of the condensate ground state. The problem of finding these excitations on an inhomogeneous condensate has been considered in a number of papers (see for example Refs. [20, 45, 56, 57]). The standard method is either by considering linear deviations around the condensate or by describing the system with an approximate Hamiltonian which can later be diagonalised. The details of these two approaches can be found in Ref. [57]; this section attempts to provide only a brief summary of the relevant theory.

3.2.1 Linear response theory

This approach is based on considering response of the system to periodic perturbations, and is a well-established method in condensed matter physics. We assume that, since the nonlinear term in the GPE couples waves travelling in opposite directions, a solution of the GPE to external periodic perturbations takes the form

$$\Psi(\mathbf{r}, t) = e^{-i\mu t} \left[\psi_g(\mathbf{r}) + \sum_i \left\{ u_i(\mathbf{r}) c_i e^{-i\omega_i t} + v_i^*(\mathbf{r}) c_i^* e^{+i\omega_i t} \right\} \right] \quad (3.1)$$

where the c_i 's are constants. Such a form of solution arises from purely physical considerations but it is also closely related to the well-known Bogoliubov transformation of operators described below. Substituting Eq. (3.1) into GPE, linearising with respect to c_i 's and equating coefficients of $e^{\pm i\omega t}$, we find a set of

equations for $\psi_g(\mathbf{r})$, $u_i(\mathbf{r})$, and $v_i(\mathbf{r})$:

$$[\mathcal{H}_0 + NU_0|\psi_g(\mathbf{r})|^2]\psi_g(\mathbf{r}) = \mu\psi_g(\mathbf{r}) \quad (3.2)$$

$$\mathcal{L}u_i(\mathbf{r}) + U_0\psi_g^2(\mathbf{r})v_i(\mathbf{r}) = \omega_i u_i(\mathbf{r})$$

$$\mathcal{L}v_i(\mathbf{r}) + U_0\psi_g^{*2}(\mathbf{r})u_i(\mathbf{r}) = -\omega_i v_i(\mathbf{r}) \quad (3.3)$$

where

$$\mathcal{L} \equiv \hat{\mathcal{H}}_0 - \mu + 2U_0|\psi_g(\mathbf{r})|^2 \quad (3.4)$$

and $\hat{\mathcal{H}}_0$ is the usual single particle Hamiltonian operator, including the trap potential. Equations (3.3),(3.4) are customarily referred to as the Bogoliubov-de Gennes (BdG) equations. Finding the solution to the above three equations gives quasiparticle wave functions and energies with the i 'th level wave function $\tilde{\psi}_i$ given by $\tilde{\psi}_i = u_i(\mathbf{r})c_i e^{-i\omega_i t} + v_i^*(\mathbf{r})c_i^* e^{+i\omega_i t}$. We note that an analytical solution is possible for the homogeneous case. For the case of trapped gas, analytical solution is possible only in the non-interacting and strong coupling (Thomas-Fermi) limits[20]; otherwise the equations must be solved numerically. The detailed numerical method starting with the conversion of the equations to a basis set notation is given in Ref. [57].

3.2.2 Diagonalisation of quadratic Hamiltonian

The second approach to calculate quasiparticle excitations is via the diagonalisation procedure for the Hamiltonian. The grand-canonical, many body Hamiltonian in the field operator formalism modified from Eq. (1.11) is given by:

$$\hat{H} = \int d^3\mathbf{r} \left\{ \hat{\Psi}^\dagger(\mathbf{r}, t) (\hat{H}_0 - \mu) \hat{\Psi}(\mathbf{r}, t) + \frac{1}{2} U_0 \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \right\} \quad (3.5)$$

where $\hat{\Psi}(\mathbf{r}, t)$ is the usual Bose field operator. One starts the diagonalisation procedure by writing the decomposition:

$$\hat{\Psi}(\mathbf{r}, t) = \psi_g(\mathbf{r}) + \hat{\delta}(\mathbf{r}, t) \quad (3.6)$$

where $\psi_g(\mathbf{r})$ satisfies the time-independent GPE:

$$\left[-\frac{\hbar^2}{2m} \nabla_r^2 + V_{\text{trap}}(\mathbf{r}) + U_0 |\psi_g(\mathbf{r})|^2 \right] \psi_g(\mathbf{r}) = \mu \psi_g(\mathbf{r}). \quad (3.7)$$

Substituting Eq. (3.6) into the Hamiltonian and discarding terms containing three or four $\hat{\delta}(\mathbf{r}, t)$ operators we are left with a Hamiltonian quadratic in $\hat{\delta}$ which is to be diagonalised using the well-known Bogoliubov transformation of the operators,

$$\hat{\delta}(\mathbf{r}, t) = \sum_i \left\{ u_i(\mathbf{r}) \hat{\beta}_i + v_i^*(\mathbf{r}) \hat{\beta}_i^\dagger \right\}. \quad (3.8)$$

After applying Eq. (3.8) and then choosing the functions $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$ to satisfy the following equations

$$\int d^3\mathbf{r} \left\{ u_i^* \left[\mathcal{L}u_j + U_0 \psi_g^2 v_j \right] + v_i^* \left[\mathcal{L}v_j + U_0 \psi_g^{*2} u_j \right] \right\} = \omega_i \delta_{ij} \quad (3.9)$$

$$\int d^3\mathbf{r} \left\{ u_i \left[\mathcal{L}v_j + U_0 \psi_g^{*2} u_j \right] + v_i \left[\mathcal{L}u_j + U_0 \psi_g^2 v_j \right] \right\} = 0, \quad (3.10)$$

the Hamiltonian reduces to

$$\hat{H} = E_0 + \sum_i \omega_i \hat{\beta}_i^\dagger \hat{\beta}_i, \quad (3.11)$$

with E_0 given by N_0 times the Ginzburg-Pitaevskii-Gross energy functional:

$$E_0 = N_0 \int d^3\mathbf{r} \psi^*(\mathbf{r}, t) \left\{ \hat{H}_0 - \mu + \frac{1}{2} U_0 N_0 |\psi(\mathbf{r}, t)|^2 \right\} \psi(\mathbf{r}, t). \quad (3.12)$$

It is clear by inspection that the BdG relations of Eqs (3.3) satisfy Eqs. (3.9)-(3.10), and are therefore sufficient to diagonalise the Hamiltonian. This establishes the connection with the linear response method discussed above.

In Eq. (3.8), $\hat{\beta}_i$ represents the annihilation operator for the quasiparticle mode i . The wave functions $u_j(\mathbf{r})$ and $v_j(\mathbf{r})$ as they appear in the Bogoliubov transformation are therefore interpreted as the amplitudes associated with the annihilation of a real particle at position $\mathbf{r}$, an action which involves both annihilation or creation of excitations on top of the condensate.

Using the transformed Hamiltonian, the evolution of the quasiparticle opera-

tors is straightforwardly given by

$$\hat{\beta}_i(t) = \hat{\beta}_i(0)e^{-i\omega_i t}. \quad (3.13)$$

If we now allow the quasiparticles to become coherent so that they have non-vanishing quantum expectation values, $\langle \hat{\beta}_i(t) \rangle = b_i(0)e^{-i\omega_i t}$, the expectation value of the field operator takes exactly the form of Eq. (3.1) in the linear response approach.

3.2.3 Properties of $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$

Equations (3.3) imply that the $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$ must satisfy the following orthogonality and symmetry relations

$$\int d^3\mathbf{r} \{u_i u_j^* - v_i v_j^*\} = \delta_{ij} \quad (3.14)$$

$$\int d^3\mathbf{r} \{u_i v_j - v_i u_j\} = 0. \quad (3.15)$$

The fact that quasiparticle operators $\hat{\beta}$ obey Bose commutation relations sets the normalisation to 1 for the $i = j$ case in Eq. (3.14). An important feature of the solutions to the BdG equations is the existence of an exact solution with $\omega = 0$, $u_0(\mathbf{r}) = \psi_g(\mathbf{r})$ and $v_0(\mathbf{r}) = -\psi_g^*(\mathbf{r})$. This condensate mode has zero norm but otherwise satisfies the orthogonality and symmetry relations of Eqs. (3.14) and (3.15), which both take the form

$$\int d^3\mathbf{r} \{\psi_g^* u_i + \psi_g v_i\} = 0. \quad (3.16)$$

It is noted, however, that $\int d^3\mathbf{r} \{\psi_g^* u_i\}$ and $\int d^3\mathbf{r} \{\psi_g v_i\}$ are not separately zero, since the excitations $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$ are *not* orthogonal to the condensate ψ_g [58].

Orthogonal solutions may be constructed by noting that, rigorously speaking, Eqs. (3.3) are not necessary conditions for the diagonalisation of the Hamiltonian[the necessary conditions are rather given by Eqs. (3.9) and (3.10)]. This then allows one to choose the excitations to be orthogonal to the condensate [59] while still diagonalising the Hamiltonian with the same eigenvalues as before. This is achieved by subtracting the overlap with the condensate from the solutions to the BdG equations. These orthogonal excitations $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$ then

obey a set of modified BdG equations[60, 61, 62]. Such modified BdG equations are introduced in Chapter 8.

3.3 Quasiparticle projection method

In a more general context, not only the excitations but also the condensate population itself changes due to interaction. We may therefore write, instead of Eq. (3.1), the wave function as

$$\Psi(\mathbf{r}, t) = e^{-i\mu t} \left[(1 + b_g) \psi_g(\mathbf{r}) + \sum_{i>0} \{ u_i(\mathbf{r}) b_i(t) + v_i^*(\mathbf{r}) b_i^*(t) \} \right]. \quad (3.17)$$

Since ψ_g and its excitations form a complete set, any wave function may in fact be expanded in this way. The expansion then explicitly includes temporal variations in both condensate and quasiparticle populations. We wish to extract these coefficients b_g , b_i in our quasiparticle projection method. For convenience, we normalise the condensate wave function to 1 and change the parameter U_0 to $C_n = N_0 U_0$ where N_0 is the number of particles in the condensate. We then consider the expressions

$$\int d^3\mathbf{r} \{ u_j^* \Psi e^{+i\mu t} - v_j^* \Psi^* e^{-i\mu t} \} = (2 + b_g + b_g^*) a_j^* + b_j \quad (3.18)$$

$$\int d^3\mathbf{r} \{ \psi_g^* \Psi e^{+i\mu t} \} = 1 + b_g + \sum_i \{ b_i a_i - b_i^* a_i^* \} \quad (3.19)$$

where the a_i 's are the overlap coefficients

$$a_i = \int d^3\mathbf{r} \{ \psi_g^* u_i \} = - \int d^3\mathbf{r} \{ \psi_g v_i \} \quad (3.20)$$

with

$$\int d^3\mathbf{r} |\psi_g|^2 = 1. \quad (3.21)$$

In addition to Eqs. (3.18) and (3.19) we also consider the quantity

$$\int d^3\mathbf{r} \{ \psi_g^* \Psi e^{+i\mu t} + \psi_g \Psi^* e^{-i\mu t} \} = 2 + b_g + b_g^* \quad (3.22)$$

where we have used Eq. (3.16) to obtain the right hand side. Since the coefficients a_i are known, the combination of this equation with Eq. (3.18) leads to deter-

mination of all coefficients b_i which can then be used in Eq. (3.19) to calculate the coefficient b_g . In this way one may decompose uniquely an arbitrary single particle wave function into a condensate and a collection of excitations. In the next section we present results relevant to this thesis from Ref. [60] which is a collaborative work between the author and Morgan *et al.*

3.4 Nonlinear mode mixing

The self interaction term in the GPE implies an intriguing possibility of nonlinear mixing of quasiparticle modes. To observe this effect explicitly, it is necessary to track how each independent mode population including the condensate population evolves over time as a result of nonlinear interactions. In order to achieve this, orthogonal projection of quasiparticle modes has to be carried out at each time step.

In order to simulate and observe the phenomenon of nonlinear mixing in BEC, an initial wave function which consists of a condensate and a certain amount of excitation in a single mode was constructed. This is achieved by setting $b_k(0)$ equal to a finite value and $b_g = b_i = 0$ for $i \neq k$ in Eq. (3.17). This wave function is then propagated in the time-dependent GPE and is analysed using the quasiparticle projection method to observe the temporal dependence of the coefficients b_i .

We note that there are a couple of subtleties involved. Firstly, the initial wave function is constructed using the $\psi_g(\mathbf{r})$, $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$ corresponding to some particular value of the chemical potential μ , which implies that the chemical potential for the constructed wave function, condensate superposed with an excitation, differs from the original μ . This is even more so when the amount of excitations is sizeable. In order to get around this inconsistency, we need to first analyse the condensate evolution using the original basis (and original μ) and from this determine the rate of rotation of the condensate phase, $e^{-i\mu_{\text{relative}}t}$, where μ_{relative} is the difference in the old and new chemical potential. By using the new μ we find new solutions to the GPE and BdG with which we reanalyse the evolution. Secondly, in view of the fact that in real experiments quasiparticle excitations are incoherent, we must recover the evolution of incoherent quasiparticles from the coherent evolution given by the GPE. This has been done by

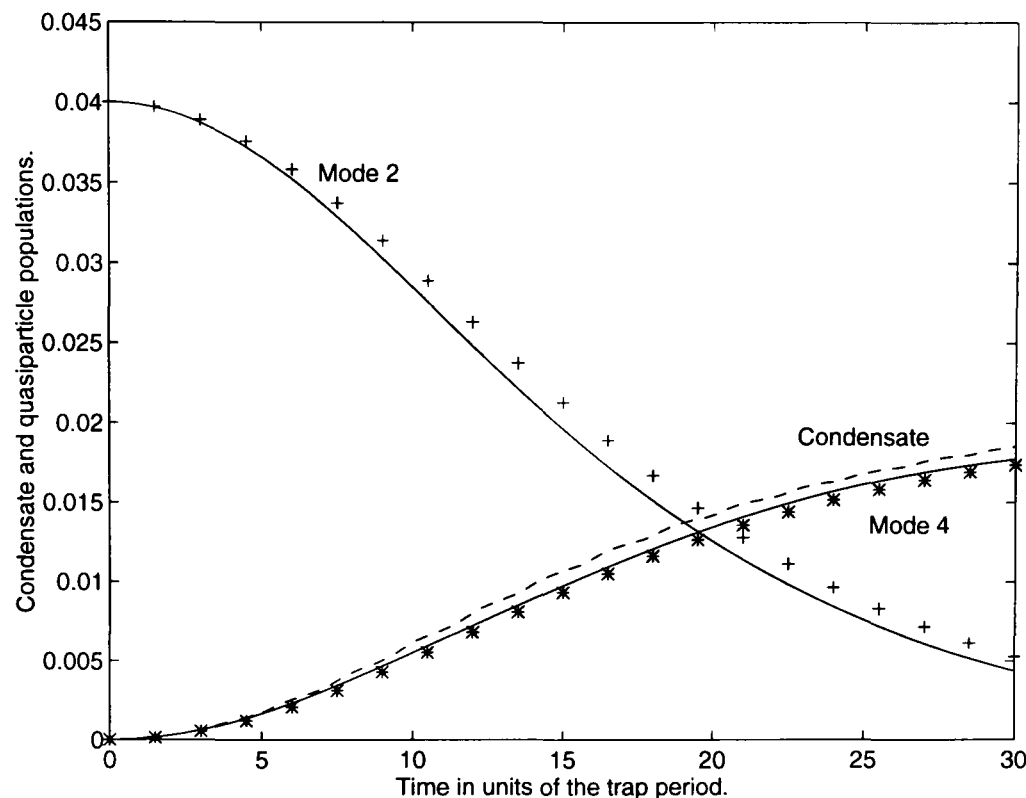


Figure 3.1: Evolution of the average quasiparticle populations and the change in the condensate population ($|1+b_g|^2-1$) for $\mu = 1$ and $|b_2(0)| = 0.2$. The pluses and asterisks are the predictions of analytical solutions for modes 2 and 4 respectively.

constructing a number of initial wave functions which differ in the phase θ_l of the initial excitation $b_k(0)$: $b_k(0) \rightarrow b_k(0)e^{i\theta_l}$, $l = 1, 2, \dots, N_S$, and then evolving separately under GPE. The final result is averaged to give the equivalent incoherent evolution of quasiparticle populations:

$$\langle |b_i|^2 \rangle = \frac{1}{N_S} \sum_S |b_i|^2. \quad (3.23)$$

We discuss the validity of this averaging process in more detail in Chapter 5. Intuitively speaking, the averaging procedure is a way to “blur” any sharply defined phase of the wave function.

The result of numerical simulations was found to give time dependent changes in quasiparticle populations akin to Rabi flopping. We have performed simulations with $|b_2(0)| = 0.2$ and 0.5 , with $\mu = 1$. They are shown in Figs. 3.1 and 3.2. One can see that the effect of the nonlinear mixing is predominantly a transfer of the quasiparticle population between modes 2 and 4. Since mode 4 is at roughly twice the energy of mode 2, this is just the frequency doubling process which we

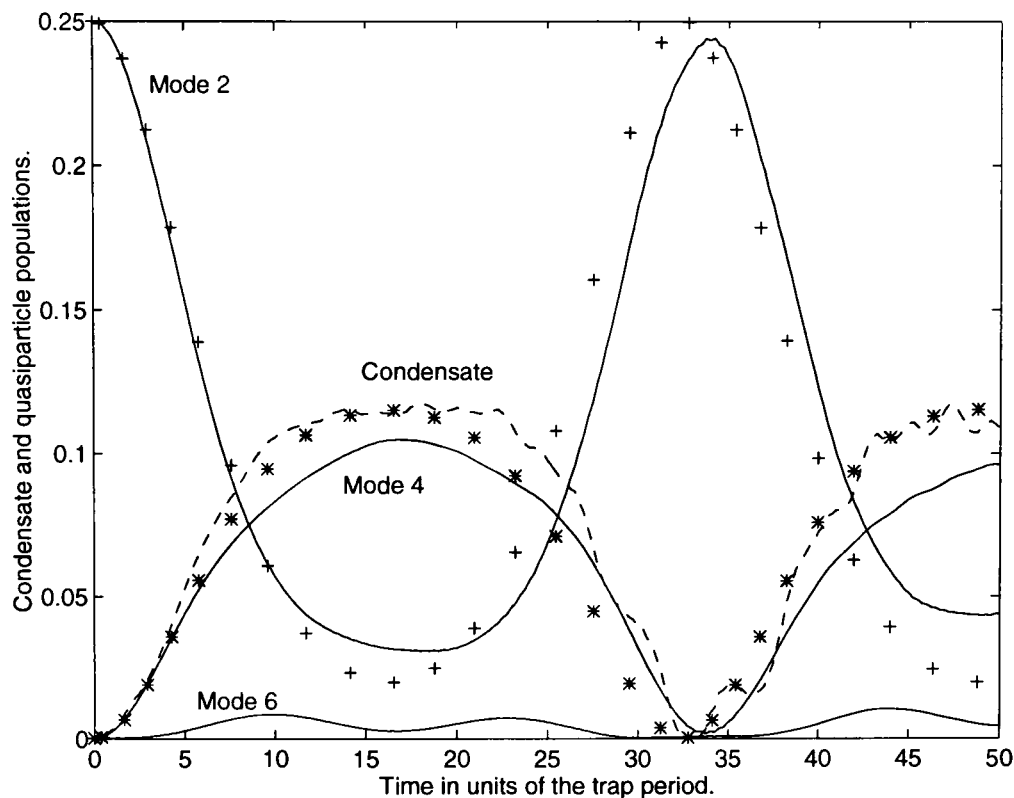


Figure 3.2: Evolution of the average quasiparticle populations and the change in the condensate population ($|1+b_g|^2-1$) for $\mu = 1$ and $|b_2(0)| = 0.5$. The pluses and asterisks are the predictions of analytical solutions for modes 2 and 4 respectively.

would expect from the form of the nonlinearity. In the case of the simulation with $|b_2(0)| = 0.5$ (Fig. 3.2), we can see that the process is reversible. This is a consequence of the fact that in a trap there is a discrete set of states rather than the continuum required for an irreversible decay of an excitation.

Also, analytical equations of motion for the coefficients b_i can be obtained by substituting the expansion of Eq. (3.17) into the time-dependent NLSE, and carrying out the projection procedure described in Sec. 3.3. Resulting equations of similar form have been studied in the context of harmonic generation in nonlinear optics[63], where it is shown that a general solution can be written in the form of elliptic integrals. These analytical solutions are shown in Figs. 3.1 and 3.2 as stars and crosses.

A number of features revealing the physics behind the mixing process can be noted from these two figures. First the rate at which the quasiparticle population is transferred between modes depends on the amount of initial excitation — with a larger initial excitation the mode mixing occurs at a faster rate and vice versa. This is to be expected from the term proportional to $|\psi|^2\psi$. Second, the change

in population of mode 2 is roughly twice that of mode 4. This is due to the conservation of energy: annihilation of two quasiparticles in mode 2 is followed by the formation of a single quasiparticle at twice the energy, i.e. in mode 4. Transfer of population from mode 4 to mode 2 is achieved via the reverse process. A third feature of the figures is that the change in the condensate population follows that in mode 4. This is a consequence of the fact that the normalisation of the wave function is conserved. Also one finds that with different values of the chemical potential μ ¹ the energy matching between mode 2 and 4 is not precise, and therefore produces a more complicated dynamics, involving particles from different modes.

In summary, we have introduced the notion of quasiparticles in this chapter and presented the method to project out the contribution of a condensate and its excitations from any wave function appearing in the NLSE. The presence of the nonlinear mixing of quasiparticles has been confirmed using the projection procedure. We have observed that the evolution is dominated by processes which conserve energy and that the initial population can be reversibly transferred to an energetically matched mode. We believe that the reversible transfer of population between modes such as those shown in Figs. 3.1 and 3.2 should be observable especially at low temperatures. The expected exponential damping of excitations at higher temperatures[64] has not, however, been observed in our simulations. In the next chapter we describe an independent way to incorporate damping in the context of GPE.

¹The chemical potential μ is identical to the eigenvalue of the GPE for the case of homogeneous system. For an inhomogeneous system, however, they differ by order $\sim 1/N$ where N is the total number of atoms in the condensate.

Chapter 4

Phenomenological damping of quasiparticle excitations

4.1 Introduction

Experiments dealing with collective excitations of BEC have indicated the presence of damping of the excitations[54, 64]. As well as measuring the energies of the excitations, these experiments have also probed the decay rates of oscillations that vary strongly with temperature[64]. Existing theoretical predictions for the decay rates are mainly for homogeneous gases (see for example Refs. [65, 66]), although some predictions for the inhomogeneous condensates have recently been published[67, 68]. For instance, a recent related work by Giorgini explores possible presence of Landau and Beliaev damping[68]. Landau damping involves two quasiparticle excitations colliding to produce a third one of different energy while Beliaev damping involves a quasiparticle colliding with the condensate itself producing two quasiparticles. Despite this, no complete theory of damping of excitations in inhomogeneous gas has been reported.

The Gross-Pitaevskii equation, which has been shown to give accurate predictions for the frequencies of elementary excitations[20, 45, 46], does not contain any mechanism for the damping of these excitations. From inspection, the first two terms in the GPE as written in Eq. (2.7) are simply the energy of a single particle in the trap while the third describes the non-dissipative effect of other particles in the system. Attempts to improve on the GPE include taking into account the correlation effects of excitations[69] and the introduction of the many-body

T -matrix[70]. These attempts so far have not produced any explicit results for damping in the inhomogeneous case.

One of the existing theories which incorporates dissipation in a quantum fluid is the phenomenological theory of superfluidity near the λ point[71]. We have adopted the theory to investigate damping in a dilute, trapped BEC numerically. The phenomenological theory of damping should be valid when the system is close to thermal equilibrium.

We begin this chapter by deriving the required modification to GPE. We then demonstrate two distinct uses of the new equation: its use in describing damping of oscillations in trapped atomic BEC, and its use as a computational tool to generate accurate eigenstates of the standard GPE.

4.2 Phenomenological theory of damping

The argument which we present below to obtain our expression for the phenomenological damping follows closely the method introduced by Pitaevskii[71]. The procedure is, in fact, a widely used one in the more general problems of dynamical critical phenomena[72].

4.2.1 Derivation

First of all, any relaxation process eventually leads to an equilibrium state. For the condensate at $T = 0$ such an equilibrium is described by the equation

$$-\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2\psi + V_{\text{trap}}(\mathbf{r})\psi + C_n|\psi|^2\psi - \mu\psi = 0. \quad (4.1)$$

This expression may be derived from minimising an appropriate energy functional or equivalently by finding the eigensolution to the time dependent GPE. Because the process we want to describe is that of relaxation, in the equation of motion for the condensate ψ ,

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{\mathcal{L}}\psi, \quad (4.2)$$

the operator $\hat{\mathcal{L}}$ cannot be Hermitian. The anti-Hermitian part of $\hat{\mathcal{L}}$ is associated with the processes by which equilibrium is approached. This anti-Hermitian part must vanish at equilibrium, that is, when Eq. (4.1) is satisfied. For the cases

where the deviation from equilibrium is small, one may therefore write the anti-Hermitian part in the form

$$i\Lambda \left(\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 \psi + V_{\text{trap}}(\mathbf{r})\psi + C_n |\psi|^2 \psi - \mu \psi \right), \quad (4.3)$$

where Λ is a dimensionless factor which is inversely proportional to the relaxation time. The Hermitian part is given by the fact that for $\Lambda = 0$, the theory must reduce to the conventional GPE at $T = 0$; the final equation including relaxation to equilibrium is, then, given by

$$i\hbar \frac{\partial \psi}{\partial t} = (1 + i\Lambda) \left\{ -\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V_{\text{trap}}(\mathbf{r}) + C_n |\psi|^2 - \mu \right\} \psi, \quad (4.4)$$

where $\Lambda < 0$ for damping.

4.2.2 Description of damping

Equation (4.4) is, in fact, a rather general equation of motion which describes evolution towards equilibrium. The standard GPE describes the motion of the mean field, ψ , which is taken to be the ensemble average of the boson field operator $\hat{\Psi}$. The mean field is customarily taken to be the condensate wave function, although it is also consistent to define it to be the condensate ground state plus any *coherent* wave function for the excited particles. Damping of elementary excitations may be described in the frame work of Eq. (4.4) by considering our mean field ψ to be broken into two parts: the condensate ground state ψ_g and a coherent excitation, $\delta\psi$, $\psi = e^{-i\mu t}(\psi_g + \delta\psi)$. Evolution in Eq. (4.4) results in the damping of $\delta\psi$ towards zero. As a simple illustration of the damping effect, we consider using the damping prescription in the homogeneous limit. Assuming that initially we have a small amount of excitations on the condensate we may write after linearising in $\delta\psi$,

$$i\hbar \frac{\partial \delta\psi}{\partial t} = (1 + i\Lambda) \left\{ -\frac{\hbar^2}{2m} \nabla_r^2 \delta\psi + V_{\text{trap}}(\mathbf{r})\delta\psi + 2U_0 |\psi_g|^2 \delta\psi + U_0 \psi_g^2 \delta\psi^* - \mu \delta\psi \right\}. \quad (4.5)$$

Letting $V_{\text{trap}}(\mathbf{r}) = 0$, and $\delta\psi = e^{-i(\omega t + \mathbf{k} \cdot \mathbf{r})} + e^{i(\omega t + \mathbf{k} \cdot \mathbf{r})}$ for the homogeneous case one obtains, after grouping and equating terms with $e^{-i\omega t}$ and $e^{i\omega t}$, the energy of

excitation as

$$\hbar\omega = (1 + i\Lambda)\sqrt{\left(\frac{\hbar k^2}{2m}\right)^2 + NU_0\frac{\hbar^2 k^2}{m}}, \quad (4.6)$$

which readily shows dissipation of energy characterised by the parameter Λ .

4.3 Approximations to Λ

Exactly how the damping occurs physically is contained in Λ , which is a measure of the relaxation rate for the system. This value for Λ is expected to depend on a variety of factors. One would, for instance, expect it to be temperature dependent, since the thermal component present in the trap is clearly going to be one of the main sources of damping for the oscillations. In the case of absorption of sound in superfluid Helium originally considered by Pitaevskii, Λ could be expressed in terms of the coefficients of second viscosity used and defined by Khalatnikov[73].

In this section, we discuss two possible avenues to evaluate Λ . First, we briefly discuss the possible use of Transport equations, noting that the theory is extremely involved even for the homogeneous case. The second method involves Quantum Kinetic Theory (QKT) which has been developed specifically with the inhomogeneous BEC in mind, and hence contains results which may be used for our purpose.

4.3.1 Transport equations

Kirkpatrick and Dorfman[74] have put forward a transport theory for a weakly interacting, homogeneous condensed Bose gas. This has been done by first deriving a closed kinetic equation for the distribution function of quasiparticles, starting from the many-body Hamiltonian. The key step in this procedure was in casting the quantum Liouville equation in a structure similar to those encountered in classical kinetic theory. The main required steps were:

- Change of reference frame to the rest frame for the superfluid.
- Transformation of the field operators using a formalised version of the mean field approximation; local Bogoliubov transformation to quasiparticle creation and annihilation operators.

- Introduction of Wigner operators for the quasiparticles.

Following this procedure and after a lengthy algebra, a kinetic equation for the quasiparticle distribution function $f(\mathbf{R}, \mathbf{k}, t)$ is obtained:

$$\left[\frac{\partial}{\partial t} + \frac{\partial}{\partial \hbar k_\alpha} (E_k + \hbar \mathbf{k} \cdot \mathbf{v}_s) \frac{\partial}{\partial R_\alpha} - \frac{\partial}{\partial R_\alpha} (E_k + \hbar \mathbf{k} \cdot \mathbf{v}_s) \frac{\partial}{\partial \hbar k_\alpha} \right] f(\mathbf{R}, \mathbf{k}, t) = C_{12} [f(\mathbf{R}, \mathbf{k}, t)], \quad (4.7)$$

where $E_k = \sqrt{\epsilon_k^2 + 2\epsilon_k n U_0}$; $\epsilon_k = \hbar^2 k^2 / 2m$; $U_0 = 4\pi \hbar^2 a / m$, and C_{12} is an integral collision operator that describes the decay of one excitation into two excitations and vice versa. Using the well-known Chapman-Enskog procedure for the classical Boltzmann equation, one then arrives at the Landau-Khalatnikov two-fluid hydrodynamics equations[74]. Transport coefficients of the shear viscosity η , thermal conductivity κ , and four bulk viscosities ζ_i , $i = 1, 2, 3, 4$ can be calculated explicitly from these equations. In principle, one may find through such procedure an explicit expression for Λ in terms of η , κ , and ζ_i and identify the damping mechanism within the context of superfluid hydrodynamics and transport coefficients. The method of solution for the corresponding integro-differential transport equation, however, becomes extremely difficult for the inhomogeneous case of a trapped atomic BEC. To date, no completely soluble theory exists for the inhomogeneous case.

4.3.2 Quantum Kinetic Theory

The quantum Kinetic Theory (QKT) for the weakly interacting trapped BEC was developed in a series of papers by Gardiner and Zoller[75]. It is essentially a formulation of quantum stochastic methods found in Quantum Optics applied to the problem of BEC. One of the main results of QKT is the description of the formation of condensates through evaporative cooling. In this subsection we give a brief description of QKT, and using a key result we estimate the value for Λ .

Brief summary of QKT

Most of the early theories on kinetics of BEC was through the Quantum Boltzmann Equation (QBE) which is essentially a classical Boltzmann equation but

modified to take into account quantum statistics[76]. The description of formation of BEC using QBE was met with numerous problems such as its inability to describe the build up of coherence. Quantum Kinetic Theory is based on the Quantum Kinetic Master Equation (QKME), equivalent of the usual Master equation treatment in quantum optics. In various limits QKME may be reduced to QBE and Quantum Boltzmann Master Equation (QBME), which is a generalised QBE that includes fluctuations in the occupation numbers rather than just their average values as in the QME. One of the features of QKT is that it includes the mean field effect i.e. the effect of condensate on other particles. This has been incorporated by dividing the system into two “bands” – the condensate band, R_C , containing all states which are significantly changed by the presence of a condensate and a non-condensate band R_{NC} which is band of energy levels containing states which are not affected significantly by the interaction with a condensate. The derivation of QKME involves separation of the field operator in the form $\hat{\Psi} = \hat{\phi} + \hat{\psi}_{NC}$ where $\hat{\phi}$ and $\hat{\psi}_{NC}$ are *operators* for the condensate and noncondensate bands respectively. ϕ is then later decomposed in the usual mean field + quasiparticle operators. R_C is described in terms of discrete trap levels while R_{NC} is taken to be thermalised. This enables treatment of systems with large number of atoms in the condensate, which was not possible previously. As a result of the decomposition, the Hamiltonian is divided into three parts, and the equation of motion for the density operator is:

$$\dot{\rho} = (\mathcal{L}_{NC} + \mathcal{L}_C + \mathcal{L}_I)\rho \quad (4.8)$$

where $\mathcal{L}_{NC}$, $\mathcal{L}_C$, and $\mathcal{L}_I$ represent the usual Liouvillian for the noncondensate band, condensate band and the coupling respectively. By tracing over the non-condensate band, one obtains the QKME for the condensate density operator, $\rho_C = \text{Tr}_{NC}(\rho)$. Considering only terms highest in order N in the master equation one obtains a stochastic master equation for the population in the condensate band, $p(N)$:

$$\begin{aligned} \dot{p}(N) = & 2NW^+(N-1)p(N-1) - 2(N+1)W^+(N)p(N) \\ & + 2(N+1)W^-(N+1)p(N+1) - 2NW^-p(N) \end{aligned} \quad (4.9)$$

where $W^\pm(N)$ are the rate factors. W^+ denotes transition into the condensate band while W^- represents transition out of the condensate band, in a similar manner to the standard birth-death master equations[77].

Estimate of Λ

$W^+(N)$ gives the rate at which the thermal particles above the condensate band enter the condensate due to collisions. Although the description of the process of evaporative cooling was the primary goal in deriving QKME, the main assumptions in calculating $W^+(N)$ were rather general:

- The condensate does not readily act back on the thermal component to change its temperature.
- The ground state wave function is very sharply peaked compared to the spatially dependent distribution function for the cloud of noncondensate atoms.
- The non-condensate band has a Maxwell-Boltzman distribution rather than a Bose-Einstein distribution. (Low average occupation number)
- The range of condensate band energies is negligible compared to that of noncondensate band. (In fact, we consider only the condensate level)
- Scattering processes into or out of quasiparticle levels within the condensate band is ignored (This also follows from the narrowness of the condensate band.)

These assumptions are expected to be valid when one considers quasiequilibrium situations. An initial estimate for the damping coefficient Λ , then, may be made by noting that, physically, Λ represents the rate at which the noncondensate components turn into the condensate which is, in practice, the transition probability $W^+(N)$. Using the reported values from the MIT experiment[54] as an example, and the expression in Ref. [78]

$$W^+(N) = \frac{4m(akT)^2}{\pi\hbar^3} e^{2\mu/kT} \left\{ \frac{\mu_N}{kT} K_1 \left(\frac{\mu_N}{kT} \right) \right\}, \quad (4.10)$$

where $K_1(z)$ is a modified Bessel function, we obtain $\Lambda \sim W^+(N)/\omega \approx -0.03$, for $T \approx T_c/10$ and $a \approx 3.45\text{nm}$. Here, ω was taken to be the trap frequency relevant to the oscillatory motion, that is $\omega = 2\pi \times 19\text{Hz}$.

We note that an extended theory which does not make the above set of assumptions except the first two has been put forward very recently[79].

4.4 Simulations of Damping

In order to simulate the experimental results as closely as possible, the breathing mode, the second lowest excitation, has been populated by an arbitrary amount and the evolution of this population over time has been plotted. The time evolution of the condensate plus excitation was carried out using Eq. (4.4). In practice, such a state is generated by, for instance, applying time dependent perturbations to the confining potential initially and then observing the subsequent behaviour of the condensate after turning off the perturbation. Exactly how the excitations damp using this formalism can be analysed quantitatively using the method of quasiparticle projection as discussed in the previous chapter. We write a general wave function ψ using the Bogoliubov transformation of fluctuations about the condensate mean field as in Eq. (3.17) and use the orthogonality relations to extract the coefficients b_g and b_i uniquely at any point in time.

Figure 4.1(a) shows the population of mode 2 over time as well as the population in the condensate mode $|b_g|^2$ for various values of Λ . An initial population of 0.25 means $|b_2|^2 = 0.25$. The corresponding ground state population is shown in the lower part of the plot. We see that for smaller values of Λ , i.e. when the excited component does not damp out quickly over time, there is a greater interplay between the ground and the excited state populations due to nonlinear mixing.

The width of the condensate is indeed what is actually measured in the experiment, and therefore this is plotted as a function of time in Fig. 4.1(b). The general shape reported in Ref. [64] of the form $A \exp(-\Lambda t) \sin(2\pi\nu t + \phi) + B$ is clearly reflected in this figure. The solid curve gives what is expected for the MIT experiment[54] (i.e. $\Lambda \approx -0.03$). The corresponding damping time is then approximately 200 ms, which is of the same order of magnitude as the experimental damping time of 250 ms. In real experiments, excitations such as quadrupole

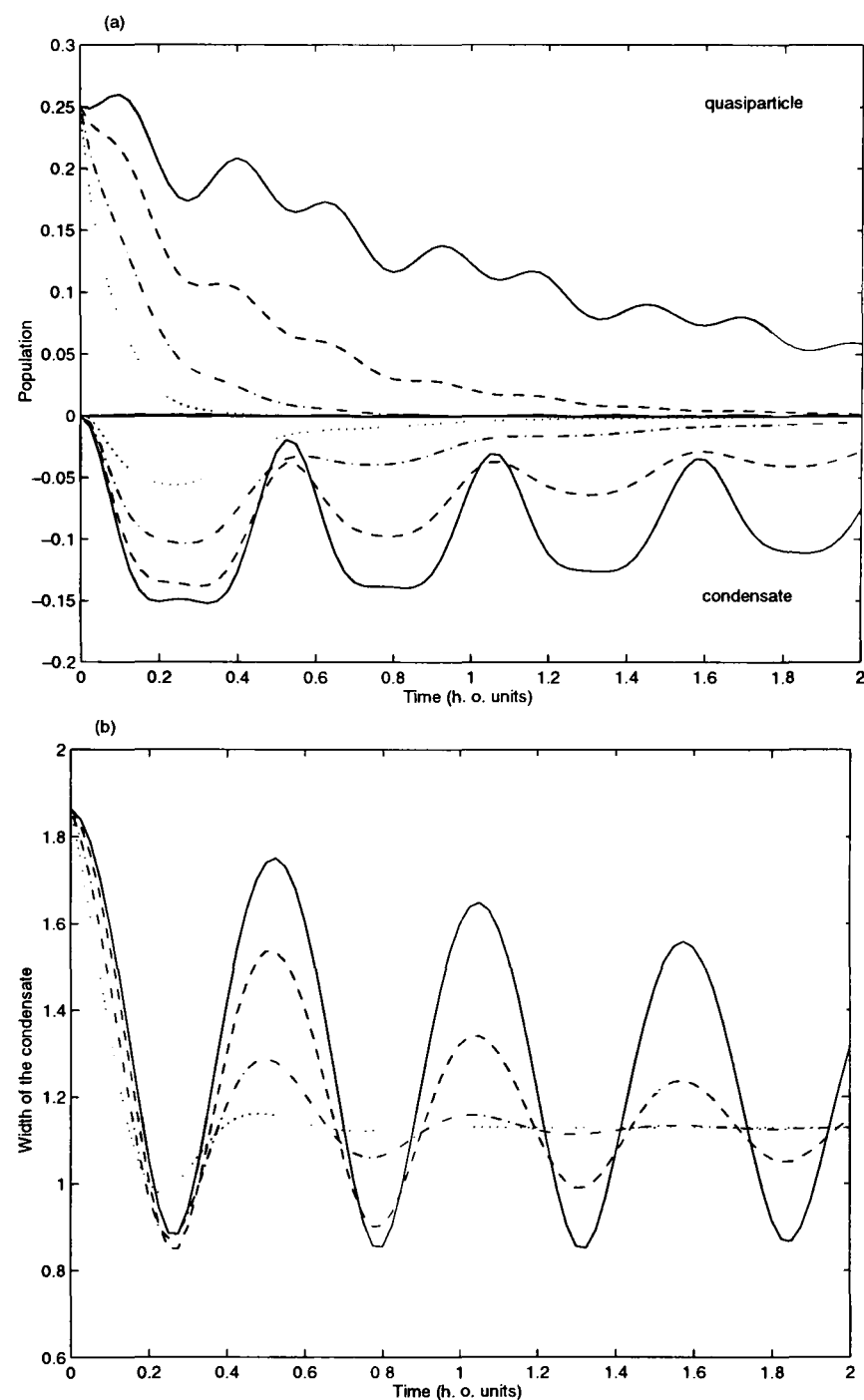


Figure 4.1: (a) Population of the breathing mode, $|b_2|^2$, over time for various values of Λ . Solid, dashed, dot-dashed, and dotted lines indicate Λ of -0.03 , -0.1 , -0.25 , and -0.5 respectively. The lower half of the plot shows the corresponding variation in $|b_g|^2$. (b) Variation of the width of the trapped condensate over time. The width is measured by the standard deviation of x , the position, weighted by the corresponding condensate density. The line shapes are as in (a).

and monopole modes are excited, and a full 3D GPE would therefore be required to justifiably compare the predictions with experiment. It is clear, however, that the description of damping should be satisfactory where an exact theoretical formalism is not needed: for instance, when Λ may be treated as a parameter to be obtained from an experiment.

One of the ways to characterise different descriptions of damping is to see its

dependence on energy. For instance, in the homogeneous gas, it is well known that the damping rate increases as k^2 when the relaxation process is due to thermal conduction and viscosity[72]. We note that the Pitaevskii prescription gives a damping rate which has a linear dependence on the mode energy, with the high energy components being damped out more rapidly. This aspect may be seen from the equation of motion Eq. (4.4), and it can also be confirmed by explicitly calculating the damping rate of the quasiparticle populations, $|b_i|^2$, for various values of i by linearisation of Eq. (4.4). Defining the damping rate as:

$$\gamma = \frac{1}{\tau_{1/2}}, \quad (4.11)$$

where $\tau_{1/2}$ is the time it takes for the population to damp down to half of its original value, i.e. $|b_i(\tau_{1/2})|^2 = 0.5|b_i(0)|^2$, we have plotted the damping rate for modes 2 to 10 in Fig. 4.2 for $\Lambda = -0.5$. On the same figure is the time-evolution of population of modes 2 to 5 as an illustration. We see here that the damping rate does indeed increase linearly. This type of dependence of damping rate on the energy of excitation can also be observed from the analytical expression for the homogeneous case, Eq. (4.6), where the damping rate is approximately proportional to k in the non-linear regime of large number of condensate particles, and proportional to k^2 in the kinetic regime of large k and smaller non-linearity. These results show that the phenomenological damping prescription does indeed model a viscous (frictional) damping in which higher energy modes are damped out faster than the low energy counterparts.

4.5 Calculation of eigenstates

In this section we discuss the second possible use of the damping equation: calculation of the eigenstate to GPE. This is an essential first step in many numerical simulations involving a trapped BEC and a reliable solution is crucial. Usual computational issues such as the CPU time it takes to “grow” a solution to GPE with high non-linearity should also be addressed. We show that the phenomenological theory of damping can be used very effectively as a numerical tool in finding numerical solutions to GPE.

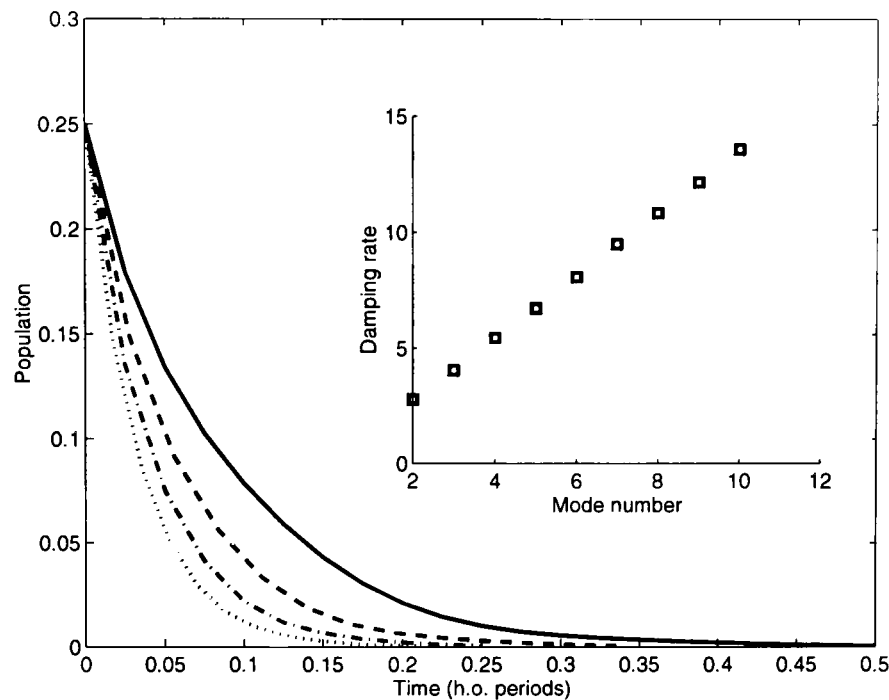


Figure 4.2: Evolution of population for different modes. Modes 2 to 5 are represented respectively by Solid, Dashed, Dash-Dot, and Dotted lines. Inset: Damping rate τ for various different modes.

Numerical procedure

From Eq. (4.4), we see that the eigenstate of the time-independent GPE is itself a solution. Using the fact that any wave function may be written as the condensate plus quasiparticles, the eigenstate to GPE can be found numerically by initially choosing an arbitrary function (preferably close to the desired solution e.g. for a condensate in a trap, a Gaussian) and running the routine with a pre-determined value of μ and Λ . However, it is to be noted that, since the equation is non-hermitian, the evolution does not conserve the norm of ψ . It is therefore necessary, in using this method, to proceed by first running the routine with an estimate of C_n for the chosen μ until convergence, and then later adjusting C_n from the renormalisation of ψ ,

$$\int |\psi(\mathbf{r})|^2 d\mathbf{r} = 1. \quad (4.12)$$

The correct C_n for the chosen μ is then given by the initial estimate divided by the final normalisation constant.

The value of Λ cannot be increased indefinitely for faster convergence, as this

results in numerical instability. It was found that we get numerical instability when $\Lambda t_{\text{step}} > 0.03$ where t_{step} is the size of the incremental time step in numerical integration. The onset of numerical instability is independent of the total length of simulation and the size of the non-linearity constant C_n . One may understand this from the fact that the damping per time step is roughly given by $e^{-\Lambda t_{\text{step}}}$ so that $e^{-0.03} \approx 0.97$ implies a reduction in the amplitude by about 3% per numerical time step. Since the typical step size used is of the order of 10^{-3} harmonic oscillator units, this, in fact, represents a complete decay on a time scale of order a period.

Features of the method

The phase profile of a stationary condensate is by definition flat. As an indication of the accuracy of the solution, the phase across the condensate for the damping simulation with $\Lambda = -2$, $C_n = 50$ running for a range of integration times of the order $t = 15/\omega$ have been evaluated. A rapid convergence to a single-valued phase across the condensate was observed within the time scale. A similar simulation with the adiabatic method showed maximum variation in phase of order 10^{-3} radians compared to 10^{-7} radians for the damping method. The time taken to grow a condensate with a large C_n is also much shorter than using conventional method. As a rough indication, an evolution time of $t = 10/\omega$ was required for growing an eigenstate with $C_n = 100$ and $\Lambda = -2$ when using the damping method while it took us $t = 500/\omega$ using the adiabatic method; in real time on a Sun SPARC station 10, these running times corresponded to roughly 10 minutes and 3 hours respectively.

We note also that the method is able to handle simulations of different experimental configurations such as the confining trap of an arbitrary shape. The vortex eigenstate in a trap may also be obtained numerically by using this damping prescription; one needs only to start with the first excited harmonic oscillator state which has an odd parity. One of the corollaries of the damping method is that although parity is conserved the number of zero crossings is not; if we started with, say, the 3rd excited harmonic oscillator state, the resulting solution is still the state with one zero crossing. The phase profile of such a condensate displays a clear π phase jump at the origin, while being flat everywhere else.

4.6 Discussion

We have presented in this chapter a modified Pitaevskii damping formalism adopted to the case of trapped atomic BEC. The formalism provides a framework for a complete theoretical description of damping as one makes more exact analytical predictions for the damping constant, Λ . The damping prescription also turned out to be a useful numerical tool in calculating time-independent eigenstates to the non-linear Schrödinger equation.

An immediate extension of the formalism is to introduce different damping rates Λ_ν for quasiparticle levels ν , where Λ_ν is a function of quasiparticle population in other levels. This would then enable a description of damping in line with the existing Landau and Beliaev damping theories. Since we have used here one Λ for all modes (this follows from our argument on describing coherent excitations), our formalism can be thought to be describing an overdamping of excitations in the long wavelength limit.

As a further investigation, a delta-correlated noise term $\mathcal{F}(x, t)$ may be added in the Pitaevskii equation such that we have

$$i\hbar \frac{\partial \psi}{\partial t} = -(1 + i\Lambda) \left\{ \frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 \psi + V_{\text{trap}}(\mathbf{r})\psi + C_n |\psi|^2 \psi - \mu \psi \right\} + \mathcal{F}(x, t), \quad (4.13)$$

with

$$\langle \mathcal{F}(x, t) \mathcal{F}(x', t') \rangle = \eta \delta(t - t') \delta(x - x'). \quad (4.14)$$

This enables, among others, modelling of the operation of cw-atom laser, with the output characterised by Λ and the noise of the lasing mode specified by the strength of the driving term $\mathcal{F}(x, t)$. In a recent work, Graham[80] has proposed a description of phase diffusion of a condensate in an analogous manner to the Schawlow-Townes model. The expression for the parameter Γ_0 which is equivalent to our Λ was found to be, from the consideration of Landau and Beliaev scattering processes and using the Fermi's golden rule,

$$\Gamma_0 = A_0 \left(\frac{ak_B T}{d_0 \hbar \bar{\omega}} \right)^2 \ll 1, \quad (4.15)$$

where $d_0 = \sqrt{\hbar/m\bar{\omega}}$ with $\bar{\omega}$ being the geometric mean of the trap frequencies, and A_0 a numerical coefficient of the order 1. This expression has a very similar

structure to $W^+(N)$ used in this chapter, indicative of the consistency of the two different approaches.

Finally, we note that a pertinent question to be addressed is how an initially zero-temperature condensate “warms up” due to the ever-present noise. The equilibrium solution of Eq. (4.13) via the fluctuation-dissipation theorem is expected to give us an indication of the amount of quasiparticles generated in an open system. The result of such an investigation will clearly have important implications in the operation of an atom laser.

Chapter 5

Evolution of BEC at finite temperatures

5.1 Introduction

Despite its validity over a very wide range of experimental situations, the main limitation of the GPE is that it is a zero temperature equation which doesn't take into account excitations. In this chapter, we discuss how to describe finite temperature BEC in equilibrium, as well as methods to simulate temporal evolution of a finite temperature BEC. Although most interesting properties of BEC are manifest because of its coherent condensate at $T = 0$, the presence of a thermal component enriches the physics of BEC.

We begin this chapter by first reviewing the self-consistent, time-independent Hartree-Fock-Bogoliubov (HFB) formulation. We also briefly discuss recent work on improving the HFB formalism. Most importantly in this chapter, we introduce a mathematically rigorous way to simulate finite temperature effects using the GPE. The appeal of “finite temperature” simulation using the “zero-temperature” GPE lies in its feasibility; it turns out that the time-dependent HFB equations are, in fact, computationally far too demanding to be practical[81], making it necessary to seek alternative methods of simulation.

Finally, we present a related method to simulate time-dependent finite temperatures using approximate solutions to the mode functions $u_j(\mathbf{r})$ and $v_j(\mathbf{r})$. The method is suitable for problems where $u_j(\mathbf{r})$ and $v_j(\mathbf{r})$ are difficult to find, and where more or less qualitative study of finite temperature effects are required.

Simulations of evaporative cooling in 2D are included as an illustration.

5.2 Finite temperature BEC

5.2.1 HFB Equations

Description of finite temperature BEC using HFB formalism is achieved by self-consistent inclusion of correlations of excited particles. The main variables introduced in the formalism are the population of the excited particles and the anomalous pairing[69]. The procedure is essentially identical to that described previously in the diagonalisation of the Hamiltonian to find quasiparticle wave function i.e. we start from the same Hamiltonian, Eq. (1.11) and use the field operator decomposed in the form of Eq. (3.6). The difference is that we include terms of up to 4th order in $\hat{\delta}$, whereas previously we have ignored terms greater than quadratic in $\hat{\delta}$. The higher order terms, namely the 3rd and 4th order terms, are then reduced to quadratic order by way of factorisation approximations:

$$\hat{\delta}^\dagger \hat{\delta} \hat{\delta} \approx 2\langle \hat{\delta}^\dagger \hat{\delta} \rangle \hat{\delta} + \langle \hat{\delta} \hat{\delta} \rangle \hat{\delta}^\dagger \quad (5.1)$$

$$\hat{\delta}^\dagger \hat{\delta}^\dagger \hat{\delta} \approx 2\langle \hat{\delta}^\dagger \hat{\delta} \rangle \hat{\delta}^\dagger + \langle \hat{\delta}^\dagger \hat{\delta}^\dagger \rangle \hat{\delta} \quad (5.2)$$

$$\hat{\delta}^\dagger \hat{\delta}^\dagger \hat{\delta} \hat{\delta} \approx 4\langle \hat{\delta}^\dagger \hat{\delta} \rangle \hat{\delta}^\dagger \hat{\delta} + \langle \hat{\delta}^\dagger \hat{\delta}^\dagger \rangle \hat{\delta} \hat{\delta} + \langle \hat{\delta} \hat{\delta} \rangle \hat{\delta}^\dagger \hat{\delta}^\dagger \quad (5.3)$$

Rearranging the resulting equation and introducing the Bogoliubov transformation, the equations to diagonalise the Hamiltonian are found to be:

$$\left\{ -\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m} + V_{\text{trap}}(\mathbf{r}) - \mu + \tilde{U}_0 \left[|\psi(\mathbf{r})|^2 + 2\tilde{n}(\mathbf{r}) + \tilde{m}(\mathbf{r}) \right] \right\} \psi(\mathbf{r}) = 0 \quad (5.4)$$

$$\hat{\mathcal{L}}_{\text{HFB}}(\mathbf{r}) u_j(\mathbf{r}) + \tilde{U}_0(\mathbf{r}) \psi^2(\mathbf{r}) v_j^*(\mathbf{r}) = \hbar \omega_j u_j(\mathbf{r}) \quad (5.5)$$

$$\hat{\mathcal{L}}_{\text{HFB}}(\mathbf{r}) v_j(\mathbf{r}) + \tilde{U}_0(\mathbf{r}) [\psi^*(\mathbf{r})]^2 u_j(\mathbf{r}) = -\hbar \omega_j v_j(\mathbf{r}) \quad (5.6)$$

where $\tilde{n}(\mathbf{r}) \equiv \langle \hat{\delta}^\dagger \hat{\delta} \rangle$ denotes the density of excited particles and $\tilde{m}(\mathbf{r}) \equiv \langle \hat{\delta} \hat{\delta} \rangle$ denotes anomalous pairing of non-condensate particles. $\psi(\mathbf{r})$ is the condensate wave function, and the hermitian operator $\hat{\mathcal{L}}_{\text{HFB}}$ is defined by

$$\hat{\mathcal{L}}_{\text{HFB}}(\mathbf{r}) = -\frac{\hbar^2 \nabla_{\mathbf{r}}^2}{2m} + V_{\text{trap}}(\mathbf{r}) - \mu + 2\tilde{U}_0 \left[|\psi(\mathbf{r})|^2 + 2\tilde{n}(\mathbf{r}) \right]. \quad (5.7)$$

These equations are then solved numerically as discussed below. We shall also note here that, so far, various modifications of the formalism have been proposed in order to improve on some of the shortcomings of the theory. The issue of gaplessness is described below; the problem of spontaneously broken symmetry and the inherent number non-conserving nature of the theory is dealt with in a modified HFB formalism discussed in Chapter 8.

5.2.2 Gapless theories

It is well-known by now that, in violation of Goldstone's theorem [82], the HFB formalism predicts a gap in the single-particle excitation spectrum of homogeneous gases[83]. We discuss here briefly the required approximations to the formalism to obtain what is known as "gapless" theories.

Popov Approximation

The HFB theory takes account of the lowest order (or pair) anomalous average of the Bose field operator, $\tilde{m}(\mathbf{r})$. The $\tilde{m}(\mathbf{r})$ which becomes crucial in the case of net attractive interactions (in which case it may lead to a competing BCS-like phase transition[84]), causes irregularities in the equations since the term doesn't appear symmetrically with respect to the terms involving U_0 . Popov has found an approximation to overcome the problem of the gap in the spectrum by setting these anomalous averages to zero everywhere[69, 85, 86]. The resulting HFB-Popov theory has been successfully employed in a variety of calculations[87, 88, 89]; for instance frequencies of elementary excitations calculated via the HFB-Popov theory have been found to be in excellent agreement with the experiments of Jin *et al.*[64] at low temperatures.

Further gapless theories

There have been several attempts at improving even the HFB-Popov theory prompted by the rather unexpected experimental disagreement in the excitation frequencies for high temperatures ($T > 0.6T_c$, where T_c is the transition temperature). The inherent limitations of the HFB-Popov theory are twofold: (i) it assumes that the condensate moves through a static thermal cloud[68, 70, 90, 91] and (ii) it does not take into account the full effects of the medium on the inter-

atomic collisions. Proposed alternative gapless theories include work by Zaremba *et al.*[92] which discusses how to go beyond the approximation of a static thermal cloud and treat the coupled dynamics of condensed and excited atoms under the assumption of local thermodynamic equilibrium for the excited states. In another proposal for alternative gapless theory, Proukakis *et al.*[93] addresses the second of the above limitations of HFB-Popov by considering the effects of the medium on the atomic collisions. This leads to the replacement of the two-body T-matrix by the many-body T-matrix. A detailed discussion of the two-body and many-body T-matrix and their respective domains of validity can be found in Ref. [70, 90, 94, 95]. The proposed theory gives an effective interaction between two atoms which is both temperature and density dependent, as opposed to the HFB-Popov approach for which it is constant; the effective interaction U_0 is modified in this theory to $\tilde{U}_0$ where

$$\tilde{U}_0 = U_0 \left[1 + \frac{\tilde{m}(\mathbf{r})}{\psi^2(\mathbf{r})} \right]. \quad (5.8)$$

This new effective interaction was shown to be consistent with the analytical expressions in the homogeneous limit [90, 95].

We note that, so far, none of the improved theories match the experiment exactly at higher temperatures, suggesting further work is needed to fully describe the condensates at high T . In this thesis, we work with the Popov approximation and limit our analysis to the lower temperature regimes.

5.2.3 Self-consistent numerical analysis

The numerical procedure for solving the HFB equations has been reported in the literature[87, 88] and can be summarised in the following steps

1. Solve Eqs. (5.4)-(5.6) in the zero temperature limit of $\tilde{n}(\mathbf{r}) = \tilde{m}(\mathbf{r}) = 0$. One thus obtains an initial value for the condensate wave function $\psi(\mathbf{r})$, as well as the quasiparticle functions $u_j(\mathbf{r})$ and $v_j^*(\mathbf{r})$.
2. Calculate $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$ by transforming to a quasiparticle basis:

$$\tilde{n}(\mathbf{r}) = \sum_j \left\{ \left[|u_j(\mathbf{r})|^2 + |v_j(\mathbf{r})|^2 \right] N_Q(E_j) + |v_j(\mathbf{r})|^2 \right\} \quad (5.9)$$

$$\tilde{m}(\mathbf{r}) = \sum_j u_j(\mathbf{r}) v_j^*(\mathbf{r}) [2N_Q E_j + 1] \quad (5.10)$$

where the quasiparticle populations $N_Q(E_j)$ are given by the Bose-Einstein distribution $N_Q(E_j) = 1/(e^{\beta E_j} - 1)$ with $\beta = 1/k_B T$.

3. Re-solve Eqs. (5.4)-(5.6) using the new values of $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$, and iterate to convergence.

For the Popov approximation, we set $\tilde{m}(\mathbf{r}) = 0$. Using MATLAB, the routine was found to converge fairly quickly in time of order of minutes.

5.3 Temporal evolution at $T > 0$

5.3.1 Motivation

The HFB theories in various approximations discussed above are theories for the thermal equilibrium cases. It is noted that a full description of BEC dynamics at finite temperatures requires a time-dependent HFB treatment, which unfortunately is computationally prohibitive. We discuss in this section how to simulate finite temperature BEC using GPE, which provides us with a way to simulate the quantum field using a classical counterpart. This involves treating the quasiparticle operators to be coherent, which is essentially the same method we used to simulate the nonlinear mixing of single mode excitation. The trajectories are then averaged in order to simulate incoherence of the thermal excitations. The argument presented here is based on a recent paper by Kagan and Svistunov[96]. The use of a classical field to represent a quantum field is in fact a relatively common approximation in a wide range of physical contexts as it is often the only approach which is expected to be accurate for practical purposes. We note that such a study involving classical evolutions has also previously been explored in Ref. [97].

5.3.2 Approximations using classical fields

For the specific case of BEC, Kagan and Svistunov give a justification for the use of the GPE even when no condensate is present and when the system is far from

equilibrium[96]. This is possible, these authors argue, *provided* that the single particle modes are highly occupied

$$n_{\mathbf{k}} \gg 1. \quad (5.11)$$

This condition may be satisfied at both low and high temperatures. At very low temperatures almost all the atoms are in the same single particle state; at high temperatures relevant excited states (single particle or quasiparticle) become highly occupied. Also, from an alternative point of view, Eq. (5.11) is clearly satisfied for any quasiparticle population *observable* by an experimenter. The high occupation number implies approximation by coherent excitations; the coefficients b_i in Eq. (3.17) are then taken to have a well defined phase in addition to a well defined amplitude. The equation of motion for the excitations, then, becomes none other than the GPE.

Justification of the method follows from the consideration of the density matrix for the system. The density operator for the condensate at finite temperatures, $W_{\mathbf{k}}$, can be written in the occupation number representation:

$$W = \prod_{\mathbf{k}} W_{\mathbf{k}}, \quad W_{\mathbf{k}} = \sum_{n_{\mathbf{k}}} Q_{\mathbf{k}}(n_{\mathbf{k}}) |n_{\mathbf{k}}\rangle \langle n_{\mathbf{k}}|. \quad (5.12)$$

where $Q_{\mathbf{k}}$ is a smooth quasicontinuous function of $n_{\mathbf{k}}$. However, it is well known that, partly as a result of how the coherent states are defined, a representation in the coherent basis such that the states span all phases and amplitudes is entirely equivalent to the occupation number state representation. In other words, another possible expression for the density operator is:

$$W = \int \mathcal{D}\alpha Q(\alpha) |\Phi(0, \alpha)\rangle \langle \Phi(0, \alpha)| \quad (5.13)$$

where

$$\mathcal{D}\alpha = \prod_{\mathbf{k}} d(\rho_{\mathbf{k}}^2) \frac{d\phi_{\mathbf{k}}}{\pi}, \quad Q(\alpha) = \prod_{\mathbf{k}} Q_{\mathbf{k}}(\rho_{\mathbf{k}}^2) \quad (5.14)$$

and $\Phi(0, \alpha)$ are the direct product of coherent states which are eigen functions of the field operator:

$$\Phi(0, \alpha) = \prod_{\mathbf{k}} |\alpha_{\mathbf{k}}\rangle \quad (5.15)$$

where $\alpha_{\mathbf{k}} = \rho_{\mathbf{k}} e^{i\phi_{\mathbf{k}}}$. It can be shown from the definition of $\Phi(0, \alpha)$ and the second

quantised Hamiltonian Eq. (1.11) that the state at time t is a coherent state such that

$$\hat{\psi}\Phi(t, \alpha) = \psi(t)\Phi(t, \alpha) \quad (5.16)$$

where the eigen value $\psi(t)$ obeys the GPE. Hence each separate coherent state of the ensemble evolves following an independent trajectory and the statistical matrix at time t is given by

$$W(t) = \int \mathcal{D}\alpha Q(\alpha) |\Phi(t, \alpha)\rangle \langle \Phi(t, \alpha)| \quad (5.17)$$

which is diagonal in a coherent state representation, with no correlation between the phases of the various coherent states in the ensemble. In order to represent the evolution of the density matrix, therefore, we can perform many classical simulations with various initial phases and then average over these phases.

An important point to note is that for almost all practical purposes, the evolution of a generic classical field with a particular choice of $\alpha \equiv \{\phi_{\mathbf{k}}, \rho_{\mathbf{k}}\}$ is *representative* of the overall evolution of the system, as the trajectories that make up the statistical ensemble are essentially similar to each other. We exploit this characteristic in our finite temperature simulations in Chapter 6.

5.4 Evaporative cooling simulation in 2D

It is possible to simulate approximately evolution of finite temperature BEC using GPE without finding explicit functions of $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$. This follows from the observation that at higher temperatures, the higher modes are closely approximated by the modes of simple harmonic oscillator, so that the initial high temperature state can be prepared using these modes. This is desirable when one wants to investigate 2 or 3D condensates where finding the quasiparticle mode functions becomes too demanding due to the enormous number of degeneracy and dimensionality spanned by the mode basis. The idea is then not to seek detailed temperature properties but to test the validity of the GPE to model such processes as evaporative cooling. The quasiparticle mode mixing studied in Chapter 3 and the evaporative cooling process are, in fact, closely related in that the mechanism for the nonlinear mixing and the rethermalisation mechanism in evaporative cooling both arise from the interaction term $C_n|\psi|^2\psi$ in the GPE.

In this section, some key results of simulations which have been published by the author jointly with Marshall *et al.* are reported as an illustration of the application of finite T simulations. Readers are referred to Ref. [98] for a more detailed account.

5.4.1 Generation of thermally excited state

In order to simulate a “hot” condensate in 2D, a self-consistent, thermally excited state was created adiabatically and added on top of the condensate. It was done by first forming an initial state, $\Psi_i(\mathbf{r}, t)$, which can be written

$$\Psi_i(\mathbf{r}, t) = \sum_{n,m}^{O,P} |a_{nm}| e^{i\alpha_{nm}} \psi_{nm}(\mathbf{r}, t) \quad (5.18)$$

where O, P are the mode-cut-off numbers, α_{nm} is the mode phase described by random variables on interval $(0, 2\pi)$, and ψ_{nm} are the two dimensional SHO mode functions. $|a_{nm}|$ is the modulus of the mode amplitude such that $|a_{nm}|^2 = 1/(e^{(n+m+1)/\beta} - 1)$. The random phases simulate the incoherence of the thermal cloud. This initial state, $\Psi_i(\mathbf{r}, t)$, was then propagated using a 2D-GPE where the interaction term is adiabatically increased from zero to its final value over the first half of the mixing time, and the mean field was allowed to equilibrate over the following half.

The results of the numerical simulation of the thermally-excited state generation is shown in Fig. 5.1 which show the density $\rho(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2$ of the thermal state. The initially square geometry of the cloud is now circular as to be expected from a thermal condensate in a cylindrical trap. Evaluation of the population in each mode after adiabatic following showed that the state does indeed approximate a thermal state with a Bose-Einstein distribution for its mode population.

5.4.2 Simulation of cooling

The process of evaporative cooling in which the most energetic atoms are removed from the trap may be modelled by the absorption in the edges of the condensate, simulating the RF-scalpel used in real experiments. To model this, we modify our trapping potential by adding a time dependent absorbing potential: $V_{\text{trap}} \longrightarrow$

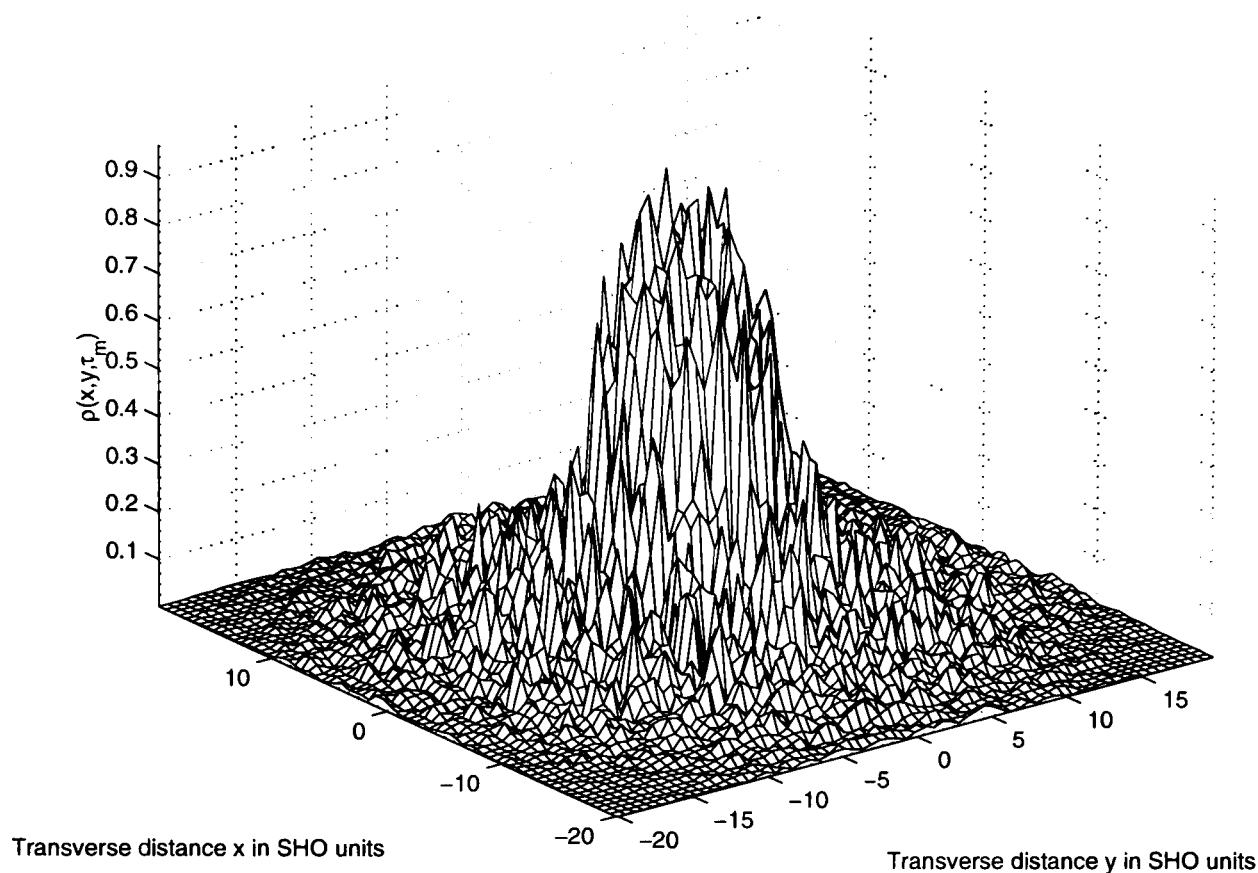


Figure 5.1: Surface plot of the mean field density of a typical thermally-excited state, Ψ_T , after mixing time $\tau_m = 80$ in h.o. units.

$V_{\text{trap}} - iA(\mathbf{r}, t)$ where $A(\mathbf{r}, t)$ is a Super-Gaussian:

$$A(\mathbf{r}, t) = A_0 \left(1 - e^{-(r/r_e(t))^{2m}} \right). \quad (5.19)$$

This choice of $A(\mathbf{r}, t)$ gives us a smooth profile of absorption to preclude the introduction of computational errors. Here $r_e(\tau)$ defines the position where the function takes non-zero values and A_0 determines the effectiveness of the cooling which is related to the intensity of the RF-field. A result of such evaporative cooling simulation is shown in Fig. 5.2.

The evidence that the thermally-excited state has cooled include the much smoother density of the condensate, which implies that the velocity, $\mathbf{v}(\zeta) = \frac{-i\hbar}{2m\rho(\zeta)}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*)$, of the initially thermally-excited state has been reduced. The shape of the resulting condensate density has a profile with a greater similarity to that of the ground state of the GP equation. Also, the phase of the thermally-excited state was found to be much more uniform, and to have large

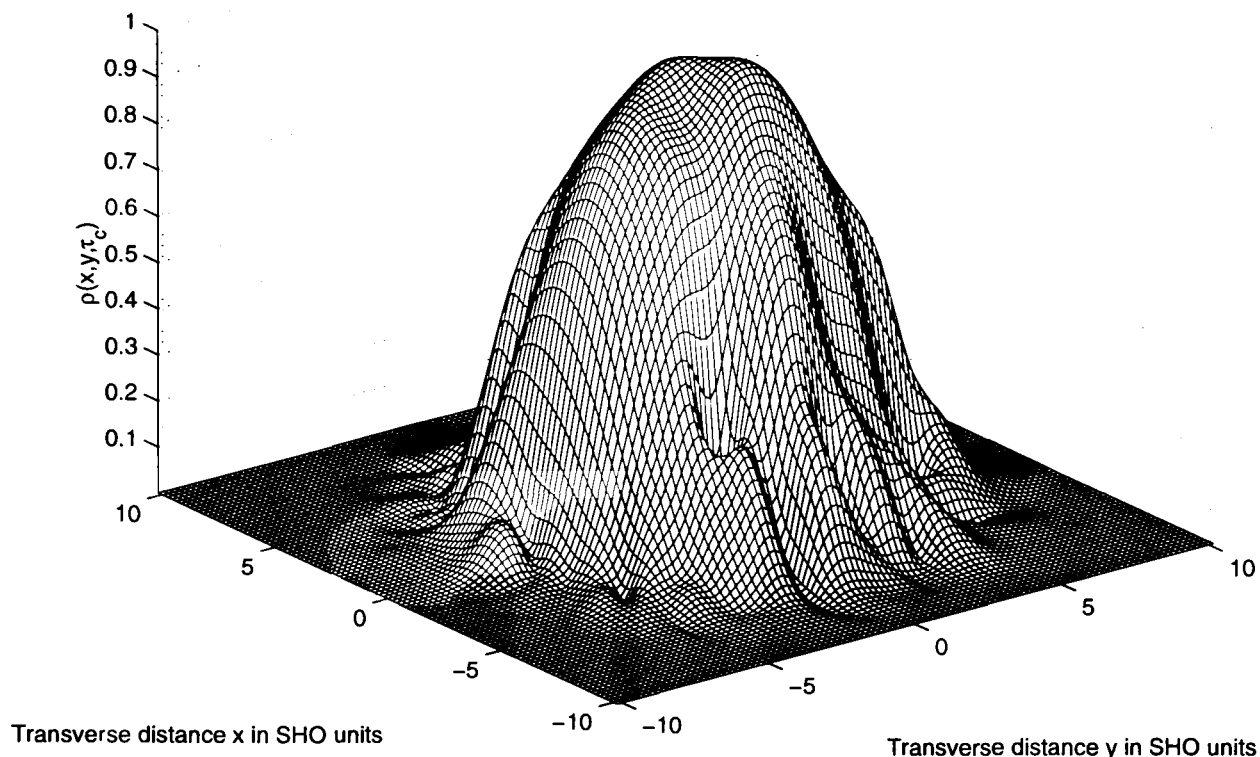


Figure 5.2: Surface plot of the mean field density of an evaporatively cooled state, Ψ_C , after a cooling time $\tau_c = 60$ in h.o. units.

coherent areas. This gives direct evidence that the thermally-excited state now predominantly consists of a ground state with only a small number of modestly populated excited states producing the phase fluctuations.

In addition to the cooling we have observed in our simulations that a vortex state could be trapped in the condensate through a rapid cooling scheme in which the initial radius of the super Gaussian is smaller than the size of the thermally excited state[98]. The resulting trapped vortex state is robust and remains with the condensate until the spatial confinement, due to the evaporative cooling, causes the state to be energetically unfavourable at which point it disappears. This method of vortex trapping may be directly applicable to two-dimensional experimental situations if the experiment is setup so that it makes “deep cuts” in the initial stages of cooling.

The possibility of creating self-consistent thermally-excited states and the numerical simulation of these states in two dimensions allows us to deal with a number of issues such as vortex interactions, coherence properties of thermally-

excited states, and accurate models of Bose-condensation experiments.

Chapter 6

Quantum carpet interferometry

6.1 Introduction

We have proposed in Chapter 2 a method to split and focus a condensate using an external potential, and also by modulating the interatomic scattering length[99]. In addition to direct focusing and beam splitting, an integral part of the field of atom optics is matter-wave interferometry[38]. In this Chapter, we propose a novel method to perform interferometry with BEC which should be immediately realisable with the current technology. It bases on the phenomenon of intermode traces, which is an aspect of quantum interference. Several theoretical studies of such phenomena for ordinary non-condensed wave packets have been carried out recently[100], showing in the spacetime probability distribution unique patterns called the “quantum carpets.”

In this Chapter, we show that these quantum carpets may also be observed with a BEC, and that the phenomenon may be utilised in measuring the temperature of the condensate. For this case, the required phase shift is induced by the density-dependent nonlinear interaction within the condensate. We note that accurate temperature measurement of ultracold atoms remains an important and pertinent experimental challenge, as indicated by a recent publication in this area[101].

6.2 Quantum carpets

6.2.1 Linear quantum carpets

The controlled preparation and measurement of wave packets is currently an active field of research. For example, wave packets in optical lattices, ion traps and molecules have been studied recently by several different authors[102]. A major aspect of interest in such systems is the spatio-temporal evolution of wave packets, or the quantum carpets. These spatio-temporal patterns in quantum mechanical probability $|\psi|^2$ are characterised by a regular net of canals and ridges (minima and maxima of probability, respectively) which run along straight lines in space time. The shapes are explained by careful consideration of solutions of appropriate Schrödinger's equation[100]. We note that similar patterns arise in the near field of a diffraction grating illuminated with light. Indeed, the space-time probability distribution $|\psi(x, t)|^2$ can be mapped directly onto field intensity $|\mathcal{E}(x, z)|^2$ where z is the direction of propagation.

A number of different linear systems¹ have been found to generate quantum carpets. For example, particle confined to an infinite potential well, evolution of an initially homogeneous wave function, and angular wave packets[103]. In this subsection, we briefly describe the example of the wave packet evolution in an infinite square well.

The equation that describes the linear quantum carpet is the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} \psi(x, t), \quad (6.1)$$

with the boundary conditions $\psi(x = \pm L) = 0$ due to the square well potential. The time evolution of the wave function of the particle $\psi(x, t)$ can be expressed in the form

$$\psi(x, t) = \sum_{n=1}^{\infty} \psi_n u_n(x) \exp\left(-2\pi i n^2 \frac{t}{T}\right) \quad (6.2)$$

where n is an integer quantum number, and

$$u_n(x) = \sqrt{\frac{1}{L}} \cos\left(\frac{n\pi}{2L} x\right) \quad (6.3)$$

¹The term “linear” is used here to describe a system of uncondensed atoms.

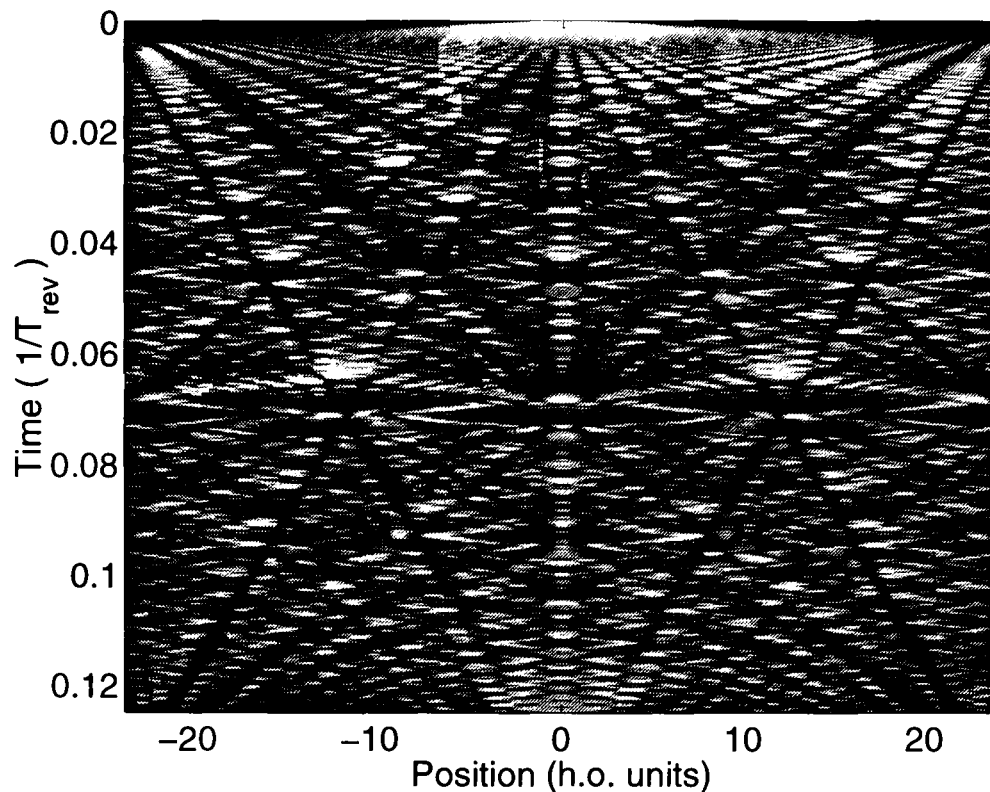


Figure 6.1: Quantum carpet generated with the Gaussian wave packet. $L = 24a_{rmHO}$ in harmonic oscillator units. The carpet is shown up to time of evolution $t = \frac{T_{rev}}{8}$, where T_{rev} is the time of revival, Eq. (6.5).

are the energy eigen functions. The expansion coefficients ψ_n are defined by

$$\psi_n = \int_{-L}^L dx \psi(x, t=0) u_n(x), \quad (6.4)$$

and

$$T \equiv \frac{16ML^2}{\pi\hbar} \quad (6.5)$$

is the revival time such that $\psi(x, t=T) = \psi(x, t=0)$. With an initial wave function $\psi(x, t=0)$ as Gaussian, we get a number of interesting features such as a perfect revival of the wave function at time T after weaving regular carpet patterns in space-time. Several quantum carpets formed under different initial conditions have so far been simulated and studied. An example of the quantum carpet generated with the Gaussian wave packet in a square well is given in Fig. 6.1.

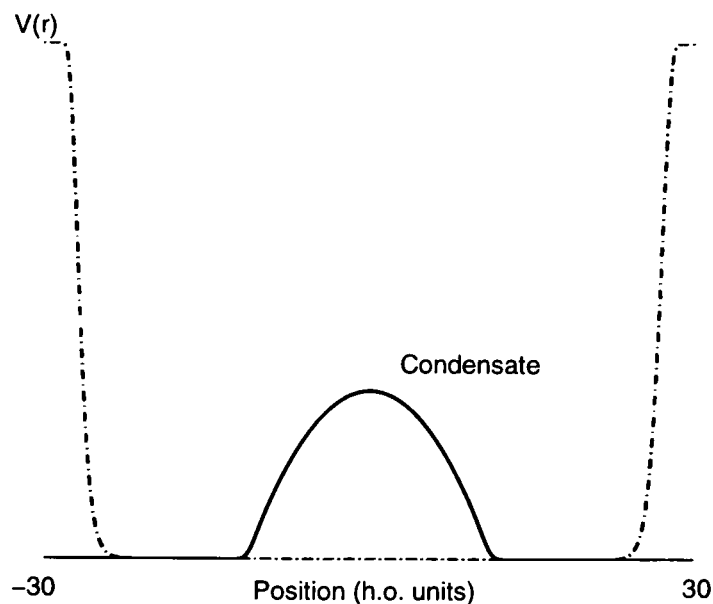


Figure 6.2: Schematic diagram of initial condition

6.2.2 Quantum carpets with BEC

Until now quantum carpets with BEC have never been investigated. The main advantage of BEC is that the quantum carpet can be formed with N atoms, as opposed to a few wave packets for uncondensed atoms. This allows, for the first time, a possibility to observe experimentally the general phenomenon of quantum carpets. In order to construct a quantum carpet for BEC, we propose to turn off the initial confining trap potential and place the BEC in a “harder” potential of the form r^ξ where $\xi \gg 2$. For simplicity, we propose to use an inverted super-Gaussian, $V_{\text{box}}(\mathbf{r})$ as our potential:

$$V_{\text{box}}(\mathbf{r}) = \frac{L^2}{2} \left[1 - \exp\left(-\frac{\mathbf{r}}{\sigma}\right)^m \right] \quad (6.6)$$

where L is defined to be half the total transverse length of the potential in harmonic oscillator units of length, and $\sigma = 0.9L$. With $m = 42$, the potential closely approximates a box of length $2L$. Experimentally, this potential is expected to be well approximated by using parallel sheets of optical fields. The potential V_{box} is equivalent in the optical context to a narrow slit, which provides a boundary condition for Maxwell’s equations. The initial configuration is shown in Fig. 6.2.

The difference between the linear quantum carpets and the carpet with BEC apart from the shape of the initial wave function is that the dynamics is described

by the GPE for the case of the condensate. As a result of introducing V_{box} , the condensate first undergoes an expansion, and then reflects at the walls acting as atomic mirrors. It then interferes with itself with varying degrees over time producing complex intensity profiles or “fringe patterns.” We note that, as to be expected, the exact shape of the carpet pattern is dependent on the potential V_{box} used. The presence of nonlinearity alters the pattern quite dramatically, and as a result, the carpet no longer repeats itself exactly.

Numerical simulation of Eq. (2.7) was carried out in 1D: we note that similar ideas may be applied to either a spherically symmetric or a cigar shaped condensate in 3D. For example, a trap with a box potential in the one direction while maintaining a tightly confining harmonic potential in the remaining two directions may be constructed. Assuming weak directional coupling in the condensate motion, this would produce a pattern due to interference in one specific direction only, effectively giving results for a 1D carpet. Alternatively, a 3D cube potential may be used to generate complex 2D interference patterns, for which a method to characterise a generalised visibility would be needed.

The pattern for $L = 30a_{\text{HO}}$, $T = 0$ and evolution time of 0 to $5\tau_{\text{HO}}$ where a_{HO} is one harmonic oscillator length and τ_{HO} is one harmonic oscillator period is shown in Fig. 6.3. This represents total integration time of approximately 30 ms for a trap with frequency $\omega = 2\pi \times 150\text{Hz}$. We note that with a nondestructive imaging technique, the shortest probe pulse duration of order 1 ms has been used[104]; this gives sufficient temporal resolution to observe the carpet structure in real experiments, in particular with a set of repeated measurements made at various different reference times. For this result, we used nonlinearity C_n of 500 which, in 1D, corresponds to approximately 10000 Rubidium atoms in the trap of frequency $\omega = 2\pi \times 150\text{ Hz}$. These numbers are typical for experiments carried out around the world based on Rubidium.

From the figure, we see canals at various angles weaving a quantum carpet, which is distinct from the reported carpets for the uncondensed atoms and other wave packets. The most important difference is that even for much longer integration times the fractional revivals of the wave function does not appear. Due to the interaction, the wave packet spreads much more rapidly; this can be related to the time dependent excitation of higher momenta due to particle collisions. We note that the sizes and the resolution of the observed patterns depend strongly on

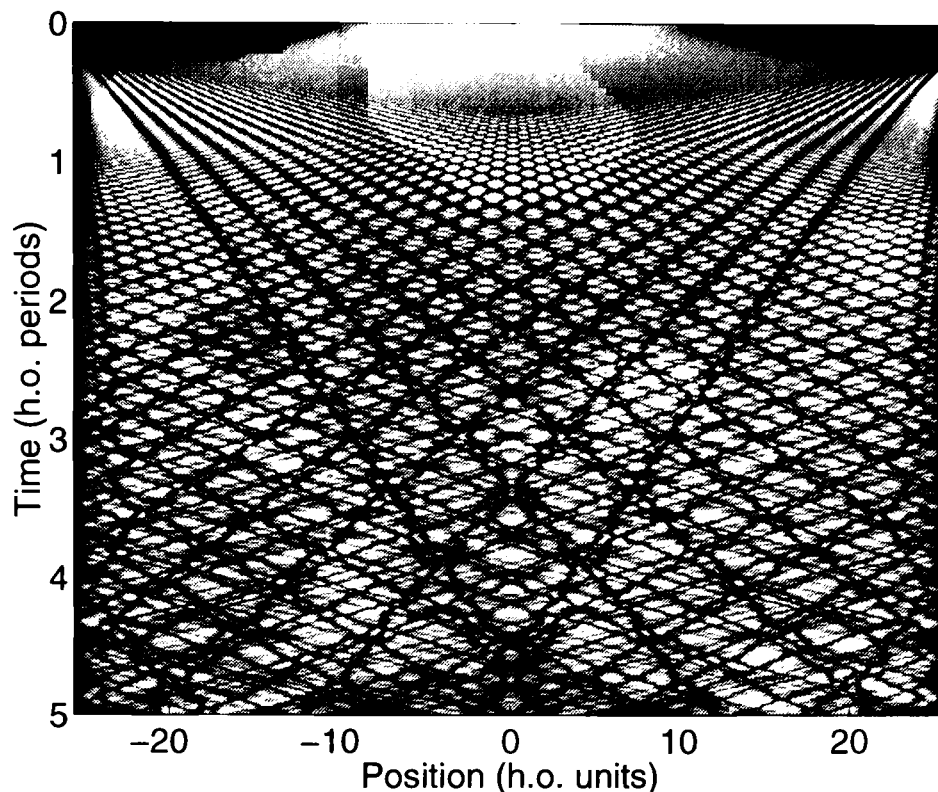


Figure 6.3: Quantum carpet for $T = 0$ condensate. $C_n = 500$, and $L = 30a_{rmHO}$ in harmonic oscillator units.

factors such as the nonlinearity C_n and the length $2L$ of the box. In particular, the pattern becomes more distinct and the canals become ridges and vice versa with fewer number of atoms or smaller nonlinearity.

6.3 Analysis of a carpet

There are a number of ways which can be used to analyse the pattern of a quantum carpet. In this section we present attempts to understand the structure of the quantum carpets by analysing the time-dependent wave function, ψ . We present here two possible ways: a more “intuitive”, simple accumulation of probabilities and the use of Wigner representation which renders a more physical interpretation of the state in phase space[100]. We note that, compared to the linear counterpart, the interatomic interactions complicate the analysis considerably, limiting our scope of investigations to those of numerical solutions.

6.3.1 Accumulation of probabilities

Accumulation of probabilities is perhaps the simplest way to analyse a quantum carpet. We first expand the wave function in a basis set; practically any kind of basis may be used, although for simplicity we choose to expand $\psi(x, t)$ in the eigen solutions of free particle in the box.

$$\psi(x, t) = -\frac{i}{2\sqrt{L}} \sum_{n=-\infty}^{\infty} \Psi_n(t) \exp \left\{ 2\pi i \left[n \frac{x}{4L} - n^2 \frac{t}{T} \right] \right\} \quad (6.7)$$

where $T \equiv 16ML^2/\pi\hbar$ as before. The expansion coefficients, Ψ_n , for the negative values of n is defined by $\Psi_{|n|} = -\Psi_{-|n|}$ and for $n = 0$ by $\Psi_0 = 0$. Writing $\Psi_n(t) \equiv A_n(t)e^{i\alpha_n(t)}$, where $A_n(t) = |\Psi_n(t)|$, the resulting probability distribution is:

$$P(x, t) = \frac{1}{4L} \sum_{m, n=-\infty}^{\infty} A_n(t) A_m(t) e^{-i(\alpha_m(t) - \alpha_n(t))} \times \exp \left\{ 2\pi i \left[(n - m) \frac{x}{4L} - (n^2 - m^2) \frac{t}{T} \right] \right\}. \quad (6.8)$$

By substituting $n - m \equiv 2k$, $n + m \equiv 2l$ that is $n \equiv l + k$, $m \equiv l - k$ for the even sums $n + m$ and differences $n - m$, and $n - m \equiv 2k + 1$, $n + m \equiv 2l + 1$ that is $n \equiv l + k + 1$, $m \equiv l - k$ for the odd sums and differences, the probability simplifies to

$$P(x, t) = \frac{1}{2L} \sum_{l=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} G_{k,l}^{\text{even}}(t) e^{i\beta_{k,l}^{\text{even}}(x,t)} + G_{k,l}^{\text{odd}}(t) e^{i\beta_{k,l}^{\text{odd}}(x,t)}, \quad (6.9)$$

where we have defined the weight factors

$$G_{k,l}^{\text{even}}(t) \equiv A_{l+k}(t) A_{l-k}(t), \quad (6.10)$$

$$G_{k,l}^{\text{odd}}(t) \equiv A_{l+k+1}(t) A_{l-k}(t), \quad (6.11)$$

and the phases

$$\begin{aligned} \beta_{k,l}^{\text{even}}(x, t) &\equiv \alpha_{l+k}(t) - \alpha_{l-k}(t) + 2\pi k \frac{x}{2L} - 8\pi kl \frac{t}{T}, \\ \beta_{k,l}^{\text{odd}}(x, t) &\equiv \alpha_{l+k+1}(t) - \alpha_{l-k}(t) + 2\pi \left(k + \frac{1}{2}\right) \frac{x}{2L} \end{aligned} \quad (6.12)$$

$$- 8\pi(k + \frac{1}{2})(l + \frac{1}{2})\frac{t}{T}. \quad (6.13)$$

The spatio-temporal lines in space with constant phase is then given by $\beta_{k,l}^{\text{even/odd}}(x, t) = \beta_0$. Along these lines the probability contribution

$$P_{k,l}^{\text{even/odd}} \equiv \frac{1}{2L} G_{k,l}^{\text{even/odd}}(t) e^{i\beta_{k,l}^{\text{even/odd}}(x,t)} \quad (6.14)$$

does not change and structures emerge. For the linear case, G is time-independent and can be given by an analytical expression; only numerical results are possible for the nonlinear case. From the knowledge of the factor $G_{k,l}^{\text{even/odd}}(t)$ and lines of constant phase, the spatio-temporal carpet structures may be explained completely.

6.3.2 Wigner distribution

For the nonlinear case, we found that the essence of the pattern formation can be demonstrated most effectively using the Wigner representation. The probability density of the condensate at a given spatio-temporal coordinate, $P(x, t)$, can be recast in the form of the Wigner distribution $\Phi^{(W)}(x, p)$ [100]:

$$P(x, t) = \frac{\pi\hbar}{2L} \sum_{m,n=-\infty}^{\infty} (-1)^{mn} \Phi^{(W)}[\chi_{m,n}(x, t), p_m] \quad (6.15)$$

where $p_m \equiv m\pi\hbar/(2L)$ and

$$\chi_{m,n}(x, t) \equiv \frac{x}{L} - m\frac{t}{T_{\text{lin}}/2} - n. \quad (6.16)$$

We have introduced the revival time for the linear case, $T_{\text{lin}} \equiv 16ML^2/\pi\hbar$. The Wigner function is defined as:

$$\Phi^{(W)}(x, p, t) \equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy \phi\left(x + \frac{y}{2}, t\right) \phi^*\left(x - \frac{y}{2}, t\right) \exp(-ipy/\hbar), \quad (6.17)$$

where $\phi(x, t) \equiv \psi(x, t) - \psi(-x, t)$, that is a superposition of the wave function minus its mirror image at each time t , which gives us a way to incorporate the effect of the reflecting walls on the wave packet. The x distribution of the Wigner function for a given momentum p_m yields information about which structure to see

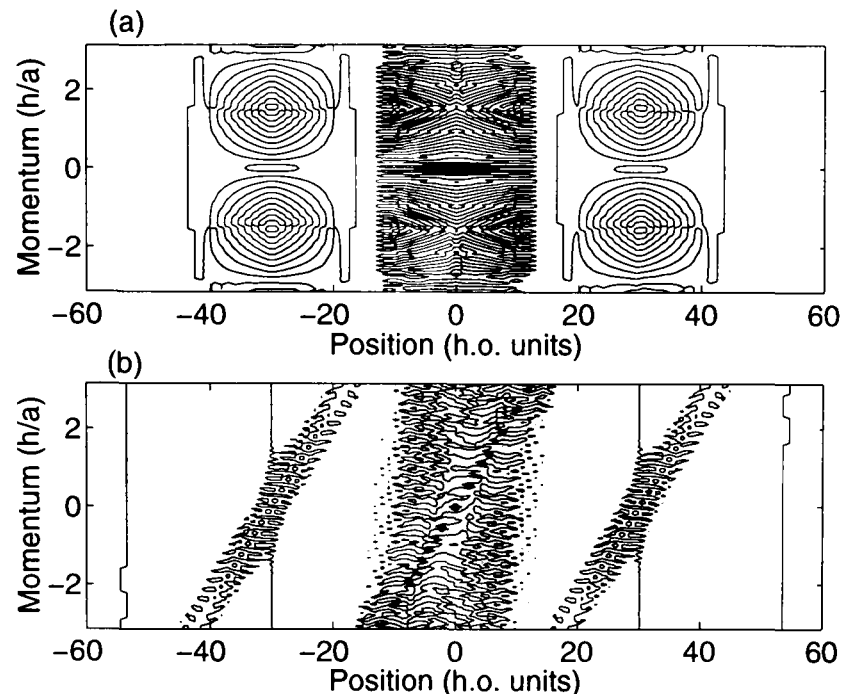


Figure 6.4: The Wigner function $\Phi^{(W)}(x, p)$ for the carpet in Fig. 1 at times (a) 0 and (b) $\frac{\tau_{HO}}{4}$, where τ_{HO} denotes the harmonic oscillator period.

in a certain direction of the carpet. For instance, the fringes near $x = 0$ indicate the observed canal structures on the carpet as an interference effect. Likewise, for a given value of x the corresponding value of p shows the direction of the moving patterns. We find that with BEC, the distributions of the single momentum component of the initial Wigner function do not follow classical trajectories; they evolve in a more complicated manner due to interactions (Figure 6.4). The shape of the BEC carpet structures is then explained by the very complex interplay of the momentum redistribution from the external boundary condition and the effect of the internal interatomic interactions. Through the Wigner plot we are able to see clearly the dynamics of how the carpet is formed.

With the absence of analytical solutions, one may state that the Wigner plots are just another convenient way to plot a quantum carpet, the dynamics of which are contained all within the GPE. It is more meaningful, therefore, to look for possible applications of the quantum carpets. In the next section we address this issue.

6.4 Quantum carpet as a thermometer

Of particular interest is the presence of any parametric dependence for the carpet structures. We propose a temperature measurement scheme as an application of the phenomenon of quantum carpets. As an introduction to the general idea behind such a measurement scheme, we briefly introduce the main concepts used in a recent interferometric experiment[101]. We then discuss how the quantum carpet thermometry has been carried out via the finite temperature BEC simulation using GPE.

6.4.1 Interthermometry

It has been established only very recently that a technique of interferometry may be used to infer the temperature of the ultracold atoms. An interferometer is traditionally used to determine external effects such as gravity by observing its effect on the phase shift. Another quantity one can measure is the change in coherence or what is called the coherence length. In the context of interferometry, the change in coherence is given by the changes in fringe visibility V defined in Eq. (2.14):

$$V = \frac{P_{\max} - P_{\min}}{P_{\max} + P_{\min}}. \quad (6.18)$$

In the context of conventional interferometry, one writes:

$$P \propto \sum_{i=1}^N \int_{-\infty}^{+\infty} |\psi_i(x)|^2 dx \quad (6.19)$$

where N denotes the total number of atoms and $\psi_i(x)$ is a superposition state of the two arms of the interferometer for the i th atom. i.e. $\psi_i(x) = f_i(x) + g_i(x - a)$ where $f_i(x)$ and $g_i(x - a)$ are separated by distance a . The quantity P therefore represents an incoherent mixture of N superposition states. Substituting Eq. (6.19) into the definition of visibility, one gets

$$V(a) \propto \sum_{i=1}^N \int_{-\infty}^{+\infty} \text{Re}[f_i^*(x)g_i(x - a)]dx, \quad (6.20)$$

which implies that by simply taking the Fourier Transform of the visibility as a function of separation, we obtain:

$$\int_{-\infty}^{+\infty} V(a) e^{-ika} da \propto \sum_{i=1}^N \text{Re}[F_i^*(k) G_i(k)], \quad (6.21)$$

where $F_i(k)$ and $G_i(k)$ represent the momentum distribution of the i th wave packet, where we used the convention in which the capitals are used to denote Fourier transforms of corresponding functions. Convolution theorem of Fourier transforms was used. Assuming $F_i(k)$ and $G_i(k)$ are proportional, the Fourier transform represents the momentum distribution of the atomic ensemble from which the temperature may be determined. Experimentally, therefore, the coherence length as a function of separation between the two arms of interferometer, a , gives us the temperature for the ultra-cold atoms.

6.4.2 Quantum carpet thermometry

In view of the fact that there exist finite amount of quasiparticle excitations at $T > 0$ which will alter the interference fringes in some way, we propose to use quantum carpets as a new and useful way to measure the temperature of the ultracold atoms. We present in this subsection finite temperature simulation of quantum carpets using a set of coherent excited state populations evolved under the GPE, which gives a representation of typical measurement result from actual experiments. We then define quantities to characterise the temperature from the carpets.

In order to simulate “*Interthermometry*” with quantum carpets, it is necessary to evolve finite temperature BEC in time. We approach this problem in the manner we have discussed in the previous chapter. That is, by way of a set of coherent evolutions which represent typical classical trajectories. We start by writing our coherent excitation to be consistent with the Bogoliubov transformation, as done in Chapter 4:

$$\psi(\mathbf{r}) = e^{-i\mu t} \left[\psi_g(\mathbf{r}) + \sum_i \{u_i(\mathbf{r}) b_i + v_i^*(\mathbf{r}) b_i^*\} \right], \quad (6.22)$$

where μ is the chemical potential and the index i denotes quasiparticle energy levels. However, noting that “standard” Hartree-Fock-Bogoliubov treatment re-

quires

$$\langle b_i^\dagger b_i \rangle = \frac{1}{e^{E_i/kT} - 1} \quad (6.23)$$

i.e. an equilibrium Bose-Einstein population of level i with energy E_i , we construct the wave functions corresponding to various different temperatures by taking coefficients

$$b_i = \sqrt{n_i} e^{i\phi} = \sqrt{\frac{1}{e^{E_i/kT} - 1}} e^{i\phi}, \quad (6.24)$$

as an ansatz to define the initial condition for our finite temperature carpet. For convenience, we take $\phi = 0$. The incoherence of the quasiparticles may be incorporated by averaging over various phases ϕ . Since the operator nature of b_i is not taken into account we note that, strictly speaking, the temperature T may be thought of as a unit quantifying the amount of quasiparticles rather than temperature in the exact sense of equilibrium HFB. A quantum carpet for temperature $T = 40\hbar\omega/k$ is shown in Fig. 6.5(a). At higher temperatures, distinct canals across the carpet become visible, indicative of the additional momentum components the hotter condensate possesses. Similar features were observed with linear carpets with an initial solution having non-zero initial momentum, or with a small spatial width.

As a method to quantify the temperature, we propose a measure of symmetry η defined as:

$$\eta = \int_0^{T_{\text{total}}} \int_{-L}^L |I(\mathbf{r}, t) - I(-\mathbf{r}, t)| d\mathbf{r} dt, \quad (6.25)$$

where $I(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2$ is the measured intensity distribution at point $\mathbf{r}$ and time t and $I(-\mathbf{r}, t)$ is its mirror image about the centre line in space. T_{total} denotes the total time of evolution. This measure is experimentally accessible, as it only involves integration of measured intensities over time. The variation of η as a function of temperature demonstrates $\eta \sim \sqrt{T}$ shown in Fig. 6.5(b) for lower temperatures. In order to simulate incoherent excitations, we tried averaging over simulations with random initial phase across the coefficients b_i . The somewhat rougher curves of the individual runs then clearly tended towards the result shown in Fig. 6.5(b), as to be expected. Another important and perhaps more physically intuitive quantity is an equal time correlation function

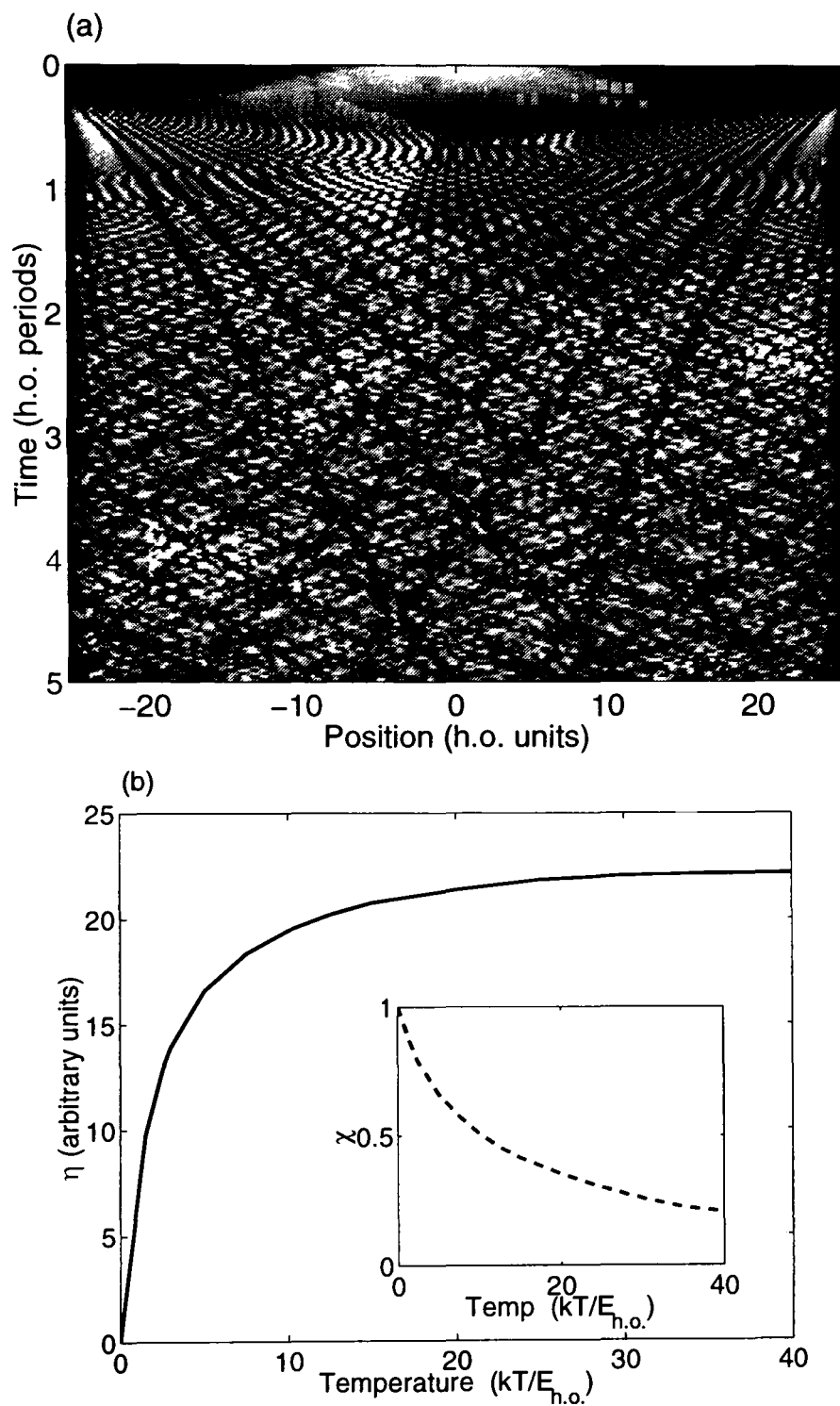


Figure 6.5: (a) Quantum carpet for $T = 40\hbar\omega/k$ condensates, using the same parameters in harmonic oscillator units as for Fig. 6.3. (b) The symmetry parameter η as a function of temperature in units of $\hbar\omega/k$. Inset: Correlation function χ as a function of temperature.

χ , which we define as

$$\chi = \frac{1}{\mathcal{N}} \int_0^{T_{\text{total}}} \int_0^L \psi^*(\mathbf{r}, t) \psi(-\mathbf{r}, t) d\mathbf{r} dt, \quad (6.26)$$

where $\mathcal{N} = \int_0^{T_{\text{total}}} \int_0^L |\psi^*(\mathbf{r}, t) \psi(-\mathbf{r}, t)| d\mathbf{r} dt$ is a normalisation constant. The

parameter χ gives a measure of coherence between the two halves of the wave packet, in a similar way to quantifying the coherence of the two arms of a Mach-Zehnder interferometer. With increasing temperature we see that the internal coherence is dramatically reduced as shown in the inset of Fig. 6.5(b).

6.5 Discussion

We have observed in this chapter the presence of quantum carpets with BEC which could be explained using similar reasoning as linear quantum carpets, except that the nonlinearity in the GPE only allows numerical analysis. The wave nature of matter exploited in a quantum carpet has enabled us to investigate its potential application as a novel near-field interferometer, in particular, its ability to gauge accurately the temperature of ultracold atoms in BEC.

One of the major limitations of the interferometric method to measure temperature or other phase-shifting quantities is the possible presence of intrinsic phase diffusion which may eventually destroy the interference patterns. This is particularly true for BEC which has atoms constantly interacting through collisions, naturally diffusing the phase. In real experimental situations, however, the phase diffusion rate is expected not to differ too greatly from that of the MIT interference experiment using sodium BEC[36], which reported a decoherence time of the order of 100 ms. Assuming that the three-body recombination rate is more or less of the same order for different atomic species, the diffusion time scale is clearly much longer than the integration times we have presented here.

The idea of temperature measurement may be applied not only in the interferometric context as done in this chapter but also in other experiments such as the Bragg scattering experiment performed recently[105]. In this case, broadening of the momentum distribution as a function of temperature is expected. Other important aspects such as two component carpets, dependence of the patterns on the potential, and the degree of revivals at longer times of evolution are expected to provide further insight into the phenomenon of quantum carpets.

Measurement of external forces due to gravity or other sources may also be made using the near-field diffraction interferometry; this involves addition of a specific form of position dependent phase shift $e^{i\Delta(\mathbf{r})}$ on the condensate wave function $\psi(\mathbf{r}, t)$. It is expected that measurements similar to the one in Ref. [106]

will be possible using the BEC quantum carpets with carefully chosen parameters and boundary conditions.

Chapter 7

Coherence and Atom Laser

In this chapter we give a brief review of the closely related concepts of coherence and atom laser. These are perhaps the most important aspects in the study of BEC, and are therefore included here as a separate chapter. This chapter acts as the bridge to the next chapter on the study of the Raman output coupler.

We begin by first reviewing briefly the concept of coherence, which was originally developed in optics, and later generalised to matter waves. We then discuss the ideal criteria for atom laser as proposed by Wiseman[107], concluding this chapter with a survey of current generation of output couplers which are realisations of the atom laser in a more broad sense.

7.1 Coherence

7.1.1 Definition of coherence

The concept of coherence of the n -th order in a quantum system was originally developed in optics to quantify the correlations of the electromagnetic field[108]. The idea of coherence in optics was first associated with the possibility of producing interference fringes when two fields are superposed. The highest degree of optical coherence was associated with a field which exhibits fringes with maximum visibility.

The first and second order correlations, and indeed n -th order correlations have been defined in the context of optics, and are important parameters which characterise the coherence of light. In general, the n -th order correlation in optics

is defined as

$$G^{(n)}(x_1, \dots, x_n, x_{n+1}, \dots, x_{2n}) = \text{Tr}\{\rho E^{(-)}(x_1) \dots E^{(-)}(x_n) \times E^{(-)}(x_{n+1}) \dots E^{(+)}(x_{2n})\} \quad (7.1)$$

where ρ is the state of the field and $x_i = (\mathbf{r}_i, t_i)$. By considering a Young's double slit experiment it is quite easily seen that the intensity variation on the screen is given by

$$I = G^{(1)}(x_1, x_1) + G^{(1)}(x_2, x_2) + 2\text{Re}\{G^{(1)}(x_1, x_2)\} \quad (7.2)$$

so that $G^{(1)}(x_1, x_2)$ gives the fringe visibility. The first order correlation function is sufficient to account for classical interference experiments, while one needs higher order correlation functions when describing experiments involving intensity correlations such as Hanbury-Brown and Twiss experiment. Using the Schwarz inequality for the correlations which may be generalised to n -th order, normalised first order coherence function is defined to be

$$g^{(1)}(x_1, x_2) = \frac{G^{(1)}(x_1, x_2)}{\sqrt{G^{(1)}(x_1, x_1)G^{(1)}(x_2, x_2)}}, \quad (7.3)$$

where $g^{(1)} = 1$ implies full coherence and $g^{(1)} = 0$ implies total incoherence. The definitions of optics are directly applicable to matter waves when one replaces the electric field operator $E^{(+)}(\mathbf{r}, t)$ with those of the quantum field operator, $\hat{\Psi}(\mathbf{r}, t)$. The definition of first order coherence is then straight forwardly given by

$$g^{(1)}(\mathbf{r}_1, t_1; \mathbf{r}_1, t_1) = \frac{\langle \hat{\Psi}^\dagger(\mathbf{r}_1, t_1) \hat{\Psi}(\mathbf{r}_2, t_2) \rangle}{\sqrt{\langle \hat{\Psi}^\dagger(\mathbf{r}_1, t_1) \hat{\Psi}(\mathbf{r}_1, t_1) \rangle \langle \hat{\Psi}^\dagger(\mathbf{r}_2, t_2) \hat{\Psi}(\mathbf{r}_2, t_2) \rangle}}. \quad (7.4)$$

On the other hand, the intensity correlations or the second order coherence gives indications of counting statistics that distinguishes quantum from classical behaviour. Different sources of light give different photon counting statistics. The counting statistics can be broadly categorised as being Poissonian (i.e. the variance in the number distribution, $V(n)$, equals the mean number of detection, $\bar{n}$), super-Poissonian ($V(n) > \bar{n}$), or sub-Poissonian ($V(n) < \bar{n}$). The relationship between the photon counting statistics and the intensity correlation in optics can be seen by writing $g^{(2)}$ as an equal-time and equal position correlation[109]:

$g^{(2)}(0) = \frac{\langle a^\dagger a^\dagger a a \rangle}{\langle a^\dagger a \rangle \langle a^\dagger a \rangle} = 1 + \frac{V(n) - \bar{n}}{\bar{n}^2}$. A super-Poissonian counting statistics such as those from a thermal source implies $V(n) = \bar{n}^2$ and $g^{(2)} = 2$ for large average photon number $\bar{n} \gg 1$ while a coherent state with a Poissonian counting statistics, $V(n) = \bar{n}$ gives $g^{(2)} = 1$.

As for the matter wave field, we first decompose the field operator into its mean field and fluctuation, $\hat{\Psi}(\mathbf{r}) = \psi(\mathbf{r}) + \hat{\delta}$ and substitute into the definition. One then obtains for the equal time, equal position intensity correlation:

$$g^{(2)}(\mathbf{r}, t) = \frac{\langle \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \rangle}{\langle \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \rangle \langle \hat{\Psi}^\dagger(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}, t) \rangle} \quad (7.5)$$

$$= 1 + \frac{1}{n^2(\mathbf{r})} \left\{ 2\text{Re} \left[|\psi(\mathbf{r})|^2 \tilde{n}(\mathbf{r}) + (\psi^*(\mathbf{r}))^2 \tilde{m}(\mathbf{r}) \right] + |\tilde{n}(\mathbf{r})|^2 + |\tilde{m}(\mathbf{r})|^2 \right\}, \quad (7.6)$$

where $\langle \hat{\delta} \rangle = \langle \hat{\delta}^\dagger \hat{\delta} \hat{\delta} \rangle = 0$. $\tilde{n} = \langle \hat{\delta}^\dagger \hat{\delta} \rangle$ and $\tilde{m} = \langle \hat{\delta} \hat{\delta} \rangle$ as in the HFB formalism and $n(\mathbf{r}) = |\psi(\mathbf{r})|^2 + \tilde{n}(\mathbf{r})$ is the total density of the particles. Detailed derivation of Eq. (7.6) involving the application of Wick's theorem on the average of product of four operators is provided in Appendix B.

7.1.2 Effects of coherence

The presence of coherent macroscopic population is what distinguishes BEC from any other quantum system. Some of the main issues related to the existence of the macroscopic coherence are interference, the Josephson effect, and decoherence.

Interference phenomena

An obvious consequence of phase coherence is the interference phenomena. This, however, was not obvious *a priori* for the trapped atomic BEC, since the system is finite-sized and interacting; the phase coherence was expected to be only approximate. In a well-known experiment carried out at MIT[36] a laser beam was used to cut a cigar-shaped atomic condensate cloud into two spatially separated parts. After switching off the confining potential and the laser, the two independent atomic clouds expanded to overlap, yielding clear interference patterns in the overlapping region. Various authors have carried out theoretical investigations of the interference phenomena based on Gross-Pitaevskii theory which assumes

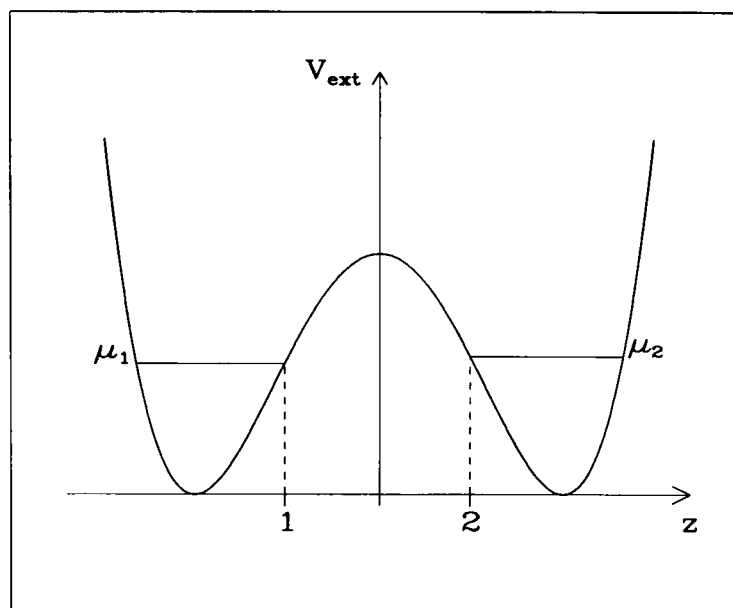


Figure 7.1: Schematic geometry of a double-well trapping potential, V_{ext} , for the Josephson effect.

from the very beginning the phase coherence of the condensate[110]; excellent agreement between the theory and experiment have been found in these works.

Josephson effect

Interesting manifestation of phase coherence is the possible occurrence of Josephson-type effects, in analogy with the well known properties of Josephson junctions in superconductors and superfluids. The physical set up consists of a double-well trap, with a barrier between the two condensates (Fig. 7.1). If the chemical potential in the two traps is different, a flux of atoms is generated. Different chemical potentials can be achieved by filling each well with a different number of atoms. If one assumes the barrier between the two wells to be high enough, then the time-independent GPE has two natural solutions, $\phi_1(\mathbf{r})$ and $\phi_2(\mathbf{r})$, localised in each potential well, and the overlap between the condensates occurs only in the classically forbidden region, where the nonlinear effects due to interactions can be ignored. The geometry of the trapped gases allows one to realise novel Josephson-type effects in BEC[111, 112].

Decoherence

An important open problem is the possible decoherence mechanisms in BEC, which could affect, or even destroy, the phase coherence in the interference and

Josephson-like experiments through phase diffusion processes. The fluctuations of the phase can have either a thermal or a quantum origin. Even at $T = 0$ the phase of the condensate must diffuse since having a fixed phase is inconsistent with atom number conservation. Many authors have investigated the problem of the quantum phase diffusion by describing the system as a coherent superposition of states with different number of atoms. This yields fluctuations in the chemical potential which defines the phase of the order parameter. Extensive discussions about the general problem of phase coherence can be found in Refs. [113].

7.2 Atom laser

It has been generally accepted right from the start that a logical step in BEC research is the construction of an atom laser as a source of coherent matter waves. We discuss in this section the criteria and models for an ideal atom laser by analogy with an optical laser[107] and then give a short review of the current experimental realisations of atom lasers, namely those that are based on output couplers for the trapped BEC. The definitions are simply a convenient working model; there is at present no universal agreement as to what an atom laser should be.

7.2.1 Definition of an ideal atom laser

An atom laser is a device used to produce an atomic field analogous to the electromagnetic field of a photon laser. For this analogy to be meaningful it is necessary to have a precise definition of a laser which applies equally to photon or atom lasers.

The fundamental principle underlying the definition is that a laser is a device which produces an output field which is well-approximated by a classical wave of fixed intensity and phase. Thus, the laser itself is treated as a black box; we are only interested in its output. The inputs are arbitrary except that they cannot themselves be laser fields of the same substrate (atoms or photons for an atom or photon laser respectively).

This fundamental principle can be quantified by requiring that the output of a laser satisfy four conditions. The first two conditions are elementary conditions that can be understood using single-boson concepts:

- (1) The output is highly directional, and ideally has a single transverse mode.
- (2) The longitudinal spatial frequency of the output beam has a small spread in the sense that $\delta k \ll \bar{k}$.

The second two conditions require many-boson concepts and are most easily stated using quantum field theory. Under the first two conditions the output field of a laser may be described by a field operator $b(t)$ satisfying $[b(t), b^\dagger(t')] = \delta(t-t')$.

The intensity operator

$I(t) = b^\dagger(t)b(t)$ measures the output boson flux in units of bosons per second.

Using these quantities the final two conditions can be stated as

- (3) The output intensity fluctuations are small in the sense that $\forall \tau \neq 0 \quad |\langle I(t+\tau), I(t) \rangle| \ll \langle I \rangle^2$, where $\langle I(t+\tau), I(t) \rangle = \langle I(t+\tau)I(t) \rangle - \langle I(t+\tau) \rangle \langle I(t) \rangle$.
- (4) The output phase fluctuations are small in the sense that $\int d\tau |b^\dagger(t+\tau)b(t)| \gg 1$.

Only when operating “above threshold” will it satisfy the final two conditions above. For the laser to be above threshold requires that the transfer of bosons from source to laser output mode be at least comparable to incoherent losses. In this regime there is a negative correlation between the number of source excitations and the number of bosons in the laser mode. This provides the self-regulation of intensity which enables condition (3) to be satisfied. By contrast, condition (4) may be satisfied for a laser above threshold simply because the intracavity boson number is very large.

7.2.2 Atom laser models

There has so far been many models of atom lasers. Atoms cannot be created out of energy (as can photons and other gauge bosons), and this means that the source for atoms must be a mode (or set of modes) of the atom field. Typically these modes would exist in a trap for atoms and the laser mode itself would be the lowest mode of that trap (although this is not necessarily so). The mechanisms which have been proposed for transferring atoms from the source to the laser mode fall into two classes: optical cooling [35, 114, 115, 116] and evaporative cooling [34, 117, 118].

Optical cooling is the reduction in the kinetic energy of atoms by the transfer of energy and momentum between the atoms, optical laser beams, and spontaneously emitted photons. Because of unwanted processes such as photon reabsorption, the calculated linewidth in Ref. [35] far exceeded the ideal limit, but was still small enough to satisfy condition (4). However, the calculation ignored many complicating factors such as interatomic collisions, so it remains to be seen whether it really would be possible to build an atom laser based on this or any other method of optical cooling.

Evaporative cooling appears a more promising route to an atom laser because unlike optical cooling it has already produced Bose condensation of atoms. What is unclear about this type of laser is whether it could satisfy condition (4). Using the simple model proposed by Holland *et al.* [34], it was shown in Ref. [118] that the linewidth of an atom laser based on evaporative cooling would typically be much larger than the output flux, so that condition (4) would not be satisfied. This is closely linked to the laser dynamics because the same *s*-wave two body scattering Hamiltonian causes both the undesired self-interaction energy of the laser mode and the desired coupling between the source and the laser modes (evaporation).

7.2.3 Current experimental progress

In the previous two sections we have discussed the criteria for an ideal atom laser. In a more general context, however, different groups of people (whether in theory, experiment, or applications) require quite different properties from a laser, and have different expectations about how a “typical” laser should behave. This implies that the stringent definition above may be relaxed in many practical situations. In particular, as long as the most basic requirement of an atom laser, that a *coherent* and *intense* matter wave should be generated, is fulfilled, one may rightfully claim to having constructed a rudimentary atom laser. By coherence, first order coherence suffices for most applications. With BEC the beam is already intense – compared to population per mode of only 10^{-12} for a thermal atomic beam, a BEC has a macroscopic number of atoms within a mode.

So far, there have been quite a few proposals for generating a pulsed or continuous beam of coherent atoms based on various schemes that output couple pre-formed condensates. The simplest uncontrolled way to generate a coherent

pulse of atomic matter-waves from a trapped condensate is to switch-off the trapping potential and let the atomic cloud expand ballistically. This is analogous to cavity dumping for an optical laser. A more controlled way to extract the atoms require a coupling mechanism between confined quantum states and a propagating atoms. Recently, pulsed, quasi-continuous and continuous atom lasers have been realised and these are briefly summarised below.

Pulsed atom laser

The first output coupler reported for a BEC[37] was essentially based on the Stern-Gerlach effect. A short RF pulse rotated the spins of the condensate by a variable angle and the inhomogeneous magnetic trapping field separated the atoms into trapped and outcoupled components. By using a series of RF pulses, a sequence of coherent atom pulses could be formed. An output coupler could be realised by applying resonant RF radiation for a variable pulse duration and causing Rabi oscillations of the atoms' magnetic moments. The spins of the atoms were rotated between spin up (trapped state) and spin down (untrapped state) resulting in output coupling efficiency cycling between 0 and 100%. Alternatively, the RF was swept through resonance and depending on the speed of the sweep, the fraction of untrapped atoms could be controlled.

Quasi-continuous atom laser

Instead of using an RF coupling which simply converts the internal state of the atoms from the trapped to the untrapped state which then fall under gravity, a quasi-continuous atom laser was constructed recently at NIST[119]. This has been achieved through using a stimulated Raman process for the coupling transition. A net momentum kick was provided in the absorption-stimulated emission cycle and the resulting momentum distribution of the output atoms became much narrower than that achieved under ballistic expansion. In addition, the beam became highly directional; by changing the angle between the wavevectors $\mathbf{k}$ of the Raman lasers, and using higher order ($2n$ -photon) Raman transitions, it was possible to impart any momentum from 0 to $2n\hbar\mathbf{k}$. The quasi-continuous output was achieved by a repeated extraction of a small fraction of the condensate, with the rate of output fast enough that the wave packets overlap with each other. Maximum pulse rate of 20kHz has been achieved.

Continuous atom laser

In April this year, a continuous output beam was reported from the group at Munich[120]. A collimated and monoenergetic beam of atoms was continuously extracted over a period of up to 100 ms using weak RF field. In this set up, the outcoupled condensate falls under the gravitational force. Their output coupling mechanism is the application of RF-pulses to flip the spins of atoms in a small region, and the result can be visualised as a small spatially localised leak in the trapping potential. Such continuous wave output coupling could only be achieved by minimising the magnetic field fluctuations that the trapped atoms experience; the Munich group used a novel magnetic trap of the quadrupole and Ioffe configuration (QUIC) trap which is particularly compact and operates at a current of just 25 A. This output coupler could also be used to perform a spectroscopic measurement of the condensate (condensate population as a function of RF frequency).

Chapter 8

Adiabatic output coupling of BEC at finite temperatures

8.1 Introduction

In this chapter, we analyse the properties of an output coupler for BEC based on stimulated Raman transitions. As discussed previously, output coupling is an essential step in the drive to construct an atom laser. We note that although general features concerning the generation of the output in the recent output coupling experiments[37, 119, 120] are fairly well understood, detailed properties of the construction of the output beam and the evolution inside the trap have not been investigated so far.

Recent theoretical treatments of output couplers for condensates have concentrated either on a single-mode non-interacting trapped condensate[121, 122] or on the mean field treatment for the condensate[123, 124, 125]. Under these conditions the output beam is assumed to be extracted out of a trap at absolute zero temperature. Real condensates, however, appear at finite temperatures, where one expects thermal excitations to play a major role.

We present in this chapter a theory of weak output coupling from a trapped BEC at finite temperatures. We describe both the short-time and long-time behaviour of the output beams. The first and second order coherence properties of the output atoms are also investigated. By applying the self-consistent HFB theory we are able to identify three kinds of processes that contribute to the output: a coherent fraction emerging from the condensate, a thermal fraction

emerging from the thermal excitations in the trap in a similar manner to quantum evaporation in liquid ^4He [126], and a component arising from a remarkable process of pair breaking, involving the simultaneous creation of an output atom and an elementary excitation inside the trap[127].

We begin this chapter by first deriving the equations of motion for the evolution of the dynamic variables. We then present in Section 8.3 a quasi-steady-state formalism, which enables us to obtain the properties of the output atoms. We demonstrate the results by numerical one-dimensional examples in Sections 8.4 and 8.5. A number of aspects in the evolution of the internal modes of the system are discussed in Section 8.6. Finally, a summary and discussion section is provided.

8.2 The two-level output coupling model

In this section we first of all describe our model for output coupling from a trapped Bose gas into free output modes. We then derive the equations of motion for the field operators for atoms in different internal states, and present a general form of solution that can be solved specifically.

8.2.1 Description of the model

Our model assumes that the atoms are initially confined by a trapping potential in thermal equilibrium at a finite temperature in an atomic level $|t\rangle$. Then a coupling interaction is switched on, which induces transitions to an untrapped free state $|f\rangle$. We use the field operator $\psi_t(\mathbf{r})$ to describe the amplitude for the annihilation of a trapped atom at point $\mathbf{r}$ and the field operator $\psi_f(\mathbf{r})$ to describe the corresponding amplitude for a free atom. The Hamiltonian has the form

$$\mathcal{H} = H^{(\text{in})} + H^{(\text{out})} + H_{\text{int}}, \quad (8.1)$$

where $H^{(\text{in})}$ and $H^{(\text{out})}$ describe the dynamics of the trapped and untrapped atoms respectively while H_{int} describes the coupling between the two atomic states.

$H^{(\text{in})}$ is given by the usual Hamiltonian used throughout the thesis; we write

it out again here to introduce consistent notations for this chapter.

$$\begin{aligned}
 H^{(\text{in})} = & \int d^3\mathbf{r} \psi_t^\dagger(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V_t(\mathbf{r}) \right] \psi_t(\mathbf{r}) \\
 & + \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \psi_t^\dagger(\mathbf{r}) \psi_t^\dagger(\mathbf{r}') U_{tt}(\mathbf{r} - \mathbf{r}') \psi_t(\mathbf{r}') \psi_t(\mathbf{r})
 \end{aligned} \quad (8.2)$$

where we denote by U_{tt} the inter-particle repulsive potential between the trapped atoms.

As for the free output atoms, the significant effect of their (elastic) collisions with the trapped atoms must be taken into account. In addition, we consider a small rate of output from the trap, so that the output atoms are dilute. This enables us to neglect the interactions between the free atoms themselves and any inelastic collisions with the trapped atoms. The Hamiltonian for the output atoms is then given by

$$\begin{aligned}
 H^{(\text{out})} = & \int d^3\mathbf{r} \psi_f^\dagger(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V_f(\mathbf{r}) \right] \psi_f(\mathbf{r}) \\
 & + \int d^3\mathbf{r} \int d^3\mathbf{r}' \psi_f^\dagger(\mathbf{r}) \psi_t^\dagger(\mathbf{r}') U_{tf}(\mathbf{r} - \mathbf{r}') \psi_f(\mathbf{r}') \psi_t(\mathbf{r})
 \end{aligned} \quad (8.3)$$

where $V_f(\mathbf{r})$ is the non-trapping potential that influences the propagation of the output free atoms and U_{tf} is the collisional interaction between the trapped and free atoms, which is in general different from the interaction U_{tt} . We use the δ -function form for the inter-particle potentials

$$U_{tt}(\mathbf{r} - \mathbf{r}') = U_0 \delta(\mathbf{r} - \mathbf{r}') \quad (8.4)$$

$$U_{tf}(\mathbf{r} - \mathbf{r}') = U_1 \delta(\mathbf{r} - \mathbf{r}') \quad (8.5)$$

where $U_0 = 4\pi\hbar^2 a_{tt}/m$ and $U_1 = 4\pi\hbar^2 a_{tf}/m$ are proportional to the s-wave scattering lengths a_{tt} and a_{tf} for trapped-trapped and trapped-free collisions, respectively. We assume a repulsive interaction between the atoms, i.e. $U_{0,1} > 0$.

For the interaction Hamiltonian H_{int} , we consider coupling by an electromagnetic field which induces transitions between the levels $|t\rangle$ and $|f\rangle$. In the dipole and rotating wave approximation the electromagnetic coupling mechanism is described by the following Hamiltonian, which can be easily generalised to describe

any kind of linear coupling such as tunnelling:

$$H_{\text{int}} = \hbar \int d^3\mathbf{r} \lambda(\mathbf{r}, t) \psi_f^\dagger(\mathbf{r}) \psi_t(\mathbf{r}) + h.c. \quad (8.6)$$

Here $\lambda(\mathbf{r}, t)$ denotes the amplitude of coupling between trapped and untrapped magnetic states. The form of $\lambda(\mathbf{r}, t)$ depends on the type of coupling used. Typical mechanisms are a direct (one-photon) radio-frequency transition and an indirect (two-photon) stimulated Raman transition. In any electromagnetic induced processes the coupling amplitude can be written as

$$\lambda(\mathbf{r}, t) = \bar{\lambda}(\mathbf{r}, t) e^{i(\mathbf{k}_{\text{em}} \cdot \mathbf{r} - \Delta_{\text{em}} t)} \quad (8.7)$$

where $\bar{\lambda}$ is slowly varying in space and time. $\bar{\lambda}$ can be either time-independent, to describe a continuous electromagnetic wave, or pulse shaped. Here $\hbar \mathbf{k}_{\text{em}}$ and $\hbar \Delta_{\text{em}}$ measure the net momentum and energy transfer from the electromagnetic field to an output atom. In an RF coupling scheme, λ is the Rabi frequency $\Omega(\mathbf{r}, t) = \langle \hat{p} \rangle \mathcal{E}(\mathbf{r}, t) / \hbar$ (or $\langle \hat{\mu} \rangle \mathcal{B}(\mathbf{r}, t) / \hbar$) corresponding to the flipping of the atomic electric (or magnetic) dipole $\langle \hat{p} \rangle$ (or $\langle \hat{\mu} \rangle$) in the electric (or magnetic) field $\mathcal{E}(\mathbf{r}, t)$ ($\mathcal{B}(\mathbf{r}, t)$). Δ_{em} is the detuning of the electromagnetic field frequency from the transition frequency and $\mathbf{k}_{\text{em}}$ is negligible compared to the initial momentum distribution of the atoms. In the stimulated Raman coupling, two laser beams are used to induce a transition from $|t\rangle$ to $|f\rangle$ through an intermediate level $|i\rangle$, and

$$\bar{\lambda}(\mathbf{r}, t) = \frac{\Omega_{ti}^*(\mathbf{r}, t) \Omega_{fi}(\mathbf{r}, t)}{\Delta_i} \quad (8.8)$$

where Ω_{ti} and Ω_{fi} are the Rabi frequencies corresponding to the intermediate transitions and Δ_i is their detuning from resonance with the two beams. Δ_{em} and $\mathbf{k}_{\text{em}}$ are the differences between the frequencies and momenta associated with the two laser beams:

$$\Delta_{\text{em}} = \omega_{1L} - \omega_{2L} - \frac{E_0^t - E_0^f}{\hbar} \quad (8.9)$$

$$\mathbf{k}_{\text{em}} = \mathbf{k}_{1L} - \mathbf{k}_{2L} \quad (8.10)$$

where $E_0^t - E_0^f$ is the energy splitting between the atomic levels $|t\rangle$ and $|f\rangle$ in the centre of the trap. Detailed derivation of these expressions, and in particular Eq. (8.8) for the Raman process is provided in Appendix C. An energy level

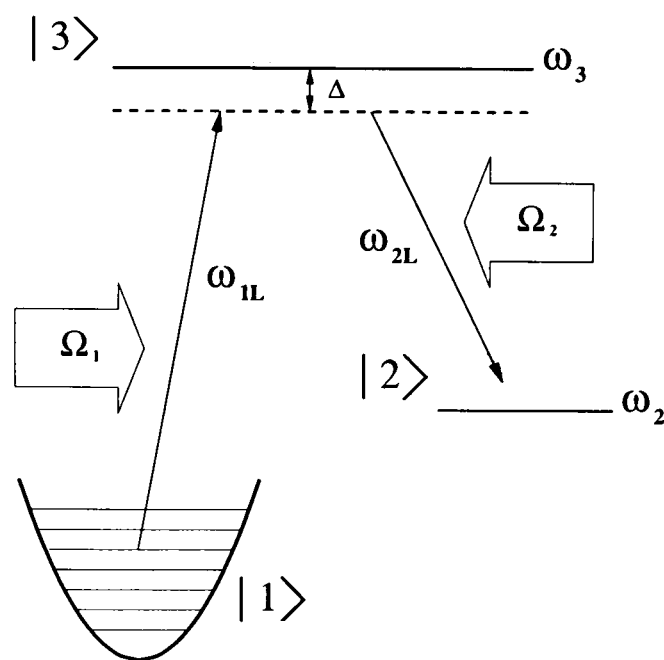


Figure 8.1: Schematic diagram of energy levels and couplings involved in the stimulated Raman process. Δ is the detuning, ω_i , Ω_i , $i = 1, 2$ are the frequencies and Rabi frequencies of the two lasers.

diagram depicting the output coupling through the stimulated Raman process is given in Fig. 8.1.

8.2.2 Equations of motion

The coupled equations of motion for the trapped and free field operators are obtained by computing their commutation relations with the Hamiltonian (8.1). We find

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\psi}_t(\mathbf{r}) = & -\frac{i}{\hbar} \mathcal{L}_t \hat{\psi}_t(\mathbf{r}) - \frac{i}{\hbar} U_0 \hat{\psi}_t^\dagger(\mathbf{r}) \hat{\psi}_t(\mathbf{r}) \hat{\psi}_t(\mathbf{r}) \\ & - i\lambda^*(\mathbf{r}, t) \hat{\psi}_f(\mathbf{r}), \end{aligned} \quad (8.11)$$

$$\frac{\partial}{\partial t} \hat{\psi}_f(\mathbf{r}) = -\frac{i}{\hbar} \mathcal{L}_f \hat{\psi}_f(\mathbf{r}) - i\lambda(\mathbf{r}, t) \hat{\psi}_t(\mathbf{r}). \quad (8.12)$$

where

$$\mathcal{L}_t \equiv -\hbar^2 \nabla^2 / 2m + V_t(\mathbf{r}), \quad (8.13)$$

$$\mathcal{L}_f \equiv -\hbar^2 \nabla^2 / 2m + V_f(\mathbf{r}) + U_1 \langle \hat{\psi}_t^\dagger(\mathbf{r}) \hat{\psi}_t(\mathbf{r}) \rangle. \quad (8.14)$$

Here we have used a mean-field approximation for the collisional effect of the trapped atoms on the untrapped ones. This approximation neglects inelastic scattering processes with the trapped atoms and other possible effects of entanglement of the output atoms with atoms in the trap. This approximation is justified in real experimental situations since the Bose gases are typically so dilute that the mean-free-path for collisions is larger than the dimensions of the atomic cloud in the trap.

8.2.3 General solutions to the equations of motion

Output atoms

The formal solution of Eq. (8.12) for $\hat{\psi}_f$ in terms of $\hat{\psi}_t$ is

$$\begin{aligned} \hat{\psi}_f(\mathbf{r}, t) = & \hat{\psi}_f^{(0)}(\mathbf{r}, t) - i \int_0^t dt' \int d^3\mathbf{r}' \\ & \times G_f(\mathbf{r}, \mathbf{r}', t - t') \lambda(\mathbf{r}', t') \hat{\psi}_t(\mathbf{r}', t'), \end{aligned} \quad (8.15)$$

where $\hat{\psi}_f^{(0)}$ satisfies the time-dependent Schrödinger equation for the free evolution of $\hat{\psi}_f$ in the absence of output coupling

$$\frac{\partial}{\partial t} \hat{\psi}_f^{(0)} = -\frac{i}{\hbar} \mathcal{L}_f \hat{\psi}_f^{(0)}, \quad (8.16)$$

and the “free” propagator $G_f(\mathbf{r}, \mathbf{r}', t - t')$ satisfies the partial differential equation

$$\frac{\partial}{\partial t} G_f(\mathbf{r}, \mathbf{r}', t - t') = -\frac{i}{\hbar} \mathcal{L}_f G_f(\mathbf{r}, \mathbf{r}', t - t') + \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') \quad (8.17)$$

The second term in Eq. (8.15) describes the transition of atoms from the trapped level $|t\rangle$ into the free level $|f\rangle$ with amplitude $\lambda(\mathbf{r}, t)$ and their subsequent propagation as free atoms.

We note that it is useful to expand the field operator ψ_f in terms of the normal modes $\varphi_{\mathbf{k}}(\mathbf{r})$ of the untrapped level

$$\psi_f(\mathbf{r}) = \sum_{\mathbf{k}} \varphi_{\mathbf{k}}(\mathbf{r}) b_{\mathbf{k}}, \quad (8.18)$$

where $b_{\mathbf{k}}$ satisfy the usual bosonic commutation relations $[b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}, \mathbf{k}'}$. $\mathbf{k}$ denotes the momentum state of the free atoms with energy $E_{\mathbf{k}} = \hbar\omega_{\mathbf{k}}$ and $\varphi_{\mathbf{k}}$ are

the time-independent solutions of the single-particle problem in the non-trapping effective potential $V_f(\mathbf{r}) + U_1\langle\psi_t^\dagger(\mathbf{r})\psi_t(\mathbf{r})\rangle$ created by the mean field effect of the collisions between the trapped and the free atoms. In principle, the solutions $\varphi_{\mathbf{k}}$ and the energies $E_{\mathbf{k}}$ may change with time due to the change in the density of the trapped atoms and the subsequent change in the effective repulsive potential near the trap. In what follows we will neglect this time-dependence under the assumption of weak output coupling and slow changes in the density of the trapped atoms.

In the absence of gravitational or other forces, at positions far away from the trap, $\mathbf{k}$ may be taken to be the wave number of a plane wave $\varphi_{\mathbf{k}} \sim e^{i\mathbf{k}\cdot\mathbf{r}}$ with $\omega_{\mathbf{k}} = \hbar k^2/2m$. In the presence of gravity, however, the modes $\mathbf{k}$ may be given asymptotically by the solutions of the Schrödinger equation in a homogeneous field. In terms of the basis functions $\varphi_{\mathbf{k}}(\mathbf{r})$, the free field operator $\psi_f^{(0)}$ is given by

$$\psi_f^{(0)}(\mathbf{r}, t) = \sum_{\mathbf{k}} \varphi_{\mathbf{k}}(\mathbf{r}) b_{\mathbf{k}}(0) e^{-i\omega_{\mathbf{k}} t} \quad (8.19)$$

and the propagator of the free atoms may be written as

$$G_f(\mathbf{r}, \mathbf{r}', t - t') = \sum_{\mathbf{k}} \varphi_{\mathbf{k}}(\mathbf{r}) \varphi_{\mathbf{k}}^*(\mathbf{r}') e^{-i\omega_{\mathbf{k}}(t-t')} \theta(t - t'). \quad (8.20)$$

It is useful to describe the evolution of the untrapped atoms in terms of the annihilation operators $b_{\mathbf{k}}$ of atoms in a specific free mode $\mathbf{k}$. The solution for this operator is obtained by multiplying Eq. (8.15) by $\varphi_{\mathbf{k}}^*$ and integrating. We then have

$$b_{\mathbf{k}}(t) = b_{\mathbf{k}}(0) e^{-i\omega_{\mathbf{k}} t} - i \int_0^t dt' \int d^3\mathbf{r} \varphi_{\mathbf{k}}^*(\mathbf{r}) \lambda(\mathbf{r}, t') e^{-i\omega_{\mathbf{k}}(t-t')} \hat{\psi}_t(\mathbf{r}, t'), \quad (8.21)$$

Solutions for the output field in Eqs. (8.15) and (8.21) require an explicit expression for the trapped field operator ψ_t . The simplest approximation is to take the first order solution in the coupling amplitude λ . This corresponds to a very weak coupling and $\psi_t(\mathbf{r}, t) \approx \psi_t^{(0)}(\mathbf{r}, t)$, where $\psi_t^{(0)}$ is the field operator of the trapped atoms without output coupling.

Trapped atoms

By substituting the solution (8.15) for ψ_f into Eq. (8.11) we obtain the following equation for the trapped field operator ψ_t

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\psi}_t(\mathbf{r}) = & -\frac{i}{\hbar} \mathcal{L}_t \hat{\psi}_t(\mathbf{r}) - \frac{i}{\hbar} U_0 \hat{\psi}_t^\dagger(\mathbf{r}) \hat{\psi}_t(\mathbf{r}) \hat{\psi}_t(\mathbf{r}) \\ & - \int_0^t dt' \int d^3 \mathbf{r}' \Gamma(\mathbf{r}, \mathbf{r}', t, t') \psi_t(\mathbf{r}', t') - i \lambda^*(\mathbf{r}, t) \hat{\psi}_f^{(0)}(\mathbf{r}), \end{aligned} \quad (8.22)$$

where

$$\Gamma(\mathbf{r}, \mathbf{r}', t, t') = \lambda^*(\mathbf{r}, t) G_f(\mathbf{r}, \mathbf{r}', t - t') \lambda(\mathbf{r}', t'). \quad (8.23)$$

In principle, two different situations may be expected from such an integro-differential equation. In the case where this equation describes coupling to output levels with a narrow available bandwidth, we anticipate Rabi oscillations of the atomic population between the trapped and untrapped levels. This kind of behaviour is expected for short times compared with the inverse of the bandwidth of the relevant output modes. Physically this means that the output atoms stay near the trap for a long enough time to perform these oscillations. However, when the bandwidth of the output modes is large, an exponential decay of the population in the trap is expected. Physically this behaviour is expected when the output atoms are fast enough to escape from the trap before the interaction couples them back into the trapped level. This kind of behaviour is expected at long times compared with the inverse of the bandwidth of the relevant output modes. In this last case Eq. (8.22) may be viewed as a Langevin equation for an interaction of a confined system with an infinite heat bath[128].

The field operators $\hat{\psi}_t(\mathbf{r})$ can be expanded, similarly to the field operator $\hat{\psi}_f$, as

$$\psi_t(\mathbf{r}) = \sum_n \phi_n(\mathbf{r}) a_n, \quad (8.24)$$

where $\phi_n(\mathbf{r})$ are the normal modes of the trap given by the solutions of the single-particle problem in the potential well $V_t(\mathbf{r})$. These eigenmodes, however, do not form a good basis, since the interaction between the atoms results in a strong mixing between the levels. The most convenient basis is the basis of condensate and excitations obtained from the HFB theory.

8.3 Quasi steady-state finite T solutions

In this section we present the properties of the output atoms under the assumption that the output coupling is very weak. In this case, the output beam of atoms can serve as a probe to the structure of the Bose gas in the trap under steady-state conditions. The solution for the output is given by Eqs. (8.15) and (8.21), where we substitute $\psi_t(\mathbf{r}, t) \approx \psi_t^{(0)}(\mathbf{r}, t)$. We give a brief description of the formalism that allows the use of the steady-state solution $\psi_t^{(0)}(\mathbf{r}, t)$ for the atoms in the trap.

It is well known that the conventional Bogoliubov theory of a Bose gas does not conserve the total number of particles. Since the situation discussed here involves the transition of atoms into untrapped propagating states, where counting the number of output atoms could be one of the possible measurements that can be performed, we choose to use a number-conserving theory in the spirit of theories recently discussed[61]. The theory enables extension of the finite temperature HFB-Popov method into time dependent cases. The main extension to the usual HFB formalism already discussed in Chapter 5 is that we include the annihilation operator for the condensate a_0 rather than assuming simply a complex wave function (completely broken symmetry) which implies total uncertainty in atom number.

The field operator of the atoms in the trap, $\psi_t(\mathbf{r}, t)$, is split into two parts both of which are now operators; a part which is proportional to the condensate wave function and the other part which represents excitations orthogonal to this state

$$\psi_t(\mathbf{r}, t) = e^{-i\Phi(t)} [\psi_0(\mathbf{r})a_0(t) + \delta\psi(\mathbf{r}, t)]. \quad (8.25)$$

Here $\Phi(t)$ is a global phase given by

$$\Phi(t) = \int_0^t \mu(t') dt', \quad (8.26)$$

where μ , the chemical potential of the system for the given global variables, is constant under steady-state conditions. The operator a_0 satisfies the commutation relation $[a_0, a_0^\dagger] = 1$ and describes the annihilation of one atom in the condensate state ψ_0 . The number of condensate atoms is represented by the operator $\hat{N}_0 \equiv a_0^\dagger a_0$. The non-condensate part, $\delta\psi$, is assumed to be orthogonal to the condensate in the sense $\int d^3\mathbf{r} \psi_0^*(\mathbf{r}, t) \delta\psi(\mathbf{r}, t) = 0$. In the number conserving

formalism $\delta\psi$ is approximated by the following Bogoliubov form:

$$\delta\psi(\mathbf{r}, t) \approx a_0 \frac{1}{\sqrt{\hat{N}_0}} \sum_j [u_j(\mathbf{r})\alpha_j(t) + v_j^*(\mathbf{r})\alpha_j^\dagger(t)]. \quad (8.27)$$

Here $\alpha_j, \alpha_j^\dagger$ are bosonic operators satisfying $[\alpha_i, \alpha_j^\dagger] = \delta_{ij}$ in the space of states with non-zero condensate number. They describe the annihilation or creation of excitations (quasi-particles), or, equivalently, transitions from an excited state j into the condensate and vice versa. This implies that the operators $\alpha_j, \alpha_j^\dagger$ *do not* commute with the condensate operator a_0 . The time-dependence of the functions ψ_0, u_j, v_j is induced only by the change in the global variables $V_t(\mathbf{r}, t), N_t(t), E_{trap}(t)$ and they are assumed to be time-independent under the steady-state conditions.

The condensate wave function ψ_0 in Eq. (8.25) is defined as the solution of the generalised steady-state Gross-Pitaevskii equation

$$\{\mathcal{L}_t - \mu + U_0[\bar{N}_0|\psi_0(\mathbf{r})|^2 + 2\bar{n}(\mathbf{r})]\}\psi_0 = 0 \quad (8.28)$$

where $\mathcal{L}_t$ is given in Eq. (8.13), while the adiabatic mean number $\bar{N}_0$ of condensate atoms and the density $\bar{n}(\mathbf{r})$ of the non-condensate atoms is calculated self-consistently by demanding

$$\bar{N}_0 + \int d^3\mathbf{r} \bar{n}(\mathbf{r}) = N_t. \quad (8.29)$$

As usual, the mean number of atoms in any excited state in equilibrium is assumed to be given by the Bose-Einstein distribution $n_j^{eq} = \frac{1}{e^{\hbar\omega_j/k_B T} - 1}$. The functions $u_j(\mathbf{r}), v_j(\mathbf{r})$ satisfy the steady-state equations

$$\begin{pmatrix} \mathcal{L}_t - \mu + 2U_0[\bar{N}_0|\psi_0|^2 + \bar{n}] & U_0\bar{N}_0\psi_0^2 \\ -U_0\bar{N}_0(\psi_0^*)^2 & -\mathcal{L}_t + \mu - 2U_0[\bar{N}_0|\psi_0|^2 + \bar{n}] \end{pmatrix} \begin{pmatrix} u_j(\mathbf{r}) \\ v_j(\mathbf{r}) \end{pmatrix} \\ = E_j \begin{pmatrix} u_j \\ v_j \end{pmatrix} + U_0\bar{N}_0 \int d^3\mathbf{r} |\psi_0(\mathbf{r})|^2 [\psi_0^*(\mathbf{r})u_j(\mathbf{r}) + \psi_0(\mathbf{r})v_j(\mathbf{r})] \begin{pmatrix} \psi_0(\mathbf{r}) \\ \psi_0^*(\mathbf{r}) \end{pmatrix} \quad (8.30)$$

where the second term on the right hand side ensures orthogonality of the non-condensate functions with the condensate[60]. Equation (8.30) is the finite-temperature HFB-Popov generalisation of the instantaneous steady-state orthog-

onalised Bogoliubov-de Gennes equations mentioned earlier in Chapter 3[60, 61, 62]. We note that the vectors $\begin{pmatrix} v_j^* \\ u_j^* \end{pmatrix}$ satisfy an equation similar to Eq. (8.30) with $E_j \rightarrow -E_j$; Eqs. (8.28) and (8.30) must be solved self-consistently for any given global conditions.

We assume a weak output process so that the total number of atoms in the trap does not change significantly during the application of the output coupling. Under these conditions the time-dependence of the operators a_0 and α_j is assumed to be simply

$$a_0(t) \approx a_0(0) \quad (8.31)$$

$$\alpha_j(t) \approx \alpha_j(0)e^{-i\omega_j t}. \quad (8.32)$$

It should be stressed that this time dependence is not exact even in the steady-state situation without output. This follows from the fact that the commutation relations $[a_0, \alpha_j]$ and $[a_0, \alpha_j^\dagger]$ between the condensate operator and the transition operators are non-vanishing, and therefore a mixing between the condensate and the excitations is expected.

8.4 Evolution of the output

In order to obtain the properties of the output we expand the output operator ψ_f in terms of the free modes $\varphi_{\mathbf{k}}$ of the output [Eq. (8.18)]. In the quasi-steady-state we assume $\lambda(\mathbf{r}, t) = \lambda(\mathbf{r})e^{-i\Delta_{em}t}$. Using the form (8.25) and (8.27) of ψ_t and the assumptions (8.31) and (8.32), we obtain from Eq. (8.21) the following equation for the annihilation operators of the free output modes

$$b_{\mathbf{k}}(t) \approx e^{-i\omega_{\mathbf{k}}t} \left\{ b_{\mathbf{k}}(0) - i \left\{ \lambda_{\mathbf{k}0} D(\Delta_{\mathbf{k}0}, t) a_0(0) + a_0 \frac{1}{\sqrt{\hat{N}_0}} \right. \right. \\ \left. \left. \times \sum_j [\lambda_{\mathbf{k}j+} D(\Delta_{\mathbf{k}j+}, t) \alpha_j(0) + \lambda_{\mathbf{k}j-} D(\Delta_{\mathbf{k}j-}, t) \alpha_j^\dagger(0)] \right\} \right\}, \quad (8.33)$$

where

$$\lambda_{\mathbf{k}0} = \int d^3\mathbf{r} \varphi_{\mathbf{k}}^*(\mathbf{r}) \lambda(\mathbf{r}) \psi_0(\mathbf{r}) \quad (8.34)$$

$$\lambda_{\mathbf{k}j+} = \int d^3\mathbf{r} \varphi_{\mathbf{k}}^*(\mathbf{r}) \lambda(\mathbf{r}) u_j(\mathbf{r}) \quad (8.35)$$

$$\lambda_{\mathbf{k}j-} = \int d^3\mathbf{r} \varphi_{\mathbf{k}}^*(\mathbf{r}) \lambda(\mathbf{r}) v_j^*(\mathbf{r}) \quad (8.36)$$

are the matrix elements of $\lambda(\mathbf{r})$ between the wave functions of collective states of the Bose gas and the output states. In addition,

$$D(\Delta, t) = i \frac{e^{-i\Delta t} - 1}{\Delta} \quad (8.37)$$

and

$$\Delta_{\mathbf{k}\eta} = \mu + \Delta_{em} + E_\eta - \hbar\omega_{\mathbf{k}} \quad (8.38)$$

for $\eta = 0, j+, j-$, where $E_{j+} = E_j$ and $E_{j-} = -E_j$.

This result enables us to calculate various properties of the output from the trap, assuming Bose-Einstein statistics for the initial quasiparticle populations inside the trap. For the initial state we assume that all the other correlation functions between different operators $a_0, \alpha_j, \alpha_j^\dagger$ vanish, except for the diagonals

$$\langle a_0^\dagger a_0 \rangle = N_0 \equiv n_0^t \quad (8.39)$$

$$\langle \alpha_j^\dagger \alpha_j \rangle = n_j \equiv n_{j+}^t \quad (8.40)$$

$$\langle \alpha_j \alpha_j^\dagger \rangle = n_j + 1 \equiv n_{j-}^t. \quad (8.41)$$

8.4.1 Output spectrum

The number of output atoms $n_{\mathbf{k}} \equiv \langle b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \rangle$ in a given mode $\mathbf{k}$ of the free atomic level can be written as a sum of discrete contributions from the different levels of the trapped gas

$$n_{\mathbf{k}}(t) \equiv \langle b_{\mathbf{k}}^\dagger(t) b_{\mathbf{k}}(t) \rangle = n_{\mathbf{k}}^0(t) + \sum_j [n_{\mathbf{k}}^{j+}(t) + n_{\mathbf{k}}^{j-}(t)]. \quad (8.42)$$

This implies that the output beam is a mixture of three different components, 0, $j+$, and $j-$. The total number of output atoms is given by $N_{out} = \int d^3\mathbf{r} n_{out}(\mathbf{r}) = \sum_{\mathbf{k}} n_{\mathbf{k}}$. Each term $\eta = 0, j+, j-$ in Eq. (8.42) has the form

$$n_{\mathbf{k}}^\eta(t) = |\lambda_{\mathbf{k}\eta}|^2 |D(\Delta_{\mathbf{k}\eta}, t)|^2 n_\eta^t \quad (8.43)$$

where n_η^t are defined in Eq. (8.39)-(8.41) above. The time dependence of $n_{\mathbf{k}}^\eta$ is governed by the function

$$|D(\Delta_{\mathbf{k}\eta}, t)|^2 = \frac{1}{2} \left[\frac{\sin(\Delta_{\mathbf{k}\eta} t/2)}{\Delta_{\mathbf{k}\eta}/2} \right]^2. \quad (8.44)$$

This function has a spectral width that decreases with time as $\delta\omega_{\mathbf{k}} \sim \pi/t$. After a time comparable to the inverse of the spectral width $\delta\omega_\eta$ of the matrix elements $\lambda_{\mathbf{k}\eta}$, the output from the internal level η is mainly generated in a narrow range of energies around

$$\hbar\omega_{out}^\eta = \mu + \Delta_{em} + E_\eta \quad (8.45)$$

and the rate of output $dn_{\mathbf{k}}/dt$ into these specific modes becomes constant with time. It is then given by the Fermi golden rule

$$\frac{dn_{\mathbf{k}}}{dt} = \pi \sum_{\eta} n_\eta^t |\lambda_{\mathbf{k}\eta}|^2 \delta(\omega_{\mathbf{k}} - \omega_{out}^\eta). \quad (8.46)$$

We note also that in the limit of long times D behaves asymptotically as

$$|D(\Delta_{\mathbf{k}\eta}, t)|^2 \sim \pi \delta(\Delta_{\mathbf{k}\eta}) t. \quad (8.47)$$

These results suggest that by changing the frequency of the output coupling electromagnetic field and scanning through different values of Δ_{em} one may scan through the magnitude of the matrix elements $|\lambda_{\mathbf{k}\eta}|$. It is, in fact, straightforward to explain physically each of the three processes from the solution for the long time limit Eq. (8.47). The terms proportional to n_0^t and n_{j+}^t describe respectively processes where, after gaining extra energy $\hbar\Delta_{em}$ from the electromagnetic field, atoms initially populating the condensate (energy μ) and an elementary excitation (energy $\mu + \hbar\omega_j$) leave the trap with respective kinetic energies $\hbar\omega_{\mathbf{k}} = \mu + \hbar\Delta_{em}$ and $\hbar\omega_{\mathbf{k}} = \mu + \hbar\omega_j + \hbar\Delta_{em}$. The term proportional to n_{j-}^t describes a process where the energy $\hbar\Delta_{em}$ supplied by the electromagnetic field is sufficient to excite an initially ground state atom to a free momentum state with kinetic energy $\mu + \hbar\Delta_{em} - \hbar\omega_j$, thereby leaving a counterpart atom in an excited trap state with energy $\mu + \hbar\omega_j$ by conservation of energy.

The total number of output atoms as a function of Δ_{em} in our one-dimensional example is shown in Fig. 8.2. The condensate component, $\sum_{\mathbf{k}} n_{\mathbf{k}}^0$ and the excita-

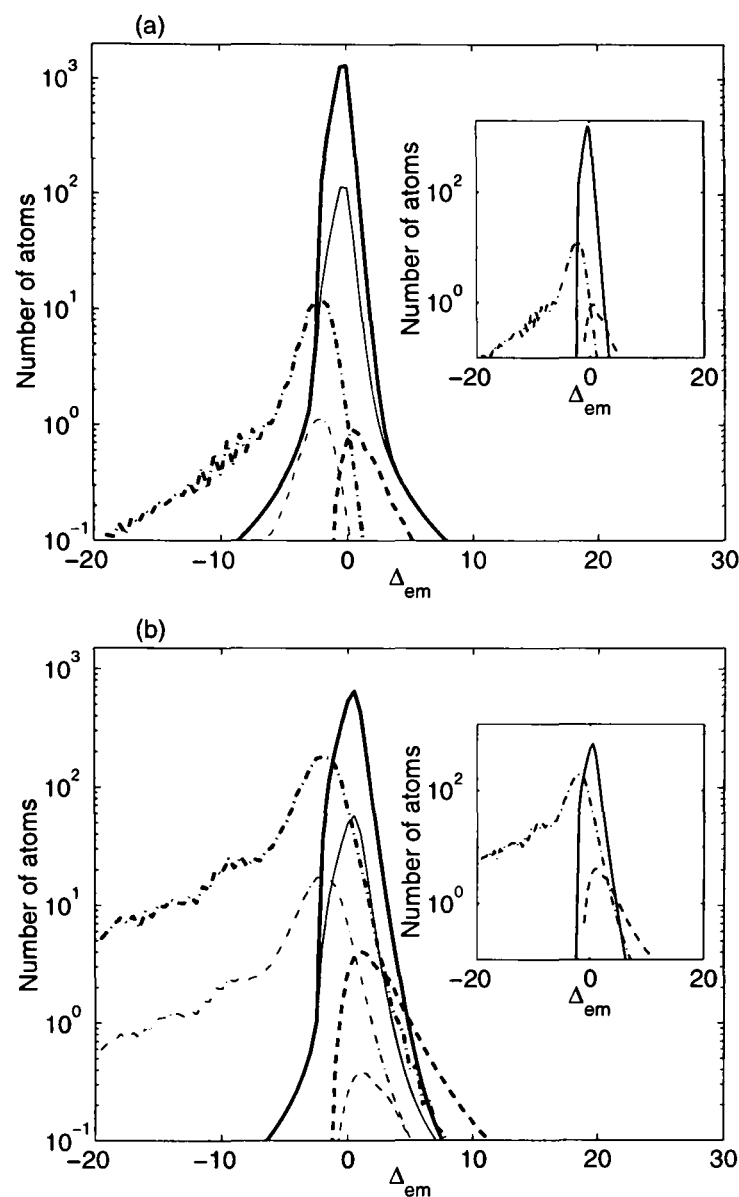


Figure 8.2: The condensate component, $\sum_{\mathbf{k}} n_{\mathbf{k}}^0$ and the excitations $\sum_{j,\mathbf{k}} n_{\mathbf{k}}^{j+}$, $\sum_{j,\mathbf{k}} n_{\mathbf{k}}^{j-}$ are plotted for the output times of $t = 10/\omega$ (thin lines) and $t = 100/\omega$ (bold lines). Figures (a) and (b) correspond to temperatures $T = 10\hbar\omega/k$ and $T = 150\hbar\omega/k$ respectively. The inset shows the corresponding graph in the limit of the long time or continuous output. In all these plots, the solid, dashed and dot-dashed lines indicate processes denoted by 0, $j+$, and $j-$ respectively.

tions $\sum_{j,\mathbf{k}} n_{\mathbf{k}}^{j+}$, $\sum_{j,\mathbf{k}} n_{\mathbf{k}}^{j-}$ are plotted for the output times of $t = 10/\omega$ (thin lines) and $t = 100/\omega$ (bold lines). Figures (a) and (b) correspond to temperatures $T = 10\hbar\omega/k$ and $T = 150\hbar\omega/k$ respectively. The inset shows the corresponding graph in the limit of the long time or continuous output. The solid, dashed and dot-dashed lines indicate processes denoted 0, $j+$, and $j-$ respectively, and we see that they are separated out by having different Δ_{em} . Another way to describe the Δ_{em} -dependent output spectrum is that low (or negative) values of Δ_{em} give rise to a thermal output leading to an evaporative cooling of the trapped gas

(“stimulated quantum evaporation”) while high values of Δ_{em} give rise to an increase in the number of excitations (“heating”). Output atomic beams with the best coherence properties are expected for medium values of Δ_{em} , where the condensate atoms are coupled most efficiently out of the trap. This is investigated more fully in the next subsection. We anticipate that the process corresponding to the higher values of Δ_{em} points to the existence of pairs of correlated atoms in the ground state in the trap, which are broken when one atom is forced out. This process occurs in the limit of weak (adiabatic) coupling and should be differentiated from non-adiabatic processes that may contribute to the generation of new elementary excitations[62, 129].

The width of the spectrum as a function of Δ_{em} is governed by the width Δk_i of the initial atomic distribution and the additional momentum k_{em} . The best separation between the different terms is therefore achieved for $k_{em} = 0$, where the width of the output spectrum as a function of Δ_{em} reflects the initial momentum distribution inside the trap. We note also that at short enough times, the output condensate population remain sizeable even for large values of $|\Delta_{em}|$ and hence the output beam is in general a mixture of particles from the various different physical processes over all values of Δ_{em} . Mathematically, this is simply a consequence of the property of the sinc function which describes the shape of the spectrum. Physically, the broadening of spectrum is a consequence of the Heisenberg uncertainty principle; at the cost of knowing the finite time of interaction, one has greater uncertainty in energy. We see from Fig. 8.2(b) that at high enough temperatures such as $T = 150\hbar\omega/k$, and at long enough times such as $t = 100/\omega$ one can produce output beams not dominated by the condensate, even for positive values of Δ_{em} . This suggests that the separation of the various components in the output should be observable experimentally.

8.4.2 Output density

The density of output atoms at a given point $\mathbf{r}$ is written in terms of the operators $b_{\mathbf{k}}$ as

$$n_{out}(\mathbf{r}) = \sum_{\mathbf{k}, \mathbf{k}'} \varphi_{\mathbf{k}}^*(\mathbf{r}) \varphi_{\mathbf{k}'}(\mathbf{r}) \langle b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \rangle. \quad (8.48)$$

This quantity is also expandable as a sum over discrete contributions from the levels in the trap

$$n_{out}(\mathbf{r}) = N_0 |\Psi_f^0(\mathbf{r}, t)|^2 + \sum_j [n_j |\Psi_f^{j+}(\mathbf{r}, t)|^2 + (n_j + 1) |\Psi_f^{j-}(\mathbf{r}, t)|^2], \quad (8.49)$$

where for each $\eta = 0, j+, j-$

$$\Psi_f^\eta(\mathbf{r}, t) = \sum_{\mathbf{k}} \varphi_{\mathbf{k}}(\mathbf{r}) D(\Delta_{\mathbf{k}\eta}, t) \lambda_{\mathbf{k}\eta}. \quad (8.50)$$

Far from the trap, and in the steady state limit, each component $\Psi_f^\eta(\mathbf{r})$ in the output beam is a wave of finite spatial extent. In the absence of gravitation or other directional forces this wave is roughly given far from the trap by

$$\Psi_f^\eta(\mathbf{r}, t) \sim \theta(r - v_f^\eta t) \sum_{\mathbf{k}} \delta(\hbar \mathbf{k}^2 / 2m - \omega_{\mathbf{k}}) \lambda_{\mathbf{k}\eta} e^{i\mathbf{k} \cdot \mathbf{r}} \quad (8.51)$$

where

$$v_f^\eta = \sqrt{2\hbar\omega_{\mathbf{k}}^\eta / m}. \quad (8.52)$$

This shows that different spectral components of frequency $\omega_{\mathbf{k}}^\eta$ travel at different velocities v_f^η and, consequently, the composition of the output beam at a given point changes over time. In our one-dimensional demonstration each output energy $\hbar\omega_k$ corresponds to two values of k representing right- and left-propagating waves. Since the magnitude of the matrix elements $\lambda_{\mathbf{k}\eta}$ for these two modes are equal, the output beam corresponding to a given component η forms a standing wave and as a result the density $n_{out}^\eta(\mathbf{r})$ becomes oscillatory. This aspect is demonstrated in the next subsection where we discuss the coherence of the output, as these two concepts are very closely related.

8.5 Coherence of the output

In this section we calculate the coherence properties of the output coupled atoms at finite temperatures using the definitions derived in the previous chapter. Recent related works on coherence of BEC include investigation of finite temperature effects within the trap[130], and also studies into the third order correlations as a probe of collisional processes[131]. These works are concerned with atoms en-

tirely within the trap, and therefore do not necessarily indicate the coherence of the condensate in the context of an atom laser.

As discussed above, an output beam weakly coupled from a Bose-gas at finite temperature is a mixture of quasi-monochromatic beams originating from the condensate and the different internal excitations in the trap. The nature of this mixture depends on the frequency, shape and momentum transfer from the electromagnetic field, and the coherence properties are correspondingly affected. Another important aspect that affects the coherence is the time-dependent density of the output atoms; the changing composition of the output beam is an important factor in determining the coherence of the output.

8.5.1 First-order coherence

The first-order, two-point coherence defined in Eq. (7.4) typically takes the maximal value for $\mathbf{r} = \mathbf{r}'$ (i.e. $g^{(1)}(\mathbf{r}, \mathbf{r}) = 1$) and drops to zero for large separation $|\mathbf{r} - \mathbf{r}'|$, for the case of random or thermal mixture of many modes. Highly monochromatic beams, however, are characterised by the fact that $g^{(1)} = 1$ even for large $|\mathbf{r} - \mathbf{r}'|$, implying perfect fringe visibility even if widely separated parts of the beam interfere. Following the quasi-steady-state solution for $\psi_f(\mathbf{r})$ in Eq. (8.21) we find a more compact notation for Eq. (7.4):

$$g^{(1)}(\mathbf{r}, \mathbf{r}', t) = \sum_{\eta=0,j+,j-} \frac{1}{\sqrt{n_{out}(\mathbf{r})n_{out}(\mathbf{r}')}} N_{\eta}[\Psi_f^{\eta}(\mathbf{r})]^* \Psi_f^{\eta}(\mathbf{r}). \quad (8.53)$$

The coherence is maximal if only one of the terms from the sum over η is dominant. In Fig. 8.3(a) the first order coherence of the output atoms as a function of $|\mathbf{r} - \mathbf{r}'|$ is plotted for three different values of detuning $\Delta_{em} = -5, 0, 5$, demonstrating the typical behaviour in the different regimes of output. We show $g^{(1)}(\mathbf{r})$ with respect to the coherent atoms at the centre of the trap. The sign of $g^{(1)}$ changes corresponding to the position of maxima and minima of the fringes. The fringe visibility itself is given by the magnitude of the coherence function, so that for $\Delta_{em} = 0$ the output is fully coherent. The solid line corresponds to $T = 10\hbar\omega/k$; dashed lines shows the case of temperature $T = 150\hbar\omega/k$. Figs. 8.3(b) and (c) are the corresponding output density $n_{out}(\mathbf{r})$ at $T = 10\hbar\omega/k$ and $150\hbar\omega/k$ respectively. In our one-dimensional example, the output density corresponding to the condensate, $n_f^0(x)$, vanishes periodically at distinct points; even if the

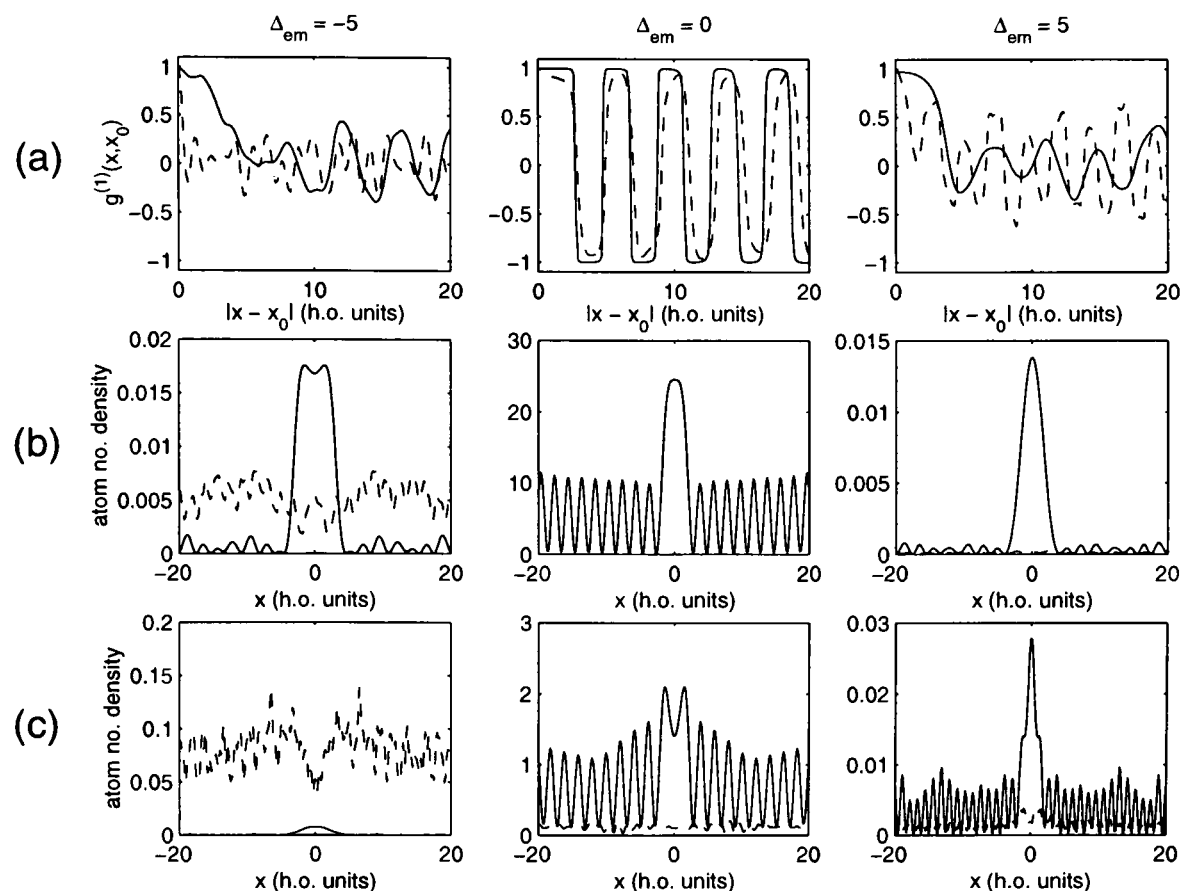


Figure 8.3: First order coherence $g^{(1)}(\mathbf{r}, \mathbf{r}', t)$ as a function of $|\mathbf{r} - \mathbf{r}'|$, $\mathbf{r}' = 0$, and the density of output atoms for different values of detuning ($\Delta_{em} = -5, 0, 5$) and temperature ($T = 10\hbar\omega/k, 150\hbar\omega/k$). The output is for time $t = 100/\omega$. The top row denoted (a) gives the plot of $g^{(1)}$ for different values of Δ_{em} . Solid line: temperature $T = 10\hbar\omega/k$; Dashed line: $T = 150\hbar\omega/k$. Rows (b) and (c) show the density of the output atoms, again for the three values of Δ_{em} . Row (b) corresponds to results at temperature $T = 10\hbar\omega/k$, (c) for temperature $T = 150\hbar\omega/k$. Solid line: condensate density; Dashed line: excited particle density.

condensate component is dominant in most of the space, the coherence drastically decrease near these points where the thermal part of the output dominates. One can see that at these points $g^{(1)} \approx 0$.

In practice, one would measure coherence using stationary detectors at fixed points in space $\mathbf{r}$. This implies that, experimentally, the two-point coherence at $\mathbf{r}$, $\mathbf{r}'$ would be determined by the actual number of atoms with velocity $v_f > r/t$ and $v_f > r'/t$ registering at the detector after time t . We have therefore investigated the time dependence of the first order coherence and the density of the output atoms $n(\mathbf{r})$. Since the case of most importance is the potential application of the output coupler as an atom laser we consider $\Delta_{em} = 0$. Figure 8.4 is laid out in exactly the same way as in Fig. 8.3 except that we now show the time-dependence

instead of the Δ_{em} dependence. The times displayed are $t = 1, 5, 50/\omega$. The case of $t = 100/\omega$ has been already shown as the middle column of Fig. 8.3. We see that for $t = 1$ i.e. a very short time of evolution the shapes of the atom density matches closely that of the initial condensate distribution. This case may also be viewed as modelling a very rapid, pulsed switching on of the output coupling. The coherence length is clearly not long for this case as the atoms have not propagated far enough. As time passes, for example $t = 5/\omega$ one can see how the wave packet has spread quite significantly. In particular one sees that there are points in space where $n(\mathbf{r})$ is still negligible while the coherence plot already gives something similar to the $t = 100/\omega$ case of Fig. 8.3. This is because, although the absolute value of the complex ψ_f may vanish for larger values of $\mathbf{r}$ we are calculating here on two-position correlations at $\mathbf{r}, \mathbf{r}'$. and the function ψ_f itself is not vanishing are large $\mathbf{r}$.

8.5.2 Second-order coherence

The second order coherence has been defined in Eq. (7.6) in terms of $\psi_0(\mathbf{r})$, $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$. The terms involving $\tilde{n}(\mathbf{r})$ and $\tilde{m}(\mathbf{r})$ give the finite temperature effect on the coherence. Noting that the anomalous pair correlations $\tilde{m}(\mathbf{r})$ are usually approximated by zero under the Popov approximation, the question that arises is whether to apply this approximation for the output beams. This can be answered in two ways. On a more practical level, we find that $\tilde{m}(\mathbf{r})$ cannot be ignored because, with the Raman output coupler, we can deliberately choose to make the effect of $\tilde{m}$ significant. Another way is to say $\tilde{m}(\mathbf{r})$ can not be zero because the Popov approximation is only relevant in a trapped condensate. The main effect of the Popov and other similar approximations is mainly small shifts in energies of excitations[70, 93]. We assume these differences are not as crucial in modelling an output coupler.

The intensity correlation at the centre of the trap as a function of detuning and the spatially dependent correlations for various temperatures have been calculated. Typical examples are displayed in Fig. 8.5. In both Fig. 8.5(a) and (b) solid line represents a zero temperature result while the dashed line gives the result for $T = 150\hbar\omega/k$. Referring back to the shape of the output spectrum Fig. 8.2, one can see clearly that if the term originating from the condensate is dominant then the intensity correlation equals 1 while in the other regions where

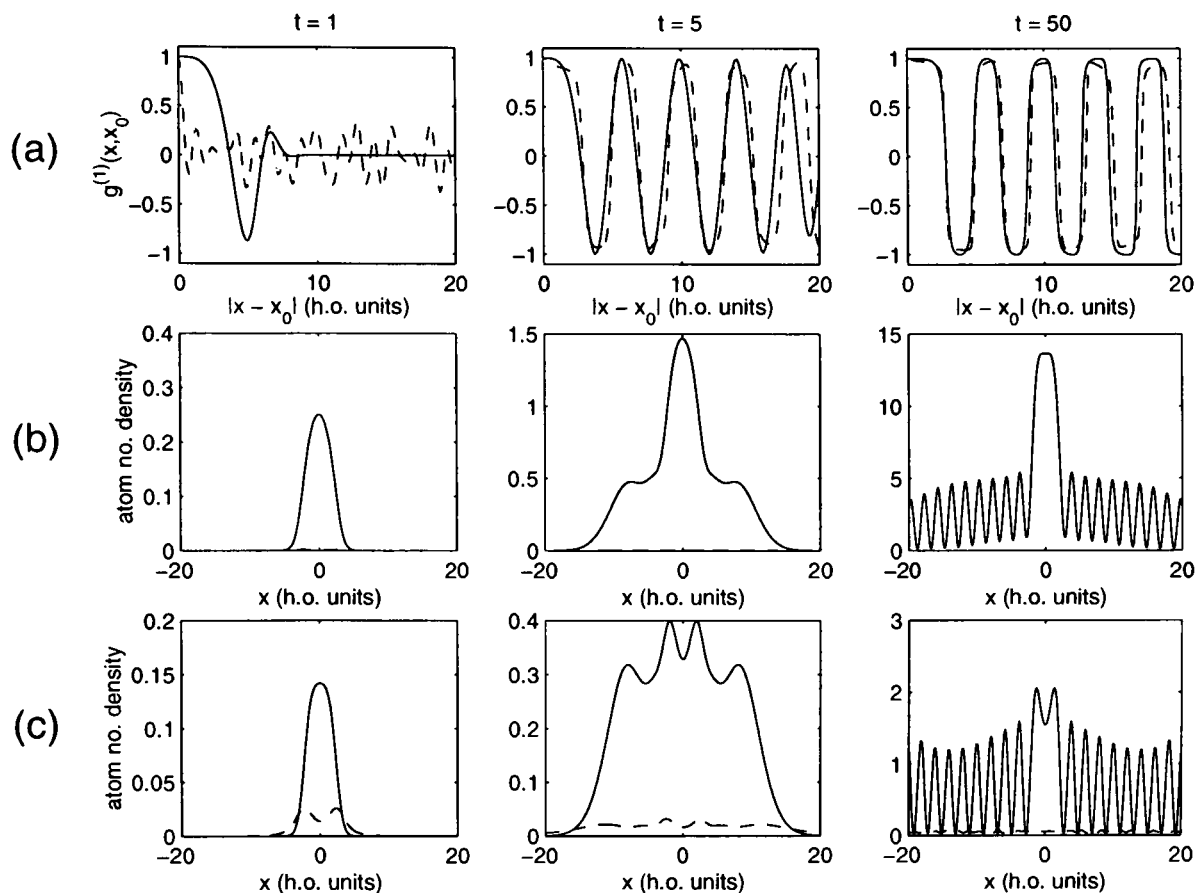


Figure 8.4: First order coherence $g^{(1)}(\mathbf{r}, \mathbf{r}', t)$ as a function of $|\mathbf{r} - \mathbf{r}'|$, $\mathbf{r}' = 0$, and the density of output atoms for different times ($t = 1/\omega, 5/\omega, 50/\omega$) and temperature ($T = 10\hbar\omega/k, 150\hbar\omega/k$). The top row denoted (a) gives the plot of $g^{(1)}$ for different values of t . Solid line: temperature $T = 10\hbar\omega/k$; Dashed line: $T = 150\hbar\omega/k$. Rows (b) and (c) show the density of the output atoms, again for the three values of t . Row (b) corresponds to results at temperature $T = 10\hbar\omega/k$, (c) for temperature $T = 150\hbar\omega/k$. Solid line: condensate density; Dashed line: excited particle density.

thermal components are dominant, $g^{(2)}(0) = 2$. This implies that optimal coherence properties may be achieved by focusing and tuning the spatial shape of the laser beams to overlap with the condensate wave function $\psi_0(\mathbf{r})$. The position dependent intensity correlation $g^{(2)}(\mathbf{r})$ for the detuning $\Delta_{em} = 0$ is constant for very low temperatures but shows oscillations between 1 and 2 for the higher temperature case. Similarly to the first order coherence, this spatial dependence can be traced to the amount of condensate at each point in space. We note that the position dependent second order coherence is found to be uniformly 2 in space for large values of $|\Delta_{em}|$. The fact that the second order correlation of the output does drop to 1 for Δ_{em} close to zero proves that the terminology “atom laser” is very appropriate for BEC coupled out of a trap.

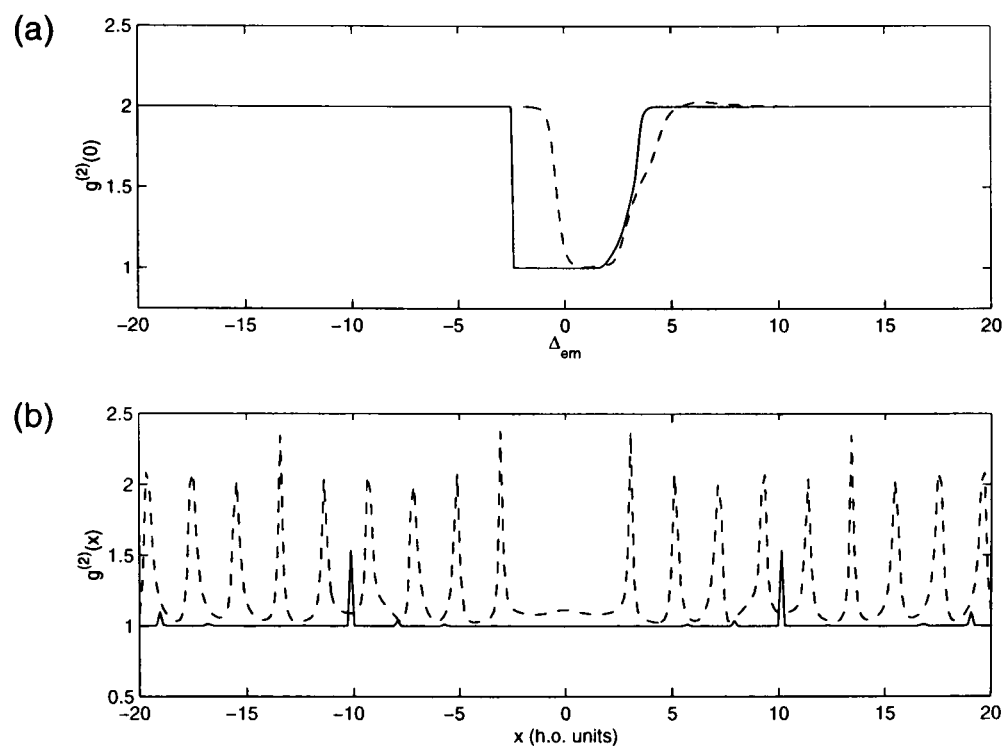


Figure 8.5: (a) Equal time and position second order coherence at the centre of the trap, $g^{(2)}(0)$, as a function of detuning Δ_{em} . Solid line: temperature $T = 0\hbar\omega/k$; Dashed line: $T = 150\hbar\omega/k$. (b) Position dependent intensity correlation $g^{(2)}(\mathbf{r})$ for the detuning $\Delta_{em} = 0$. Solid line: temperature $T = 0\hbar\omega/k$; Dashed line: $T = 150\hbar\omega/k$.

8.6 Dynamics of the trapped gas

We have investigated the properties of the output; for completeness we very briefly discuss in this section the internal dynamics of the trapped atomic Bose gas during the output coupling process. The internal dynamics are described by solutions to Eq. (8.22). We note that during output coupling, the number of trapped atoms populating the condensate state and each of the excited states change in a different way due to different transition amplitudes from the trapped to the output states.

Essentially the mode populations redistribute depending on which value of Δ_{em} has been used. For negative and intermediate values of Δ_{em} one expects decrease in the quasiparticle population. The level with energy which matches the energy supplied by the electromagnetic field is affected most. For positive values of Δ_{em} , we expect the growth in population in the corresponding broken pair.

For longer times it is possible to replace the set of linear integro-differential

equations by a set of linear differential equations; a Markovian approximation may be made which transforms the integro-differential equation into an ordinary differential equation, which can then be solved analytically. Also, it is noted that a full solution of linear integro-differential equations may, in principle, be given by perturbative iterations. It is therefore possible to solve by iteration accurately for shorter times of evolution such that the population of the different excitation levels are not changed significantly from their initial values.

We note that the coherence of the output atoms also tells us about coherence properties of atoms inside the trap; the coherence of the trapped Bose gas is expected to be altered as a direct consequence of the output coupling. In simple terms, when the output atoms are mainly those of condensates we expect the coherence of the internal atoms to drop, if only because the amount of coherent condensate fraction decreases.

8.7 Discussion

We have investigated in this chapter detailed properties of the output coupler based on stimulated Raman process. In particular, in view of recent success at NIST of creating a quasi-continuous atomic beam based on a Raman output coupler, a more detailed theoretical analysis was needed. The effect of incoherent excitations has been included to give a more realistic model, and such inclusion through the self-consistent HFB methods provided us with an important demonstration of the ever-present collisional effects in BEC. Even at zero temperature, the output beam may contain predominantly excited particles for a range of Δ_{em} . Excitations that are present even at zero temperature form an important aspect of the commonly observed interacting Bose-condensed systems such as superfluid ^4He .

The measurement of the spectrum of a weakly coupled output as a function of the coupling parameters should be an excellent tool for probing the quantum state of a trapped atomic Bose gas at finite temperatures. The remarkable effect of output from pair breaking in the ground state demonstrates that the output spectrum may reveal properties of the condensate that are not included in standard mean field theories. The pair breaking process, and indeed the output coupling of the condensate in general, provides an experimentally feasible method

to study quantum entanglement in a macroscopic system. The quantum theory of entanglement is currently under intense study owing to its relevance to quantum computation. So far it has rarely been studied in the context of BEC.

The formalism used here may easily be adopted to cope with output couplers of different configurations. The well-known RF-output coupler has been implicitly dealt with in this chapter; it is but one limiting case of the stimulated Raman output coupler namely $\mathbf{k}_\lambda = 0$. From a more general point of view, our formalism is a description of coupling two types of condensates, namely that represented by $\hat{\psi}_t(\mathbf{r})$ and $\hat{\psi}_f(\mathbf{r})$. Future work may include coupling out a mixture of condensates in which new Josephson-like phenomena are expected to be observed. Output coupling of condensates with negative scattering length is another possible area of investigation in the context of the atom laser, since the system has properties which differ markedly from the usual positive scattering length case. The coherence properties of such an output beam is clearly of great theoretical and practical interest.

In summary, an output coupler for BEC based on stimulated Raman process has been found to display interesting properties that partly result from the complex structure of the theory of BEC itself. It is expected that applications of such a system will lead us to a better general understanding of the phenomenon of BEC in dilute atomic gases.

Chapter 9

Conclusion

In this thesis, a number of issues that relate to the experimentally produced BEC in trapped atomic gas have been investigated. The main impetus of our study was to propose possible new experiments involving BEC. Various predictions relating to the proposed experiments have been made, and we note that some of the basic predictions such as the behaviour of BEC in an optical standing wave have been verified, while others such as the quantum carpet interferometry and the spectroscopy using Raman output couplers are already within the reach of current experimental technology. To establish our theories, existing theoretical tools such as the HFB theory in inhomogeneous systems have been employed, and others such as the quasiparticle projection method have been developed. Since useful analytical solutions are generally intractable in the case of inhomogeneous, weakly interacting BEC, numerical simulations have been used extensively.

In this chapter, we give a summary of the main results of this thesis along with some further remarks. We then proceed to discuss possible future work.

9.1 Summary of main results

There are 6 main results in this thesis on manipulation of the trapped atomic BEC. These are listed below.

(1) Our first attempt in manipulating the experimentally produced trapped BEC involved applying ideas taken from the relatively new field of atom optics. Due to the presence of interatomic interactions, it was found that the effects of

“standard” atom optical elements such as the standing wave diffraction grating are strongly modified. On the other hand, we found that application of the optical potential need not always be external to the condensate. Extending the concept of the tunability of the interatomic scattering length through the Feshbach resonance, we showed that a spatially modulated scattering length results in similar diffraction patterns; this final result is fundamentally different from conventional atom optics in that the diffraction is generated from internal, rather than external, interactions.

(2) Analogy of the physics of BEC with nonlinear optics, which is a well-established subfield of applied optics, is one of the most important aspects of BEC study. We expect that most of the progress of the field in the near future will be driven by exploiting this parallel with nonlinear optics. Very recent such example is the experiment at NIST on nonlinear atom optics and four wave mixing[132]. The main complication with BEC is that calculating the energy “eigenmodes” requires a much more involved theory of quasiparticles, in which the condensate is taken to be the quasiparticle vacuum. In a close parallel with the well-known high harmonic generation, we have successfully observed nonlinear mixing of quasiparticle populations with BEC. The major difference here again was that the nonlinear coupling between the modes is provided internally from atom-atom interactions, not by an external crystal as in traditional nonlinear optics.

(3) A further motivation for our investigation of the quasiparticle mixing was the possibility of explaining the experimentally observed damping of excitations in the trapped condensate. The reduction of quasiparticle population of, say, a “breathing mode” would be then interpreted as the damping. Study of damping is still very much an ongoing work here at Oxford[133]. In this thesis, we studied an alternative description of damping, based on the phenomenological approach of Pitaevskii. The equation derived could also be used as a numerical tool to evaluate the ground state solution to GPE which is, itself, a non-trivial numerical problem. We expect the Pitaevskii damping equation to be of particular value in further studies of BEC dynamics as it is the only equation so far that embeds self-consistent, generalised loss mechanism into the time dependent GPE.

(4) We introduced in this thesis a way to simulate finite temperature BEC evolving in time. The argument based on the work by Kagan and Svistunov was used for the first time in practical numerical simulations. As an example of the method, simulations of the finite temperature condensate in the presence of absorbing boundaries was carried out, modelling the experimental evaporative cooling process. The results confirm self-consistency of the simulation method; when the quasiparticle populations were explicitly worked out by an adiabatic following to a noninteracting system, a dramatic redistribution of the populations which indicates reduction in temperature was observed. A more rigorous theoretical basis, in particular the exact or even partial equivalence of the GPE to the Quantum Boltzmann Equation, is clearly the next step along this potentially very rich line of research.

(5) Studies of the general quantum carpet phenomenon are important in their own right for deepening our understanding of quantum mechanics. In studying the quantum carpets using BEC, and taking a slightly different view point, we found that a generalised version of atom interferometer may be formed using a quantum carpet. We found that from the interferometry, it is possible to make an indirect, but highly sensitive temperature measurement of the ultracold BEC. We note that, in conventional Fresnel diffraction experiments, changing the size of the slit shifts the position of fringes, and in some cases causes the fringes to disappear altogether. Similar effect of quantum interference should be observable with a quantum carpet. Detailed properties of quantum carpets in potential applications remains an exciting area for further study.

(6) The last method discussed in the thesis to manipulate a trapped condensate was the output coupling from a trap using Raman transitions. A variety of results were obtained from this study; in particular, the output spectrum, and the coherence of the output beams were observed. We believe that the Raman based output coupler will prove to be an essential tool in understanding important properties that go into the construction of an atom laser. For instance, the spontaneous generation of quasiparticle excitations as observed in the output is expected to have a significant effect on the beam quality.

9.2 Future work

The field of BEC has been expanding rapidly over the last few years, and the growth is expected to be enhanced even further as physicists from different backgrounds converge, and start to “speak the same language.” Proliferation of laboratories achieving the coldest temperature in the universe by way of BEC makes possible even further stimulation of growth. The state-of-the-art experimental set up used to produce BEC should become simpler as people become more aware of the exact parameters for condensation. It is quite important then that we concentrate on areas which matter most. With the current state of BEC research which, in a sense started only 4 years ago, we see that there are two main paths to follow:

1. Development of the theory of BEC by integrating various existing theories from different fields. The goal would be to form a consistent theory that is valid over various approaches that exist. Physicists from different disciplines are still approaching the problem of BEC in their own ways; for example the Green’s function approach is not so familiar to the atomic physicists. Currently there is no “standard” theoretical establishment that defines the subfield of BEC study.
2. Prediction of possible experimental results with a “quantum engineering” view point. With technological advances in areas such as cavity QED and laser cooling, the ability to engineer quantum systems is within our grasp. BEC lends particularly useful properties such as coherence of the beam and a high number of degrees of freedom. Possible candidate systems to be engineered include quantum logic gates and entangled systems.

We believe that the underlying theme in future BEC research should continue to be that of making the most of the ongoing experiments running hand in hand with the theory.

We discuss below possible extensions to the thesis as well as possible future projects involving spontaneous symmetry breaking, tomography of quasiparticles, and quantum nondemolition measurements.

9.2.1 Extensions to the thesis

As mentioned earlier in various places, some of the projects presented in the thesis have room for further study.

Quasiparticle excitation in atom optical experiments

The effect of atom optical element on the quasiparticle excitations have not yet been studied. This requires taking into account the fact that the quasiparticle basis changes as the geometry of the inhomogeneity changes. Whether one should use the quasiparticle shapes before or after the interaction would depend, among others, on the time scales involved. This is clearly of importance since the coherence of the condensate should be preserved as much as possible while it transits an atom optical element.

Nonlinear mixing in 3D

With higher degeneracy of modes in higher dimensions, it is expected that effects which could not be observed in 1D such as the damping of excitations may be observed. This clearly requires a 3D GPE solver, which is currently being developed in our group at Oxford. Further possible uses of the 3D evolver would be along the lines of work done by Schneider and Feder[134] in which a 3D condensate in a rotating trap was found to form vortex lines. We believe that topological defects could also be observed during other possible scenarios such as the collapse of condensate during a fast switching of the scattering length from positive to negative. This could possibly be a laboratory test of cosmological quenching effect, similar to the experiment originally proposed by Zurek[135] in which a rapid phase transition to the He superfluid phase is induced by a sudden change in the pressure.

3D Raman output coupler

The Raman output coupler discussed in this thesis was limited by the fact that it is a 1D system with no effects of gravity included. The fact that it is a 1D system does not allow the possibility of directional output coupling as realised in a recent experiment[119]. The repulsive potential that free atoms experience from the trapped atoms diminishes rapidly with distance, and the effect of gravity becomes

important. The gravitational potential modifies the eigen modes of the free atoms in a significant way, and therefore leads to different results when various overlap integrals are evaluated. This work would then enable more realistic predictions for experiments.

9.2.2 Study of spontaneously broken symmetry

The fact that a condensate has a definite phase has always been an issue of contention. It is generally accepted now that there is only relative phase, although this does not support the common experimental fact that a phase standard with which the relative phase is to be measured is not always present. In particular, such ideas as superfluid velocity $\nabla\phi$ depends on the seemingly absolute phase of the superfluid. The prevailing argument today is that a number state may be decomposed into coherent states so that a number state has in itself some phase information[136]. To see this, we first write the state as a statistical mixture of number states with a peak in the number distribution. It then follows that

$$\rho = \sum_n |b_n|^2 |n\rangle\langle n| = \int d\alpha |be^{i\alpha}\rangle\langle be^{-i\alpha}| \quad (9.1)$$

where $P(n) = |b_n|^2$ is the Poisson probability distribution and $|be^{i\alpha}\rangle$ are coherent states. A projection measurement onto some angle α_0 then imparts a phase. A model in which phase is generated either spontaneously or systematically is an important fundamental problem. This would then complement a study by Barnett *et al.* which showed that, in the context of the condensates, a coherent state is the most robust state against decoherence[137]. The problem is equivalent to the question ‘How does a coherent state “know” which phase to take?’ Another way to formulate the problem is by considering the process of condensation across the critical temperature: ‘How does the information about the phase of the first few atoms get transmitted to the rest?’ These important theoretical questions clearly need to be addressed.

9.2.3 Tomography of quasiparticles

The density matrix encodes all information which can be obtained about a quantum mechanical system. A particular representation of the density matrix is the

Wigner distribution[138]. The precise nature of the quasiparticle excitations has never been analysed in detail; their phase space representation in terms of Wigner functions is a novel way to understand the nature of the quasiparticle wave functions. Some preliminary work has been already done in this area by us and it shows clearly that they are qualitatively very different from the standard harmonic oscillator eigenfunctions. Of particular interest is the observation of two distinct momentum components p and $-p$ locked to each other in the function “ $v(\mathbf{r})$ ” in the Bogoliubov transformation. This gives a visual representation of the particle pairing effect. Studying and understanding the exact nature of such pairing is of particular interest as it is fundamental to such important effects as the BCS transitions.

On the experimental side, a tomographic reconstruction of the Wigner distribution would be of particular interest[139]. Phase space tomography requires a set of measured projection of the Wigner function $W(x, p)$ along different directions in phase space. A physical mixing mechanism has to be introduced, and this can be done by a combination of lenses and a free space propagation. The key idea is to change a momentum distribution into a position distribution which can then be observed with an atom detector. Such mixing mechanism is given by the free evolution which, in the case of BEC, would contain an extra term originating from the interactions:

$$H = \frac{p^2}{2m} + \int_0^t dt' \nabla U_0 |\psi(\mathbf{r}, t')|^2 \quad (9.2)$$

where U_0 is the usual interatomic interaction strength. The experiment would provide a way to directly observe the non-classical behaviour of macroscopic quantum systems.

9.2.4 Quantum Non-demolition measurements

The quantum nondemolition (QND) measurement is one of the most fascinating aspects of measurement theory[109]. The basic requirement of a QND measurement is the availability of a variable which may be measured repeatedly giving predictable results. This requires that the act of measurement itself does not degrade the predictability of subsequent measurements. Then in a sufficiently long sequence of measurements the output becomes predictable. This requirement is

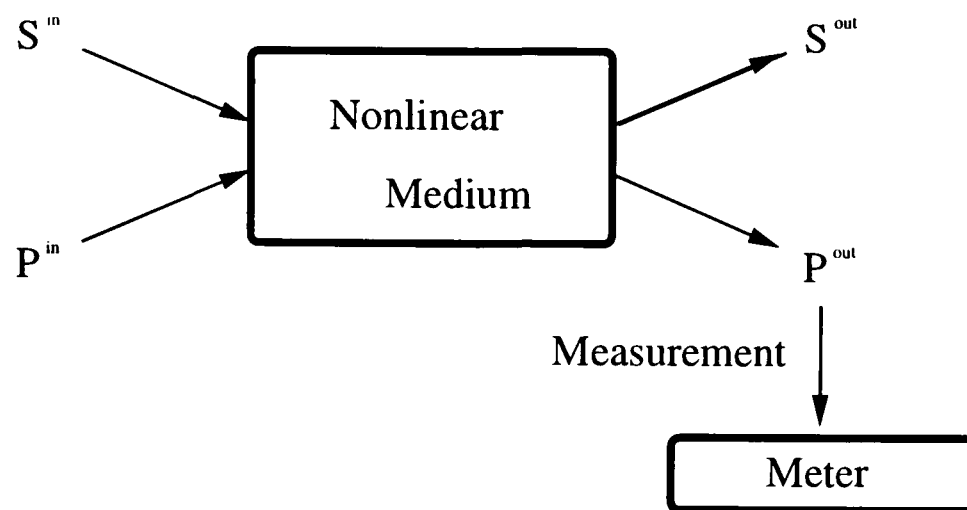


Figure 9.1: Schematic diagram of a QND measurement scheme.

satisfied if for an observable $A(t)$

$$[A(t), A(t')] = 0. \quad (9.3)$$

General idea behind the scheme is summarised in Fig. 9.1. A signal input S^{in} is coupled to a probe P^{in} by a suitable mechanism. From the measurement of probe output P^{out} one can deduce the state of the S^{in} .

Traditionally the QND measurement in quantum optical context requires a coupling which is provided by a crystal. A particle number QND scheme using a four wave mixing process is particularly promising to be directly applicable to the case of BEC[140]. The relevant interaction Hamiltonian is

$$H_{int} = \hbar \chi a^\dagger a b^\dagger b, \quad (9.4)$$

which gives mutual intensity dependent phase shift for the signal and probe fields:

$$a(t) = e^{-i\chi b^\dagger b t} a(0) \quad (9.5)$$

$$b(t) = e^{-i\chi a^\dagger a t} b(0) \quad (9.6)$$

Equations (9.5),(9.6) imply that by measuring the phase of the probe one is able to calculate non destructively the number of the signal atom number. Such QND measurements have never been carried out on a condensate previously.

Extensions of the QND scheme to other observables is expected to have far-reaching consequences in metrology and in communication systems.

Appendix A

Numerical Integration of GPE

The GPE, in dimensionless units may be written as:

$$\frac{\partial \Psi}{\partial t} = i \frac{\partial^2 \Psi}{\partial x^2} - i V(x, t) \Psi - i C n l |\Psi|^2 \Psi. \quad (\text{A.1})$$

Ψ is position dependent and hence the equation to be integrated can be viewed as a partial differential equation of the form:

$$\frac{\partial y(x, t)}{\partial t} = f(x, t, y). \quad (\text{A.2})$$

In this case, the temporal evolution is carried out at each time t_i for every point x_j . The evaluation of the RHS of equation (A.2) at a particular point x_j may require information from other spatial points if, for example, the function f contains spatial derivatives.

To overcome the complication one makes a conversion to an interaction picture as follows. First, Eq. (A.1) is rewritten as:

$$\frac{\partial \Psi}{\partial t} = \hat{D} \Psi + N \Psi \quad (\text{A.3})$$

where $\hat{D} \equiv i \frac{\partial}{\partial x^2}$ and $N \equiv -i V(x, t) - i C n l |\Psi|^2$ and is transformed to an interaction picture representation defined by:

$$\Psi_I(x, t, \tau) = e^{-\hat{D}(t-\tau)} \Psi(x, t) \quad (\text{A.4})$$

$$\Psi(x, t) = e^{+\hat{D}(t-\tau)} \Psi_I(x, t, \tau) \quad (\text{A.5})$$

It is important to note that there are two times involved in the definition of the interaction picture, namely t and τ . $\Psi_I(x, t, \tau)$ can be viewed as the interaction picture wave function at time t centred on time τ . Equation (A.3) becomes, in the interaction picture:

$$\frac{\partial \Psi_I(x, t, \tau)}{\partial t} = N_I(x, t) \Psi_I(x, t, \tau) \quad (\text{A.6})$$

where $N_I(x, t) \equiv e^{-\hat{D}(t-\tau)} N e^{+\hat{D}(t-\tau)}$. This may also be written as:

$$\frac{\partial \Psi_I(x, t, \tau)}{\partial t} = e^{-\hat{D}(t-\tau)} N \Psi(x, t) \quad (\text{A.7})$$

using equation (A.5).

The action of the operator $e^{\pm \hat{D}(t-\tau)}$ is then calculated in the momentum space, since the operator $\hat{D}$ is then simply a multiplier. For example, to calculate $e^{+\hat{D}(t-\tau)} \Psi(x, t)$, one first performs a Fast Fourier Transform (FFT) on $\Psi(x, t)$, multiplies the result by $e^{+i(t-\tau)(-2\pi kx)^2}$ and then performs the inverse Fourier transform (IFFT) back into the position space. By using a suitable sequence of Fourier Transforms and its inverse, the RHS of Eq. (A.7) at any given time t_i is evaluated.

Having determined the RHS of Eq. (A.7) for time t_i , the fourth order Runge-Kutta method (RK4) was chosen in our simulations to propagate the equation. Any numerical solution is a trade off between speed and accuracy and the fourth order Runge-Kutta algorithm provides a good balance between the two. The error in the Euler method is of order Δt^2 where Δt is the time grid spacing. By using Euler's result to obtain estimates of the solution (and hence the derivatives) within the computational step, the overall error in RK4 may be made to be of order $(\Delta t)^5$. The calculations required to implement the RK4 algorithm are:

$$\begin{aligned} \Delta y_1 &= f(t_i, y_i) \Delta t \\ \Delta y_2 &= f\left(t_i + \frac{\Delta t}{2}, y_i + \frac{\Delta y_1}{2}\right) \Delta t \\ \Delta y_3 &= f\left(t_i + \frac{\Delta t}{2}, y_i + \frac{\Delta y_2}{2}\right) \Delta t \\ \Delta y_4 &= f(t_i + \Delta t, y_i + \Delta y_3) \Delta t \\ y_{i+1} &= y_i + \frac{\Delta y_1}{6} + \frac{\Delta y_2}{3} + \frac{\Delta y_3}{3} + \frac{\Delta y_4}{6} + O(\Delta t^5) \end{aligned} \quad (\text{A.8})$$

The numerical integration may be carried out efficiently by a convenient choice for τ . Noting that $\Psi(x, t) \equiv \Psi_I(x, t, \tau)$ if $t = \tau$ and that the RK4 algorithm requires the procedure to be followed four times for each computational step, one can reduce the number of required Fourier transforms by always choosing τ to be in the middle of the step. At the end of any one such time step, one gets $\Psi_I(x, t_{i+1}, \tau = t_{i+1} - \frac{\Delta t}{2})$ which is then to be converted into $\Psi_I(x, t_{i+1}, t_{i+1} + \frac{\Delta t}{2})$ through the operation:

$$\Psi_I(x, t_{i+1}, t_{i+1} + \frac{\Delta t}{2}) = e^{+\hat{D}(\Delta t)} \Psi_I(x, t_{i+1}, t_{i+1} - \frac{\Delta t}{2}) \quad (\text{A.9})$$

This, again, is done using a sequence of FFT's. The overall saving compared with simply fixing the value of τ is a reduction in the number of FFT's which must be performed by a factor of $\frac{3}{4}$.

Appendix B

Derivation of $g^{(2)}$

Starting from the definition of the second-order correlation:

$$g^{(2)}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = \frac{\langle \hat{\psi}_f^\dagger(\mathbf{r}_1, t_1) \hat{\psi}_f^\dagger(\mathbf{r}_2, t_2) \hat{\psi}_f(\mathbf{r}_1, t_1) \hat{\psi}_f(\mathbf{r}_2, t_2) \rangle}{\langle \hat{\psi}_f^\dagger(\mathbf{r}_1, t_1) \hat{\psi}_f(\mathbf{r}_1, t_1) \rangle \langle \hat{\psi}_f^\dagger(\mathbf{r}_2, t_2) \hat{\psi}_f(\mathbf{r}_2, t_2) \rangle} \quad (\text{B.1})$$

and decomposing the field into its mean field and fluctuation,

$$\hat{\psi}(\mathbf{r}_j) = \Psi(\mathbf{r}_j) + \hat{\delta}(\mathbf{r}_j) = \Psi_j + \hat{\delta}_j \quad (\text{B.2})$$

the numerator may be expanded as:

$$\begin{aligned} & \hat{\psi}^\dagger(\mathbf{r}_1, t_1) \hat{\psi}^\dagger(\mathbf{r}_2, t_2) \hat{\psi}(\mathbf{r}_1, t_1) \hat{\psi}(\mathbf{r}_2, t_2) \\ = & |\Psi_1|^2 |\Psi_2|^2 + |\Psi_2|^2 \{ \Psi_1^* \hat{\delta}_1 + \Psi_1 \hat{\delta}_1^\dagger \} + |\Psi_1|^2 \{ \Psi_2^* \hat{\delta}_2 + \Psi_2 \hat{\delta}_2^\dagger \} \\ + & \Psi_1^* \Psi_2^* \hat{\delta}_2 \hat{\delta}_1 + \Psi_1 \Psi_2^* \hat{\delta}_1^\dagger \hat{\delta}_2 + \Psi_2 \Psi_1 \hat{\delta}_1^\dagger \hat{\delta}_2^\dagger + \Psi_1^* \Psi_2 \hat{\delta}_2^\dagger \hat{\delta}_1 \\ + & |\Psi_1|^2 \hat{\delta}_1^\dagger \hat{\delta}_1 + |\Psi_2|^2 \hat{\delta}_2^\dagger \hat{\delta}_2 + \Psi_2^* \hat{\delta}_1^\dagger \hat{\delta}_2 \hat{\delta}_1 + \Psi_2 \hat{\delta}_1^\dagger \hat{\delta}_2^\dagger \hat{\delta}_1 \\ + & \Psi_1^* \hat{\delta}_2^\dagger \hat{\delta}_2 \hat{\delta}_1 + \Psi_1 \hat{\delta}_1^\dagger \hat{\delta}_2^\dagger \hat{\delta}_2 + \hat{\delta}_1^\dagger \hat{\delta}_2^\dagger \hat{\delta}_2 \hat{\delta}_1 \end{aligned} \quad (\text{B.3})$$

All terms of single order in δ vanish by definition. Third order terms in $\hat{\delta}$ also vanish because they factorise such that one may write, for instance,

$$\langle \hat{\delta}_1^\dagger \hat{\delta}_2 \hat{\delta}_1 \rangle = \langle \hat{\delta}_1^\dagger \hat{\delta}_2 \rangle \langle \hat{\delta}_1 \rangle + \langle \hat{\delta}_1^\dagger \hat{\delta}_1 \rangle \langle \hat{\delta}_2 \rangle + \langle \hat{\delta}_2 \hat{\delta}_1 \rangle \langle \hat{\delta}_1^\dagger \rangle \quad (\text{B.4})$$

so that they vanish. Defining $n(1, 2) = \langle \hat{\delta}_1^\dagger \hat{\delta}_2 \rangle$, $m(1, 2) = \langle \hat{\delta}_1 \hat{\delta}_2 \rangle$, $n_0(1, 2) = \langle \Psi_1^* \Psi_2 \rangle$ and $m_0(1, 2) = \langle \Psi_1 \Psi_2 \rangle$, one obtains

$$\begin{aligned}
 & \langle \hat{\psi}^\dagger(\mathbf{r}_1, t_1) \hat{\psi}^\dagger(\mathbf{r}_2, t_2) \hat{\psi}(\mathbf{r}_1, t_1) \hat{\psi}(\mathbf{r}_2, t_2) \rangle \\
 = & n_0(1, 1)n_0(2, 2) + n_0(1, 1)n(2, 2) + n_0(2, 2)n(1, 1) + n(1, 1)n(2, 2) \\
 + & m_0^*(1, 2)m(2, 1) + n_0(2, 1)n(1, 2) + m_0(1, 2)m^\dagger(1, 2) + n_0(1, 2)n(2, 1) \\
 + & n(1, 2)n(2, 1) + m^\dagger(1, 2)m(2, 1). \tag{B.5}
 \end{aligned}$$

Here, Wick's Theorem was used to write the fourth order term

$$\langle \hat{\delta}^\dagger \hat{\delta}^\dagger \hat{\delta} \hat{\delta} \rangle = n(1, 2)n(2, 1) + n(1, 1)n(2, 2) + m^\dagger(1, 2)m(2, 1). \tag{B.6}$$

Writing the total density as $\bar{n}(i) = n_0(i, i) + n(i, i)$, the coherence function is written as:

$$\begin{aligned}
 g^{(2)}(\mathbf{r}_1, \mathbf{r}_2) &= 1 + \frac{1}{\bar{n}(1)\bar{n}(2)} \left\{ m_0^*(1, 2)m(2, 1) + m_0(1, 2)m^\dagger(2, 1) \right. \\
 &\quad + n_0(2, 1)n(1, 2) + n_0(1, 2)n(2, 1) \\
 &\quad \left. + n(1, 2)n(2, 1) + m^\dagger(1, 2)m(2, 1) \right\} \\
 &= 1 + \frac{1}{\bar{n}(1)\bar{n}(2)} \left\{ 2\text{Re} [n_0(2, 1)n(1, 2) + m_0^*(1, 2)m(2, 1)] \right. \\
 &\quad \left. + |n(1, 2)|^2 + |m(1, 2)|^2 \right\}. \tag{B.7}
 \end{aligned}$$

For $\mathbf{r}_1 = \mathbf{r}_2$ we get the result of Eq. (7.6) in Chapter 7.

Appendix C

Derivation of $\lambda(\mathbf{r}, t)$

The form of the coupling function $\lambda(\mathbf{r}, t)$ determines the specific type of coupling between $\hat{\psi}_f(\mathbf{r})$ and $\hat{\psi}_t(\mathbf{r})$ in the interaction Hamiltonian, H_{int} . We discuss here the stimulated Raman scheme as the coupling mechanism. A Raman coupling gives us several parameters that can be controlled: the frequency difference between the two lasers, the Rabi frequencies and the detunings from the atomic levels. In order to derive $\lambda(\mathbf{r}, t)$, we consider a non-interacting many-body Hamiltonian, where coupling between the internal atomic levels and laser fields are considered.

We consider a collection of three level atoms subjected to a pair of laser beams in a scheme appropriate to induce stimulated Raman transition from the ground atomic level $|1\rangle$ to a second ground¹ level $|2\rangle$ through a third level $|3\rangle$, far from resonance with the laser fields. In this case the system can be effectively described as a two level system while the third level is adiabatically eliminated.

We assume the following many-body Hamiltonian for a collection of non-interacting atoms

$$H = \sum_{j=1,2,3} \int d^3\mathbf{r} \psi_j^\dagger(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V_j(\mathbf{r}) + \hbar\omega_j \right] \psi_j(\mathbf{r}) + \frac{1}{2} \sum_{j=1,2} \mu_{j3} \int d^3\mathbf{r} E_{jL}(\mathbf{r}, t) \psi_3^\dagger(\mathbf{r}) \psi_j(\mathbf{r}) + h.c. \quad (\text{C.1})$$

where $V_j(\mathbf{r})$ are effective external potentials acting on the different atomic levels, μ_{j3} are the dipole moments for the transition $|j\rangle \rightarrow |3\rangle$ and $E_{jL}(\mathbf{r}, t)$ are the amplitudes of the laser fields, which we assume to have the form $E_{jL}(\mathbf{r}, t) =$

¹Or maybe meta-stable level?

$\mathcal{E}_j(\mathbf{r}, t)e^{i(\mathbf{k}_{jL} \cdot \mathbf{r} - \omega_{jL}t)}$ where the envelopes $\mathcal{E}$ are slowly varying with respect to the exponential term. The equations of motion for the three field operators are:

$$i\hbar\dot{\psi}_1 = H_1^{(0)}\psi_1 - \mu_{13}^*E_{1L}^*\psi_3 \quad (\text{C.2})$$

$$i\hbar\dot{\psi}_2 = H_2^{(0)}\psi_2 - \mu_{23}^*E_{2L}^*\psi_3 \quad (\text{C.3})$$

$$i\hbar\dot{\psi}_3 = H_3^{(0)}\psi_3 - \mu_{13}E_{1L}\psi_1 - \mu_{23}E_{2L}\psi_2 \quad (\text{C.4})$$

The solution of the equation for ψ_3 as a function of the two other field operators can be written as

$$\begin{aligned} \psi_3(\mathbf{r}, t) &= \psi_3^{(0)}(\mathbf{r}, t) + i \int_0^t dt' \int d^3\mathbf{r}' G^{(3)}(\mathbf{r}, \mathbf{r}', t - t') e^{-i\omega_3(t-t')} \\ &\quad \times \sum_{j=1,2} \Omega_j(\mathbf{r}', t') \psi_j(\mathbf{r}', t') e^{i(\mathbf{k}_{jL} \cdot \mathbf{r}' - \omega_{jL}t')} \end{aligned} \quad (\text{C.5})$$

Here $\psi_3^{(0)}$ is the freely evolving field operator of level $|3\rangle$ atoms, which we set to zero under the assumption that this level is initially unpopulated. $\Omega_j(\mathbf{r}, t) = \mu_{j3}\mathcal{E}_{jL}(\mathbf{r}, t)/2\hbar$ are the slowly varying Rabi frequencies and $G^{(3)}$ is the Green function for the evolution of the level $|3\rangle$ as it is subjected to a δ -function source. The Green's function $G^{(3)}(\mathbf{r}, \mathbf{r}', t - t')$ can be expanded in terms of the energy eigenfunctions $\varphi_{\mathbf{q}}^{(3)}(\mathbf{r})$ with energies $\hbar\omega_{\mathbf{q}}$ of the Hamiltonian $H^{(3)}$

$$G^{(3)}(\mathbf{r}, \mathbf{r}', t - t') = \sum_{\mathbf{q}} \varphi_{\mathbf{q}}^{(3)}(\mathbf{r}) \varphi_{\mathbf{q}}^{(3)*}(\mathbf{r}') e^{-i\omega_{\mathbf{q}}(t-t')} \theta(t - t')$$

We substitute the solution for ψ_3 using this expansion in Eqs. (C.2),(C.3). We then expand the functions ψ_i ($i = 1, 2$) as $\psi_i(\mathbf{r}, t) = \sum_n \varphi_n^{(i)}(\mathbf{r}) \tilde{c}_n^{(i)}(t) e^{-i(\omega_i + \omega_n^i)t}$, where $c_n^{(i)} = \tilde{c}_n^{(i)} e^{-i(\omega_i + \omega_n^i)t}$ are the annihilation operators of the eigenmodes n of the Hamiltonian $H_i^{(0)}$. Then we obtain the following equations for the slowly varying operators $\tilde{c}^{(i)}(t)$

$$\dot{\tilde{c}}_n^{(i)}(t) = \sum_{n'} \sum_{j=1,2} \lambda_{n,n'}^{ij}(t) \tilde{c}_{n'}^{(j)}(t) \quad (\text{C.6})$$

where

$$\lambda_{n,n'}^{ij} = i \int d^3\mathbf{r} \varphi_n^{(i)*}(\mathbf{r}) \Omega_i^*(\mathbf{r}, t) \sum_{\mathbf{q}} \varphi_{\mathbf{q}}^{(3)}(\mathbf{r}) e^{-i\mathbf{k}_{iL} \cdot \mathbf{r}} e^{i(\omega_i + \omega_n^i + \omega_{iL} - \omega_3 - \omega_{\mathbf{q}})t}$$

$$\times \int d^3\mathbf{r}' \varphi_{\mathbf{q}}^{(3)*}(\mathbf{r}') \varphi_{n'}^{(j)}(\mathbf{r}') e^{i\mathbf{k}_{jL} \cdot \mathbf{r}'} I(\mathbf{r}', t). \quad (\text{C.7})$$

with the time integral $I(\mathbf{r}', t)$ given by

$$I(\mathbf{r}', t) = \int_0^t dt' \Omega_j(\mathbf{r}', t') e^{i(\omega_3 + \omega_{\mathbf{q}} - \omega_j - \omega_{n'} - \omega_{jL})t'}. \quad (\text{C.8})$$

Since the variation of Ω_j with time is slow compared with the exponential oscillatory terms, we may approximate the time integral by

$$I(\mathbf{r}', t) = -i \frac{\Omega_i(\mathbf{r}', t) e^{i(\omega_i + \omega_n + \omega_{iL} - \omega_j - \omega_{n'} - \omega_{jL})t} - \Omega_i(\mathbf{r}, 0) e^{i(\omega_i + \omega_n + \omega_{iL} - \omega_3 - \omega_{\mathbf{q}})t}}{\omega_j + \omega_{n'} + \omega_{jL} - \omega_3 - \omega_{\mathbf{q}}}. \quad (\text{C.9})$$

We now assume that the detuning $\Delta_{j3} \equiv \omega_j + \omega_{jL} - \omega_3$ is much larger than the separation between the relevant translational degrees of freedom $\Delta\omega_{\mathbf{q}}$, $\Delta\omega_n$ of each atomic level and much larger than the detuning $\Delta_{ij} \equiv \omega_i + \omega_{iL} - \omega_j - \omega_{jL}$. In this case we may neglect the fast oscillating second exponent in Eq. (C.9) and the $\mathbf{q}$ dependence in the denominator. The sum over the degrees of freedom $\mathbf{q}$ in Eq. (C.7) then becomes $\sum_{\mathbf{q}} \varphi_{\mathbf{q}}^{(3)}(\mathbf{r}) \varphi_{\mathbf{q}}^{(3)*}(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$ and we obtain the following expression for $\lambda_{n,n'}^{ij}$,

$$\lambda_{n,n'}^{ij}(t) = e^{i(\omega_i + \omega_n - \omega_j - \omega_{n'})t} \int d^3\mathbf{r} \varphi_n^{(i)*}(\mathbf{r}) \lambda^{ij}(\mathbf{r}, t) \varphi_{n'}^{(j)}(\mathbf{r}) \quad (\text{C.10})$$

where

$$\lambda^{ij}(\mathbf{r}, t) = -i \frac{\Omega_i^*(\mathbf{r}, t) \Omega_j(\mathbf{r}, t)}{\Delta_{j3}} e^{i[(\mathbf{k}_i - \mathbf{k}_j) \cdot \mathbf{r} - (\omega_{iL} - \omega_{jL})]t} \quad (\text{C.11})$$

Equation (C.6) can be derived from an effective Hamiltonian

$$H = \hbar \sum_{j=1,2} \sum_n (\omega_j + \omega_n) [c_n^{(j)}]^\dagger c_n^{(j)} + \sum_{i,j} \lambda^{ij}(\mathbf{r}, t) \psi_i^\dagger(\mathbf{r}) \psi_j(\mathbf{r}) \quad (\text{C.12})$$

The diagonal part ($i = j$) in the second term of this Hamiltonian serve as an effective potential created by the laser fields. The non-diagonal terms ($i \neq j$) are the terms responsible for transitions between the internal atomic states.

In order that the laser field will not have a significant effect on the state of the atoms in the trap we assume that the effective potential created by the laser field is much smaller than the separation between the energy levels in the trap, $\Omega_1^2/\Delta \ll \Delta\omega_n$. The final form of the coupling function $\lambda(\mathbf{r}, t)$ between levels $|1\rangle$

and $|2\rangle$ is then given by

$$\lambda(\mathbf{r}, t) = \bar{\lambda}(\mathbf{r}, t)e^{-i\Delta_\lambda t} \quad (\text{C.13})$$

where

$$\bar{\lambda}(\mathbf{r}, t) = \frac{\Omega_1^*(\mathbf{r}, t)\Omega_2(\mathbf{r}, t)}{\Delta} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}} \quad (\text{C.14})$$

is slowly varying in time and

$$\Delta_\lambda = \omega_{1L} - \omega_{2L} \quad (\text{C.15})$$

is the frequency difference between the two levels.

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