Matter Wave Detection and Phase Fluctuations in Bose-Einstein Condensates

By

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Abstract

Accepted analogies between matter waves and electromagnetic waves are extended in order to show that matter waves should have mechanical properties. A semiclassical description of the continuity equations describing these mechanical properties is presented and a general expression for their flux density is obtained.

A semiclassical detection theory for matter waves is developed, drawing upon the theory of photoelectron detection and the conservation equations from fluid mechanics. It is the intrinsically dispersive nature of matter waves which is important in deriving such a theory. It is shown that the detection rate can be related to the flux of particles through the detector surface.

A fully quantum matter wave detection theory is also presented, beginning from a microscopic description of detection. Both the short-time approximation to the detection rate and its long-time correction are developed. Again it is shown that the detection rate can be related to the flux through the detector surface.

The relative phase fluctuations of two one-dimensional condensates coupled along their whole length with a local single-atom interaction is examined. The thermal equilibrium is defined by the competition between independent longitudinal thermally excited phase fluctuations and the coupling between the condensates which locally favours identical phase. The relative phase fluctuations and their correlation length are computed as a function of the temperature and the strength of the coupling.

Finally, the future potential of the work contained herein is examined.

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Chapter 1

Introduction

1.1 Historical background

Although the wave theory of light has origins as far back as Robert Hooke in 1665, it was not until significantly after James Clerk Maxwell [1] proposed his theory of electromagnetic waves that this became a widely accepted truth. Indeed, Maxwell himself did not live to see the direct experimental verification of his theory performed by Heinrich Hertz in 1888. There are, however, many phenomena which could not at that time be explained by a wave theory of light. The archetypal example of such a phenomenon is that of the photoelectric effect, which involves incident light ionising a metal. In actual fact the semiclassical theory of light is sufficient to explain the photoelectric effect [2]. Arguably the crowning achievement of physics in the 20th century was the realisation of, among others, Max Planck, Niels Bohr and Albert Einstein, that energy is imparted to the electromagnetic field in discrete packets rather than continuously. These packets were dubbed "quanta" and quantum theory was born. This allowed the photoelectric effect to be suitably explained, as the energy of the ionised electrons depends not on the intensity of the light, as a wave theory would require, but on its frequency [3] via the equation $E = h\nu$. Here ν is the frequency of the light and $h = 6.626 \times 10^{-34}$ J.s is Planck's constant. The existence of seemingly contradicting phenomena such as the photoelectric effect and observation of properties such as interference which exemplifies the wave nature of light led to the concept of wave-particle duality.

In 1925, Louis de Broglie proposed that wave-particle duality is not a concept confined to light, but is a property of all matter. This means that, given the right conditions, matter will exhibit interference and diffraction as if it was a wave. The diffraction of electrons was indeed demonstrated shortly afterwards by Davisson and Germer [4] and George Thompson. The wave nature of matter can be quantified in the simple equation

$$\lambda = \frac{h}{p},\tag{1.1}$$

where p is the momentum of the particle in question and λ is the wavelength of the corresponding matter wave. Again we see that Planck's constant is the key. If x is some characteristic length scale of the measurement, then we do not see the wave nature of matter if

$$\frac{\lambda}{x} \ll 1, \tag{1.2}$$

that is

$$\frac{h}{xp} \ll 1. \tag{1.3}$$

Thus if xp is much larger than Planck's constant we do not observe the wave nature of the system. This is satisfied in macroscopic bodies and classical mechanics is applicable in these situations.

At around the same time as de Broglie formulated the wave theory of matter, Satyendra Bose developed a new way of deriving Planck's law of radiation from a black body, treating photons as a gas of indistinguishable particles. His paper [5] was rejected by a journal referee, but later published with support from Einstein. Upon reading Bose's work, Einstein realised that the statistical approach used in the derivation could be extended from photons to massive particles. He published two papers soon after [6, 7] which formulated what would later be known as Bose-Einstein statistics. This detailed a purely statistically derived condensation of particles into the ground state in the absence of interactions, which was later dubbed Bose-Einstein condensation. The first experimental evidence for this curious state of matter came from Fritz London whilst analysing liquid helium in its superfluid state. This evidence was difficult to verify due to the strong interactions between helium atoms, which leads to a low fraction of the atoms being condensed. It would be 70 years before Einstein's prediction would be fully experimentally verified in dilute gases of weakly interacting atoms [8, 9, 10].

1.2 Overview

This thesis will cover two disconnected topics in the field of matter waves and Bose-Einstein condensates (BECs). These are matter wave detection, in which we neglect interactions between atoms, and phase fluctuations in coupled BECs, in which interactions play an essential role.

In chapter 2 we show how particles are mathematically represented in both semiclassical and quantum theories. We also introduce Bose-Einstein condensates and explore some of their properties. Chapter 3 is concerned with physical conservation laws and their quantification in the form of continuity equations. We explore these laws in the context of both fluid mechanics and electromagnetism. In chapter 4 we introduce the concept of conservation of mechanical properties of matter waves, drawing analogy with the electromagnetic theory from the previous chapter. In chapter 5 we will derive a theory of matter wave detection in the semiclassical regime, based on the theory of photoelectric detection. The problem of linking the theory thus derived to the microscopic detection process will be dealt with in chapter 6 when we extend the detection theory into the quantum regime, starting from a microscopic model of detection. In chapter 7 we turn our attention to the BECs themselves. We will examine condensates which are sufficiently elongated as to be described as one-dimensional. Such objects are not pure condensates, but are known as quasi-condensates (QCs). We consider two QCs connected via a local coupling and predict what will happen to the fluctuations of their relative phase.

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Chapter 2

Particles

2.1 Wave mechanics

In quantum mechanics the state of a system at time t is represented by a vector $|\psi(t)\rangle$ and measurable quantities are represented by linear operators called observables. The possible outcomes of a measurement of an observable \hat{A} are given by its eigenvalues λ_A . The eigenvalues define the eigenstates $|\psi_{\lambda}\rangle$ of the system such that

$$\hat{A}|\psi_{\lambda}\rangle = \lambda_{A}|\psi_{\lambda}\rangle. \tag{2.1}$$

The basic mathematical formalism and manipulation of these objects is described in [11] and knowledge of this is assumed for this thesis.

2.1.1 The position representation

In classical mechanics the dynamics of any system can be described in terms of the canonical position and momentum, denoted q and p respectively. In particular, the dynamics of any two variables u and v are related by the Poisson bracket

$$[u,v]_P = \left\{ \frac{\partial u}{\partial q} \frac{\partial v}{\partial p} - \frac{\partial u}{\partial p} \frac{\partial v}{\partial q} \right\}.$$
 (2.2)

Dirac [11] showed that any two observables \hat{u} and \hat{v} in quantum mechanics could be related via the commutator - the quantum version of the Poisson bracket. This "quantum Poisson bracket" is related to the classical version via

$$[\hat{u}, \hat{v}] \equiv \hat{u}\hat{v} - \hat{v}\hat{u} = i\hbar [u, v]_P, \qquad (2.3)$$

where \hbar is Planck's constant. The simplest case is that where \hat{u} and \hat{v} correspond to the canonical position and momentum variables. In this case the Poisson bracket is equal to unity, and so the commutator is

$$[\hat{q}, \hat{p}] = i\hbar. \tag{2.4}$$

By comparing this with the commutator of q and $\partial/\partial q$, Dirac showed that there exists a representation (a way of expressing states as a function of eigenvalues of an observable) called the position representation, in which

$$\hat{p} \equiv -i\hbar \frac{\partial}{\partial q}.$$
(2.5)

In the following we will define the properties of the position representation.

We will turn our attention to the case of a single particle in one-dimensional space. In this case the canonical position and momentum reduce to the spatial position and momentum observables \hat{x} and \hat{p} . In the position representation, the state space is spanned by the eigenvectors $|x'\rangle$ of the position operator. This means that any state can be written as a linear combination of the eigenvectors. The eigenvectors of \hat{x} are delta function normalised, meaning that

$$\langle x|x'\rangle = \delta(x-x')$$
 (2.6)

where $\delta(x - x')$ is the Dirac delta function. The basis vectors obey the completeness relation, which states that

$$\int_{-\infty}^{\infty} \mathrm{d}x' |x'\rangle \langle x'| = \hat{1}, \qquad (2.7)$$

where $\hat{1}$ is the identity operator. We can use this to show how to write an arbitrary state in terms of the eigenvectors via the equation

$$|\psi(t)\rangle = \int_{-\infty}^{\infty} \mathrm{d}x' |x'\rangle \langle x'|\psi(t)\rangle.$$
(2.8)

The quantity $\langle x'|\psi(t)\rangle$ is an important quantity in the position representation of quantum mechanics. It is a complex valued function which we call the wavefunction. We denote it by

$$\psi(x,t) \equiv \langle x | \psi(t) \rangle \tag{2.9}$$

and it is interpreted as a measure of the probability density of finding the particle at position x at time t. In fact, as ψ can be complex valued, it cannot be a probability. It is the function $|\psi(x,t)|^2 dx$ which is the probability of finding the particle not at the distinct position x, but in an infinitesimal region $x \to x + dx$. The probability of finding the particle in some portion of space is the integral of $|\psi|^2$ over the region in question. Naturally, if we consider all space we must find the particle. We quantify this with the normalisation condition

$$\int_{-\infty}^{\infty} \mathrm{d}x \, |\psi(x,t)|^2 = 1. \tag{2.10}$$

This is equivalent to the normalisation of the state vectors themselves:

$$\langle \psi(x,t) | \psi(x,t) \rangle = 1. \tag{2.11}$$

We can show this by inserting the completeness relation (2.7) in between the vectors, giving

$$\int_{-\infty}^{\infty} \mathrm{d}x' \langle \psi(t) | x' \rangle \langle x' | \psi(t) \rangle,$$

which is equivalent to (2.10).

2.1.2 Expectation values

The probabilistic nature of quantum mechanics leads us to define the average value of an observable \hat{A} for a particular state. We call this the expectation value and denote it by

$$\langle \hat{A} \rangle \equiv \langle \psi(t) | \hat{A} | \psi(t) \rangle.$$
 (2.12)

To translate this into the position representation we insert completeness relations on the left and right of the operator

$$\begin{aligned} \langle \hat{A} \rangle &= \int_{-\infty}^{\infty} \mathrm{d}x' \int_{-\infty}^{\infty} \mathrm{d}x'' \langle \psi(t) | x' \rangle \langle x' | \hat{A} | x'' \rangle \langle x'' | \psi(t) \rangle \\ &= \int_{-\infty}^{\infty} \mathrm{d}x' \int_{-\infty}^{\infty} \mathrm{d}x'' \psi^*(x',t) \langle x' | \hat{A} | x'' \rangle \psi(x'',t). \end{aligned}$$
 (2.13)

In the case where \hat{A} is a function of \hat{x} alone, say $f(\hat{x})$, the quantity $\langle x'|\hat{A}|x''\rangle$ is given by

$$\langle x'|f(\hat{x})|x''\rangle = f(x'')\delta(x'-x'').$$
 (2.14)

When \hat{A} is simply \hat{p} , we use the position representation of \hat{p} (2.5) to show that

$$\langle x'|\hat{p}|x''\rangle = -i\hbar \frac{\partial}{\partial x''}\delta(x'-x'').$$
 (2.15)

Just as the delta function is defined as the limiting value of a Gaussian function, its derivative is defined as the limiting value of the derivative of a Gaussian function. Its definition only has meaning when used to manipulate integrals.

As a result of equation (2.15), if \hat{A} is any function $f(\hat{p})$ then we can write

$$\langle x'|f(\hat{p})|x''\rangle = f\left(-i\hbar\frac{\partial}{\partial x''}\right)\delta(x'-x'').$$
 (2.16)

We can use these results to calculate the expectation values of these particular

functions, with $\hat{A} = f(\hat{x})$ giving

$$\langle f(\hat{x}) \rangle = \int_{-\infty}^{\infty} \mathrm{d}x' \psi^*(x',t) f(x') \psi(x',t).$$
 (2.17)

In the case of $\hat{A} = f(\hat{p})$ we can show that

$$\langle f(\hat{p}) \rangle = \int_{-\infty}^{\infty} \mathrm{d}x' \int_{-\infty}^{\infty} \mathrm{d}x'' \psi^*(x',t) f\left(-i\hbar \frac{\partial}{\partial x''}\right) \delta(x'-x'') \psi(x'',t)$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x'' \psi^*(x'',t) f\left(-i\hbar \frac{\partial}{\partial x''}\right) \psi(x'',t),$$
(2.18)

where we have used integration by parts to obtain the last line.

2.1.3 Particle dynamics

Any quantum system represented by the state $|\psi(t)\rangle$ undergoes dynamics according to the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle.$$
 (2.19)

We have introduced here the observable \hat{H} which represents the total energy of the system in analogy with the Hamiltonian H in classical mechanics. For example, a particle of mass m in one-dimensional free space has a classical Hamiltonian given by

$$H = \frac{p^2}{2m},\tag{2.20}$$

where p is the momentum of the particle. The Hamiltonian operator in quantum mechanics for the same system is given by

$$\hat{H} = \frac{\hat{p}^2}{2m}.$$
 (2.21)

In the position representation we use the definition (2.5) to write (2.21) as

$$\hat{H} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \tag{2.22}$$

and thus the Schrödinger equation (2.19) becomes

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t).$$
(2.23)

In general a particle will be under the influence of a potential $V(\hat{x})$ and so (2.22) becomes

$$\hat{H} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x).$$
(2.24)

We can calculate the average total energy of the system by finding the expectation value of the Hamiltonian operator

$$\langle \hat{H} \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \psi^*(x,t) \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t).$$
 (2.25)

Upon using integration by parts and the fact that the wavefunction vanishes as $x \to \pm \infty$, we can rewrite the average energy as

$$\langle \hat{H} \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \left[\frac{-\hbar^2}{2m} \left| \frac{\partial}{\partial x} \psi(x,t) \right|^2 + V(x) \left| \psi(x,t) \right|^2 \right].$$
(2.26)

The formal solution to the Schrödinger equation (2.19), in the case where the Hamiltonian is not explicitly time-dependent, is given by

$$|\psi(t)\rangle = \exp\left[\frac{-i(t-t_0)\hat{H}}{\hbar}\right]|\psi(t_0)\rangle.$$
 (2.27)

Thus the average value of an operator \hat{A} is given by

$$\langle \hat{A} \rangle = \langle \psi(t_0) | \exp\left[\frac{i(t-t_0)\hat{H}}{\hbar}\right] \hat{A} \exp\left[\frac{-i(t-t_0)\hat{H}}{\hbar}\right] |\psi(t_0)\rangle.$$
 (2.28)

Instead of the states evolving in time and the operators staying constant, we may move to a picture in which the operators evolve and the states stay constant. The former is called the Schrödinger picture and the latter the Heisenberg picture. In the Heisenberg picture we define the states to be the initial Schrödinger picture states $|\psi(t_0)\rangle$. In order to maintain the average value of the operators, we must define the Heisenberg picture operators to be

$$\hat{A}_{H}(t) = \exp\left[\frac{i(t-t_{0})\hat{H}}{\hbar}\right]\hat{A}_{S}\exp\left[\frac{-i(t-t_{0})\hat{H}}{\hbar}\right],\qquad(2.29)$$

where \hat{A}_S is the Schrödinger picture operator. By taking the time derivative of (2.29) we obtain the Heisenberg equation of motion

$$i\hbar \frac{\mathrm{d}\hat{A}_{H}}{\mathrm{d}t} = \left[\hat{A}_{H}, \hat{H}\right] + \frac{\partial\hat{A}_{H}}{\partial t},\tag{2.30}$$

where we have defined the operator

$$\frac{\partial \hat{A}_H}{\partial t} = \exp\left[\frac{i(t-t_0)\hat{H}}{\hbar}\right]\frac{\partial \hat{A}_S}{\partial t}\exp\left[\frac{-i(t-t_0)\hat{H}}{\hbar}\right]$$
(2.31)

We see immediately that the Hamiltonian itself does not evolve.

2.1.4 More general systems

In the previous subsections we have shown the important features of representing a single particle system in wave mechanics. These features generalise to systems of N particles. The only change is that if we search the entire space we will find N particles, which changes the normalisation condition (2.10) to

$$\int_{-\infty}^{\infty} \mathrm{d}x \left|\psi(x,t)\right|^2 = N. \tag{2.32}$$

We may also generalise the system to represent particles in three-dimensional space. This is done by changing the spatial integrals from one-dimensional to three-dimensional

$$\int_{-\infty}^{\infty} \mathrm{d}x \to \int_{\mathrm{all space}} \mathrm{d}^3 r.$$

The position representation of the momentum operator also becomes threedimensional with

$$\hat{\boldsymbol{p}} = -i\hbar\nabla, \qquad (2.33)$$

where the vector ∇ is defined by

$$\nabla \equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right). \tag{2.34}$$

The Hamiltonian is then written as

$$\hat{H} = \frac{-\hbar^2}{2m} \nabla^2 + V(\boldsymbol{r}).$$
(2.35)

2.2 Second quantised formalism

In the semiclassical formalism, which we have used in the previous section, we treat the field in question as a complex number. In doing this we fix the number of particles being considered. The second quantised formalism takes into account the quantum nature of a field, introducing operators which annihilate and create particles and thereby allowing for situations in which the number of particles changes.

2.2.1 Bosons and fermions

The Heisenberg uncertainty principle implies that we cannot know, with arbitrary precision, both the position and momentum of a particle simultaneously. As a result of this we cannot in principle individually mark a number of identical particles, follow their dynamics and identify them at a later point. This is the principle of indistinguishability of identical particles. A direct consequence of this principle is that there are only two types of systems allowed. These are ones where the system wavefunction is unchanged when two constituent particles are interchanged, and those where the system wavefunction changes sign under this interchange. The former of these has a "symmetric" wavefunction and its particles are called bosons, whereas the latter has an "antisymmetric" wavefunction and the particles are called fermions. As a direct result of this no two fermions can occupy the same quantum state. This restriction is known as Pauli's exclusion principle. No such principle applies to bosons, so in principle any number of bosons may occupy the same quantum state. These distinct groups are also related to the spin of the particles, with bosons having integer spin and fermions having half-integer spin. Examples of bosons include photons and phonons, and of fermions include electrons and protons. We can also see that any particle made up of an even number of fermions is a boson, whereas a particle composed of an odd number of fermions is itself a fermion. This thesis is only concerned with bosons.

2.2.2 Occupation number representation

We consider here a system of N bosons which may be in any of the (appropriately normalised) single-particle states $|\psi_1\rangle, |\psi_2\rangle, \ldots$. The state of the system may be labelled in two different ways. We may use the N single-particle states, obtaining a state of the form

$$|\Psi\rangle = |\psi_i^{(1)}\rangle |\psi_j^{(2)}\rangle \dots |\psi_k^{(N)}\rangle, \qquad (2.36)$$

where the superscript is the particle number and some of the i, j, \ldots, k may be equal. One can immediately see a problem with this, in that such labelling implies particle distinguishability.

Instead, we write the state of the system in terms of the occupation number N_i of each of the states $|\psi_i\rangle$. This may be expressed in terms of a symmetric sum of all permutations of the i, j, \ldots, k in (2.36). The occupation number states are thus given by

$$|N_1, N_2, \dots, N_l, \dots\rangle = \left(\frac{N_1!N_2!\dots N_l!\dots}{N!}\right)^{1/2} \sum |\psi_i^{(1)}\rangle |\psi_j^{(2)}\rangle \dots |\psi_k^{(N)}\rangle (2.37)$$

where the sum is over all possible permutations of i, j, \ldots, k which preserve

the occupation numbers.

We introduce the annihilation operator \hat{a}_i which decreases the number of particles in state *i* by one and multiplies the state by N_i , the initial number of particles in state *i*. Its Hermitian conjugate operator is the creation operator \hat{a}_i^{\dagger} , which increases the number of particles in state *i* by one and multiplies the state by $N_i + 1$, the final number of particles in state *i*. We quantify this via the equations

$$\hat{a}_i|N_1, N_2, \dots, N_i, \dots\rangle = \sqrt{N_i}|N_1, N_2, \dots, N_i - 1, \dots\rangle$$
(2.38)

$$\hat{a}_{i}^{\dagger}|N_{1}, N_{2}, \dots, N_{i}, \dots\rangle = \sqrt{N_{i} + 1}|N_{1}, N_{2}, \dots, N_{i} + 1, \dots\rangle.$$
 (2.39)

The factor $\sqrt{N_i}$ in (2.38) acts to ensure that the annihilation operator cannot reduce the occupation number of a state to less than zero.

We see that acting the annihilation operator followed by the creation operator leaves the total number of particles unchanged and multiplies the state by the number of particles initially in the state i:

$$\hat{a}_i^{\dagger} \hat{a}_i | N_1, N_2, \dots, N_i, \dots \rangle = N_i | N_1, N_2, \dots, N_i, \dots \rangle.$$

$$(2.40)$$

This combination of operators is known as the number operator and is given the notation \hat{N}_i . The total number operator is the sum of all of the individual number operators:

$$\hat{N} = \sum_{i=1}^{\infty} \hat{N}_i.$$
 (2.41)

We note that the annihilation and creation operators do not commute, since reversing the action involved in the number operator gives

$$\hat{a}_i \hat{a}_i^{\dagger} | N_1, N_2, \dots, N_i, \dots \rangle = (N_i + 1) | N_1, N_2, \dots, N_i, \dots \rangle.$$
 (2.42)

Also we can see that creation and annihilation operators which act on different states will always commute, and so we may write the general commutation relation in the form

$$\left[\hat{a}_{i}, \hat{a}_{j}^{\dagger}\right] = \delta_{ij}, \qquad (2.43)$$

where δ_{ij} is the Krönecker delta which is unity if i = j and zero otherwise.

It may be shown that any operator \hat{A} , which only acts on one particle at a time, can be written in terms of the annihilation and creation operators, via

$$\hat{A}_1 = \sum_{i,j} \langle \psi_i | \hat{A} | \psi_j \rangle \hat{a}_i^{\dagger} \hat{a}_j.$$
(2.44)

This can be generalised to operators which act on more than one particle at a time, so long as the operator is symmetrical with respect to all of the particles. For example a symmetrical two-particle operator may be expressed as

$$\hat{A}_2 = \frac{1}{2} \sum_{i,j,k,l} \langle \psi_i | \langle \psi_j | \hat{A} | \psi_k \rangle | \psi_l \rangle \hat{a}_i^{\dagger} \hat{a}_j^{\dagger} \hat{a}_k \hat{a}_l.$$
(2.45)

2.2.3 Field operators

Another way of expressing the second quantised formalism is via bosonic field operators which are expressed as functions of spatial position. We define these via

$$\hat{\psi}(\mathbf{r}) = \sum_{i=1}^{\infty} \langle \mathbf{r} | \psi_i \rangle \hat{a}_i$$
$$\hat{\psi}^{\dagger}(\mathbf{r}) = \sum_{i=1}^{\infty} \langle \mathbf{r} | \psi_i \rangle \hat{a}_i^{\dagger}. \qquad (2.46)$$

These field operators do not depend on the particular basis which was chosen to represent the one-particle states. Their commutators can easily be found by

$$ig[\hat{\psi}(m{r}),\hat{\psi}^{\dagger}(m{r}')ig] = \sum_{i,j}^{\infty} \langlem{r}|\psi_i
angle \langle\psi_j|m{r}'
angle \left[\hat{a}_i,\hat{a}_j^{\dagger}
ight]$$

$$= \sum_{i=1}^{\infty} \langle \boldsymbol{r} | \psi_i \rangle \langle \psi_i | \boldsymbol{r}' \rangle$$

= $\langle \boldsymbol{r} | \boldsymbol{r}' \rangle$
= $\delta(\boldsymbol{r} - \boldsymbol{r}'),$ (2.47)

where, in going from the second to the third line, we used the completeness relation for discrete states

$$\sum_{i=1}^{\infty} |\psi_i\rangle \langle \psi_i| = \hat{1}.$$
(2.48)

We may express the total number operator (2.41) in terms of the field operators via the equation

$$\hat{N} = \int_{-\infty}^{\infty} \mathrm{d}^3 r \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r})$$
(2.49)

which gives the interpretation of $\hat{\psi}^{\dagger}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})$ as the number density operator.

The interpretation of the field operator may be shown by considering its action on the zero particle state $|0\rangle$. After the field operator acts on the zero particle state, we can show that the action of the total number operator on the resulting state produced gives

$$\hat{N}\hat{\psi}^{\dagger}(\boldsymbol{r})|0\rangle = \int_{-\infty}^{\infty} d^{3}\boldsymbol{r}'\hat{\psi}^{\dagger}(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r}')\hat{\psi}^{\dagger}(\boldsymbol{r})|0\rangle
= \int_{-\infty}^{\infty} d^{3}\boldsymbol{r}'\hat{\psi}^{\dagger}(\boldsymbol{r}')\left\{\hat{\psi}^{\dagger}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}') + \delta(\boldsymbol{r}-\boldsymbol{r}')\right\}|0\rangle
= \hat{\psi}^{\dagger}(\boldsymbol{r})|0\rangle,$$
(2.50)

which shows that $\hat{\psi}^{\dagger}(\boldsymbol{r})|0\rangle$ is a one-particle state. We consider the probability amplitude for finding the particle in the state $\hat{\psi}^{\dagger}(\boldsymbol{r})|0\rangle$ at the position \boldsymbol{r}' , which is given by

$$\begin{aligned} \langle \boldsymbol{r}' | \hat{\psi}^{\dagger}(\boldsymbol{r}) | 0 \rangle &= \sum_{i=1}^{\infty} \langle \boldsymbol{r}' | \psi_i \rangle \langle \psi_i | \hat{\psi}^{\dagger}(\boldsymbol{r}) | 0 \rangle \\ &= \sum_{i=1}^{\infty} \langle \boldsymbol{r}' | \psi_i \rangle \langle 0 | \hat{a}_i \hat{\psi}^{\dagger}(\boldsymbol{r}) | 0 \rangle \end{aligned}$$

$$= \langle 0 | \hat{\psi}(\mathbf{r}') \hat{\psi}^{\dagger}(\mathbf{r}) | 0 \rangle$$

= $\delta(\mathbf{r} - \mathbf{r}').$ (2.51)

This shows that the particle in the single-particle state $\hat{\psi}^{\dagger}(\mathbf{r})|0\rangle$ is localised at \mathbf{r} . Thus the action of $\hat{\psi}^{\dagger}(\mathbf{r})$ is to create a single particle which is localised at \mathbf{r} .

The representation of operators in terms of the field operators is calculated by assuming knowledge of the position representation of the operator \hat{A} and calculating

$$\langle N_1, N_2, \dots, N_k, \dots | \hat{A} | N_1, N_2, \dots, N_k, \dots \rangle.$$
 (2.52)

The result for an operator which is a sum of single-particle operators

$$\hat{A} = \sum_{i=1}^{N} \hat{f}(\boldsymbol{r}_i)$$
(2.53)

is given by

$$\hat{A} = \int_{-\infty}^{\infty} \mathrm{d}^3 r \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{f}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}).$$
(2.54)

In general, as in the case of the Hamiltonian, \hat{f} may depend on the momentum of the particle as well, in which case the position representation of the momentum operator (2.5) is used.

The Hamiltonian is an example of an operator which is a sum of singleparticle operators. For a many particle system, the Hamiltonian in the case of a system under the influence of a potential $\hat{V}(x)$ is given by

$$\hat{H} = \sum_{i=1}^{N} \left[\frac{-\hbar^2}{2m} \nabla_i^2 + V(\boldsymbol{r}_i) \right].$$
(2.55)

The occupation number representation of this Hamiltonian may thus be ex-

pressed, using (2.54), as

$$\hat{H} = \int \mathrm{d}^3 r \left[\frac{-\hbar^2}{2m} \hat{\psi}^{\dagger}(\boldsymbol{r}) \nabla^2 \hat{\psi}(\boldsymbol{r}) + \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{V}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) \right].$$
(2.56)

If we integrate by parts and use the fact that the field operator vanishes as $r \to \pm \infty$, we obtain the equivalent form

$$\hat{H} = \int d^3r \left[\frac{\hbar^2}{2m} \nabla \hat{\psi}^{\dagger}(\boldsymbol{r}) \cdot \nabla \hat{\psi}(\boldsymbol{r}) + \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{V}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) \right].$$
(2.57)

In general the potential \hat{V} may contain nonlinearities.

2.3 Bose-Einstein condensates

Since bosons are not restricted in the number of particles which can occupy a single quantum state, it is conceivable that in a gas of bosons a macroscopic number of particles could occupy a single state. This is well known in the case of photons; it occurs in laser light where below threshold many modes are occupied, but above threshold a single mode is occupied. By analogy a similar situation must occur with massive bosons. This phenomenon is known as Bose-Einstein condensation.

To achieve Bose-Einstein condensation with a dilute gas of weakly interacting atomic bosons requires extremely low temperatures, such that the de Broglie wavelength of the particles become larger than their mean spacing. These extreme conditions make it very difficult to create a Bose-Einstein condensate (BEC) and it was not until very recently that BEC was experimentally realised in these systems [8, 9, 10] using bosonic isotopes of Rb, Na and Li. A BEC is created by cooling the atoms using optical and magnetic forces, and then cooling them again using one of a number of techniques. The BEC is then held in a magnetic trap, which is switched off after a period of time in order that the atoms may be detected. There are several techniques for detection, including shadow imaging, which is used to calculate the density of the BEC, and microchannel plate detection, which analyses the time-of-flight of the condensate atoms.

In order to model a BEC we must take account of the interactions between the particles in the system. Due to the diluteness of the gas involved in creating a BEC the only interactions which have an appreciable effect on the system are two body ones. Scattering theory tells us that the strength of the interaction between two low energy particles of mass m is given by

$$U_0 = \frac{4\pi\hbar^2 a}{m}.$$
 (2.58)

Here a is the s-wave scattering length of the particles, which in the scattering theory of collisions gives the amplitude of the scattered wavefunction in the limit of low energy, spherically symmetric collisions [12]. In the position representation the interaction potential between two particles positioned at r and r' is therefore given by

$$U(\boldsymbol{r}, \boldsymbol{r}') = U_0 \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{2.59}$$

2.3.1 Mean-field theory

In mean-field theory we consider a fully condensed system, that is one in which all of the bosons are in the same single particle state. We write this single particle state using the wavefunction $\psi_0(\mathbf{r})$, which is normalised to unity. The full system wavefunction is then the product of all of the single particle states. Thus if there are N bosons, the wavefunction is

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_N) = \prod_{i=1}^N \psi_0(\boldsymbol{r}_i), \qquad (2.60)$$

where \mathbf{r}_i are the positions variables of the *i*-th single particle system. The generalisation of the average value of an operator $\hat{A} = f(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2, \dots, \hat{\mathbf{r}}_N)$ in the position representation to a system of N identical particles is given by

$$\langle \hat{A} \rangle = \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \cdots \int \mathrm{d}^3 r_N \psi^*(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_N) f(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_N) \psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_N).$$
(2.61)

A similar generalisation occurs for $\hat{A} = f(\hat{p}_1, \hat{p}_2, \dots, \hat{p}_N)$.

When the interaction potential given by (2.59) is included in the formalism, the position representation Hamiltonian is given by

$$\hat{H} = \sum_{i=1}^{N} \left[\frac{-\hbar^2}{2m} \nabla_i^2 + V(\boldsymbol{r}_i) \right] + \frac{U_0}{2} \sum_{i \neq j; i, j=1}^{N} \delta(\boldsymbol{r}_i - \boldsymbol{r}_j).$$
(2.62)

We may therefore write the average total energy of the system as

$$\langle \hat{H} \rangle = \int \mathrm{d}^{3} r_{1} \cdots \int \mathrm{d}^{3} r_{N} \sum_{k=1}^{N} \left\{ \left[\prod_{i \neq k; i=1}^{N} \psi_{0}^{*}(\boldsymbol{r}_{i}) \right] \left[\prod_{j \neq k; j=1}^{N} \psi_{0}(\boldsymbol{r}_{j}) \right] \right.$$

$$\left. \left[\frac{\hbar^{2}}{2m} \left| \nabla_{k} \psi_{0}(\boldsymbol{r}_{k}) \right|^{2} + V(\boldsymbol{r}_{k}) \left| \psi_{0}(\boldsymbol{r}_{k}) \right|^{2} \right] \right.$$

$$+ \sum_{l \neq k; l=1}^{N} \left[\prod_{i \neq k, l; i=1}^{N} \psi_{0}^{*}(\boldsymbol{r}_{i}) \right] \left[\prod_{j \neq k, l; j=1}^{N} \psi_{0}(\boldsymbol{r}_{j}) \right]$$

$$\left. \frac{U_{0}}{2} \delta(\boldsymbol{r}_{k} - \boldsymbol{r}_{l}) \left| \psi_{0}(\boldsymbol{r}_{k}) \right|^{2} \left| \psi_{0}(\boldsymbol{r}_{l}) \right|^{2} \right\}.$$

$$(2.63)$$

Upon using the fact that the ψ_0 form an orthonormal set of functions, that is

$$\int \mathrm{d}^3 r_i \psi_0^*(\boldsymbol{r}_j) \psi_0(\boldsymbol{r}_k) = \delta_{ij} \delta_{ik}, \qquad (2.64)$$

we obtain the result

$$E \equiv \langle \hat{H} \rangle = N \int \mathrm{d}^3 r \left[\frac{\hbar^2}{2m} |\nabla \psi_0(\boldsymbol{r})|^2 + V(\boldsymbol{r}) |\psi_0(\boldsymbol{r})|^2 + \frac{N-1}{2} U_0 |\psi_0(\boldsymbol{r})|^4 \right].$$
(2.65)

We introduce the condensed state wavefunction

$$\psi(\boldsymbol{r}) = \sqrt{N}\psi_0(\boldsymbol{r}) \tag{2.66}$$

which differs from the system wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ in that it is an *N*-particle wavefunction rather than a product of single-particle wavefunctions. In a system consisting of a large number of bosons, so that $N(N-1) \simeq N^2$, the average energy of the system (2.65) may be approximated to be

$$E \simeq \int \mathrm{d}^3 r \left[\frac{\hbar^2}{2m} \left| \nabla \psi(\boldsymbol{r}) \right|^2 + V(\boldsymbol{r}) \left| \psi(\boldsymbol{r}) \right|^2 + \frac{U_0}{2} \left| \psi(\boldsymbol{r}) \right|^4 \right].$$
(2.67)

In order to find the form of ψ which minimises the energy, we use the action principle of classical mechanics

$$\delta \int_{t_1}^{t_2} \mathrm{d}t L = 0 \tag{2.68}$$

where L is the Lagrangian. In a general system with canonical position variables q_i and corresponding canonical momenta p_i , the Lagrangian is related to the Hamiltonian via the equation

$$L(\{q_i\}, \{\dot{q}_i\}, t) = \sum_i \dot{q}_i p_i - H(\{q_i\}, \{\dot{q}_i\}, t),$$
(2.69)

where $\dot{q} = \partial q / \partial t$. In our case the Hamiltonian is given by (2.67) and thus the Lagrangian is

$$L = \int d^3 r \frac{i\hbar}{2} \left[\psi^*(\mathbf{r}, t) \frac{\partial}{\partial t} \psi(\mathbf{r}, t) - \psi(\mathbf{r}, t) \frac{\partial}{\partial t} \psi^*(\mathbf{r}, t) \right] - E.$$
 (2.70)

In general, if a function J has an integral representation in the form

$$J = \int \mathrm{d}t f(q, \dot{q}, t), \qquad (2.71)$$

then J is minimised if the Euler-Lagrange equation

$$\frac{\partial f}{\partial q} - \frac{d}{dt} \left(\frac{\partial f}{\partial \dot{q}} \right) = 0 \tag{2.72}$$

holds. In our case $f \equiv L$, which is a functional of ψ and ψ^* . Thus instead of partial derivatives in the Euler-Lagrange equation we need to use functional

derivatives. Our Euler-Lagrange equation therefore becomes

$$\frac{\delta L}{\delta \psi^*} - \frac{\partial}{\partial t} \left(\frac{\delta L}{\delta \dot{\psi}^*} \right) = 0.$$
(2.73)

The functional derivative is defined as

$$\frac{\delta F[f(x)]}{\delta f(y)} = \lim_{\epsilon \to 0} \frac{F[f(x) + \epsilon \delta(x - y)] - F[f(x)]}{\epsilon}$$
(2.74)

and if we substitute (2.70) into (2.73) using this definition, we obtain the time-dependent Gross-Pitaevskii equation

$$i\hbar \frac{\partial \psi(\boldsymbol{r},t)}{\partial t} = \left[\frac{-\hbar^2}{2m} \nabla^2 + V(\boldsymbol{r}) + U_0 \left|\psi(\boldsymbol{r},t)\right|^2\right] \psi(\boldsymbol{r},t).$$
(2.75)

In the case of a stationary wavefunction, where the number of particles takes a constant value

$$N = \int_{-\infty}^{\infty} \mathrm{d}^3 r |\psi(\mathbf{r}, t)|^2, \qquad (2.76)$$

the quantity we seek to minimise is the grand canonical energy, given by

$$E' = E - \mu N. \tag{2.77}$$

Here μ is the chemical potential, the energy required to add a particle to the condensate. We do this by setting the functional derivative of equation (2.77) with respect to the condensate wavefunction to be zero, so

$$\frac{\delta E'}{\delta \psi^*} = 0. \tag{2.78}$$

This results in the time independent Gross-Pitaevskii equation

$$\mu\psi(\mathbf{r}) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + U_0 \left|\psi(\mathbf{r},t)\right|^2\right]\psi(\mathbf{r},t).$$
(2.79)

The two types of Gross-Pitaevskii equation can also be obtained by considering the second quantised operator representing the field to consist of small fluctuations about the mean field value. The lowest order expansion in the fluctuations gives the time-dependent Gross-Pitaevskii as we will show in the next subsection.

2.3.2 Second quantised theory

In section 2.2 we showed that a single particle operator may be written in the second quantised form (2.54). We may also show that an operator which is a sum of symmetric two-particle operators

$$\hat{A} = \frac{1}{2} \sum_{i \neq j} \hat{U}(\boldsymbol{r}_i, \boldsymbol{r}_j)$$
(2.80)

may be written as

$$\hat{A} = \frac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}^3 r \int_{-\infty}^{\infty} \mathrm{d}^3 r' \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{\psi}^{\dagger}(\boldsymbol{r}') \hat{U}(\boldsymbol{r}, \boldsymbol{r}') \hat{\psi}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}').$$
(2.81)

The interparticle interactions in a BEC are described in the position representation via equations (2.58) and (2.59). This two-particle potential is clearly symmetric with respect to the particles involved. The Hamiltonian for the system then becomes

$$\hat{H} = \int_{-\infty}^{\infty} \mathrm{d}^{3} r \left[\frac{-\hbar^{2}}{2m} \hat{\psi}^{\dagger}(\boldsymbol{r}) \nabla^{2} \hat{\psi}(\boldsymbol{r}) + \hat{\psi}^{\dagger}(\boldsymbol{r}) V(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) \right. \\ \left. + \frac{1}{2} U_{0} \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) \right]$$
(2.82)

We may express the Heisenberg equation of motion for the field operator $\hat{\psi}$ as

$$i\hbar \frac{\partial \hat{\psi}(\boldsymbol{r},t)}{\partial t} = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) + U_0 \hat{\psi}^{\dagger}(\boldsymbol{r},t) \hat{\psi}(\boldsymbol{r},t)\right] \hat{\psi}(\boldsymbol{r},t).$$
(2.83)

We consider here a system in which almost all of the particles are in the same (condensed) state. Thus we write the field annihilation operator as the sum of the condensate wavefunction and an annihilation operator for the

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fluctuations about this state:

$$\hat{\psi}(\boldsymbol{r},t) = \psi(\boldsymbol{r},t) + \delta \hat{\psi}(\boldsymbol{r},t)$$
 (2.84)

If we assume these fluctuations to be negligible, then we arrive at the time dependent Gross-Pitaevskii equation

$$i\hbar \frac{\partial \psi(\boldsymbol{r},t)}{\partial t} = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) + U_0 \left|\psi(\boldsymbol{r},t)\right|^2\right] \psi(\boldsymbol{r},t).$$
(2.85)

If instead of assuming the fluctuations to be negligible we assume them to be finite but small, then we obtain the spectrum of elementary excitations of the BEC.

2.3.3 Elementary excitations

This calculation was first performed by Bogoliubov [13] and we will outline it in this subsection. To simplify matters we consider the condensate to be confined to a box of volume V. From the theory of waves we know that the allowable wavenumbers for the wavefunction will be

$$k = \frac{n\pi}{V^{1/3}},\tag{2.86}$$

where n is any integer. We can treat each of these wavenumbers as a mode of the matter wave field and can therefore expand the field operators in terms of creation and annihilation operators for these modes. This yields the expressions

$$\hat{\psi}(\boldsymbol{r},t) = \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{V}} \hat{a}_{k}(t) \exp(i\boldsymbol{k}\cdot\boldsymbol{r})$$
$$\hat{\psi}^{\dagger}(\boldsymbol{r},t) = \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{V}} \hat{a}_{k}^{\dagger}(t) \exp(-i\boldsymbol{k}\cdot\boldsymbol{r}), \qquad (2.87)$$

where \hat{a}_k and \hat{a}_k^{\dagger} obey the equal time bosonic commutation relations

$$\left[\hat{a}_{k}(t), \hat{a}_{k'}^{\dagger}(t)\right] = \delta_{k,k'}.$$
(2.88)

The assumption that we make is that the interactions are weak. If there was no interaction, all of the particles would be in the zero momentum state and the total number of particles $\hat{N} = \sum_k \hat{a}_k^{\dagger} \hat{a}_k$ would be equal to the number of particles in the ground state $\hat{N}_0 = \hat{a}_0^{\dagger} \hat{a}_0$. Thus we write the condensate wavefunction as the zero momentum state in the sums (2.87). This will mean that we treat the mode operator \hat{a}_0 as a classical field a_0 with $|a_0|^2 = N_0$. The condensate wavefunction is written

$$\psi(\mathbf{r},t) = \frac{a_0(t)}{\sqrt{V}} \tag{2.89}$$

and the field operators are

$$\hat{\psi}(\boldsymbol{r},t) = \frac{1}{\sqrt{V}} \left[a_0(t) + \hat{\theta}(\boldsymbol{r},t) \right], \qquad (2.90)$$

where

$$\hat{\theta}(\boldsymbol{r},t) = \sum_{k\neq 0,k=-\infty}^{\infty} \hat{a}_k(t) \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) \equiv \sqrt{V}\delta\hat{\psi}(\boldsymbol{r},t).$$
(2.91)

The assumption of weak interactions is thus equivalent to treating $\hat{\theta}$ as a small quantity. We expand the evolution equation (2.83) to first order, assuming that there is no external potential. Upon inserting the expansion (2.90) into the evolution equation (2.83), we obtain

$$i\hbar\left[\frac{\partial a_0}{\partial t} + \frac{\partial\hat{\theta}}{\partial t}\right] = \frac{-\hbar^2}{2m}\nabla^2\hat{\theta} + \frac{U_0}{V}\left[|a_0|^2a_0 + 2|a_0|^2\hat{\theta} + a_0^2\hat{\theta}^\dagger\right],\qquad(2.92)$$

where we have neglected terms of greater than first order in $\hat{\theta}$. The time dependent Gross-Pitaevskii equation (2.75) for the condensate wavefunction (2.89) in the absence of an external potential is simply

$$i\hbar\frac{\partial a_0}{\partial t} = \frac{N_0 U_0}{V} a_0. \tag{2.93}$$

This means that to the lowest order in this calculation the condensate wavefunction rotates at frequency $N_0U_0/(V\hbar)$. We transform to a new frame

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rotating at this frequency by defining

$$\hat{a}_k(t) = \hat{b}_k(t) \exp\left(\frac{-iN_0U_0t}{V\hbar}\right); \qquad a_0(t) = b \exp\left(\frac{-iN_0U_0t}{V\hbar}\right).$$
(2.94)

In this new frame the evolution equation (2.92) becomes

$$i\hbar \sum_{\substack{k\neq 0; k=-\infty}}^{\infty} \frac{\partial \hat{b}_k}{\partial t} \exp(i\mathbf{k} \cdot \mathbf{r}) = \sum_{\substack{k\neq 0; k=-\infty}}^{\infty} \left\{ \left[\frac{\hbar^2 k^2}{2m} + \frac{N_0 U_0}{V} \right] \hat{b}_k \exp(i\mathbf{k} \cdot \mathbf{r}) + \frac{b^2 U_0}{V} \hat{b}_k^{\dagger} \exp(-i\mathbf{k} \cdot \mathbf{r}) \right\}.$$
(2.95)

The last term in the sum may be written in an equivalent form by taking $k \to -k$, and so we can remove the sum and the common phase factor and obtain

$$i\hbar\frac{\partial\hat{b}_{k}}{\partial t} = \left[\frac{\hbar^{2}k^{2}}{2m} + \frac{N_{0}}{V}U_{0}\right]\hat{b}_{k} + \frac{b^{2}}{V}U_{0}\hat{b}_{-k}^{\dagger}.$$
 (2.96)

A similar equation can be derived for the complex conjugate by taking the conjugate of (2.83). The resulting relation is

$$-i\hbar\frac{\partial\hat{b}_{-k}^{\dagger}}{\partial t} = \left[\frac{\hbar^2k^2}{2m} + \frac{N_0}{V}U_0\right]\hat{b}_{-k}^{\dagger} + \frac{b^2}{V}U_0\hat{b}_k, \qquad (2.97)$$

which together with the previous equation form a pair of coupled evolution equations for the mode operators. If we calculate the Hamiltonian to second order, which is the same approximation used in the above calculation, we obtain

$$\hat{H} = \frac{N_0^2}{2V} + \sum_{k \neq 0} \left\{ \left[\frac{\hbar^2 k^2}{2m} + \frac{2N_0}{V} \right] \hat{b}_k^{\dagger} \hat{b}_k + \frac{1}{2V} \left[b^2 \hat{b}_k^{\dagger} \hat{b}_{-k}^{\dagger} + b^{*2} \hat{b}_k \hat{b}_{-k} \right] \right\}.$$
 (2.98)

The existence of the double annihilation and double creation terms in the Hamiltonian is due to the interaction between bosons. In order to find the elementary excitations we would like to remove the coupling terms from the Hamiltonian. This is done by performing a transformation

$$\hat{b}_k = u_k \hat{\xi}_k + v_k^* \hat{\xi}_{-k}^\dagger \qquad ; \qquad \hat{b}_{-k}^\dagger = u_k^* \hat{\xi}_{-k}^\dagger + v_k \hat{\xi}_k$$
 (2.99)

to new operators $\hat{\xi}_k$ and $\hat{\xi}_{-k}^{\dagger}$, where the u_k and v_k depend only on the magnitude of k. The inverse transformation is given by

$$\hat{\xi}_{k} = \frac{u_{k}^{*}\hat{b}_{k} - v_{k}^{*}\hat{b}_{-k}^{\dagger}}{|u_{k}|^{2} - |v_{k}|^{2}} \qquad ; \qquad \hat{\xi}_{-k}^{\dagger} = \frac{u_{k}\hat{b}_{-k}^{\dagger} - v_{k}\hat{b}_{k}}{|u_{k}|^{2} - |v_{k}|^{2}}, \qquad (2.100)$$

and we use this to calculate the commutation relations between $\hat{\xi}_k$ and its conjugate. This is given by

$$\left[\hat{\xi}_{k}, \hat{\xi}_{k'}^{\dagger}\right] = \frac{\delta_{k,k'}}{|u_{k}|^{2} - |v_{k}|^{2}},\tag{2.101}$$

and if we restrict the transformation to $|u_k|^2 - |v_k|^2 = 1$ then the operator $\hat{\xi}_k$ is a bosonic annihilation operator. We may write the transformation in the equivalent form (aside from a phase factor)

$$\hat{b}_{k} = \frac{\hat{\xi}_{k} + L_{k}\hat{\xi}_{-k}^{\dagger}}{\sqrt{1 - |L_{k}|^{2}}} \quad ; \quad \hat{b}_{-k}^{\dagger} = \frac{\hat{\xi}_{-k}^{\dagger} + L_{k}^{*}\hat{\xi}_{k}}{\sqrt{1 - |L_{k}|^{2}}}, \quad (2.102)$$

where

$$L_k = \frac{v_k^*}{u_k}.\tag{2.103}$$

The $\hat{\xi}_k$ give the elementary excitations of the system. We call these operators "quasi-particle" operators, as their spectrum is the same as that for a system of non-interacting particles as we will now show.

In order to decouple the evolution equations (2.96) and (2.97) we simply find the value for L_k which removes the coupling terms. Upon substituting (2.102) into the coupled evolution equations we obtain

$$i\hbar\left[\frac{\partial\hat{\xi}_{k}}{\partial t}+L_{k}\frac{\partial\hat{\xi}_{-k}^{\dagger}}{\partial t}\right] = \left[\frac{\hbar^{2}k^{2}}{2m}+\frac{N_{0}U_{0}}{V}\right]\left[\hat{\xi}_{k}+L_{k}\hat{\xi}_{-k}^{\dagger}\right]$$

$$-i\hbar \left[\frac{\partial \hat{\xi}_{-k}^{\dagger}}{\partial t} + L_{k}^{*} \frac{\partial \hat{\xi}_{k}}{\partial t} \right] = \left[\frac{\hbar^{2} k^{2}}{2m} + \frac{N_{0} U_{0}}{V} \right] \left[\hat{\xi}_{-k}^{\dagger} + L_{k}^{*} \hat{\xi}_{k} \right] \\ + \frac{b^{\dagger 2} U_{0}}{V} \left[\hat{\xi}_{k} + L_{k} \hat{\xi}_{-k}^{\dagger} \right].$$
(2.104)

Next we multiply the second equation by L_k and add the equations so

$$i\hbar\frac{\partial\hat{\xi}_{k}}{\partial t}\left(1-|L_{k}|^{2}\right) = \hat{\xi}_{k}\left\{\left[|L_{k}|^{2}+1\right]\left[\frac{\hbar^{2}k^{2}}{2m}+\frac{N_{0}U_{0}}{V}\right]+\frac{U_{0}}{V}\left[b^{2}L_{k}^{*}+b^{\dagger 2}L_{k}\right]\right\} + \hat{\xi}_{-k}^{\dagger}\left\{2L_{k}\left[\frac{\hbar^{2}k^{2}}{2m}+\frac{N_{0}U_{0}}{V}\right]+\frac{U_{0}}{V}\left[b^{2}+b^{\dagger 2}L_{k}^{2}\right]\right\}.$$
 (2.105)

If we are to decouple the evolution equations for $\hat{\xi}_k$ and $\hat{\xi}_{-k}^{\dagger}$ then the term proportional to $\hat{\xi}_{-k}^{\dagger}$ in (2.105) must vanish, i.e.

$$\frac{U_0}{V}b^{\dagger 2}L_k^2 + 2\left[\frac{\hbar^2k^2}{2m} + \frac{N_0U_0}{V}\right]L_k + \frac{U_0}{V}b^2 = 0, \qquad (2.106)$$

which is achieved by setting

$$L_{k} = \frac{Vb^{2}}{N_{0}^{2}U_{0}} \left[E(k) - \frac{\hbar^{2}k^{2}}{2m} - \frac{N_{0}}{V}U_{0} \right].$$
(2.107)

Here we have defined

$$E(k) = \sqrt{\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + \frac{2N_0}{V}U_0\right)}.$$
 (2.108)

The decoupled equations are thus written

$$i\hbar \frac{\partial \hat{\xi}_{k}}{\partial t} = E(k)\hat{\xi}_{k}$$
$$-i\hbar \frac{\partial \hat{\xi}_{-k}^{\dagger}}{\partial t} = E(k)\hat{\xi}_{-k}^{\dagger}. \qquad (2.109)$$

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Upon substituting the value for L_k (2.107) into (2.98) we obtain

$$\hat{H} = H_0 + \sum_{k \neq 0} E(k) \hat{\xi}_k^{\dagger} \hat{\xi}_k, \qquad (2.110)$$

where

$$H_0 = \frac{U_0 N^2}{2V} + \frac{1}{2} \sum_{k \neq 0} \left[E(k) - \frac{\hbar^2 k^2}{2m} - \frac{N_0}{V} U_0 \right].$$
(2.111)

Thus the transformation (2.102) acts to diagonalise the Hamiltonian. This shows that in this approximation, the total energy is the ground state energy H_0 plus the individual energies of each of the quasi-particles, whose annihilation operators are simply $\hat{\xi}_k$. The fact that this is diagonal in $\hat{\xi}_k^{\dagger}\hat{\xi}_k$ shows that these quasi-particles do not interact to this level of approximation. One can extend the approximation to the next level and show weak interaction between the quasi-particles [13], but this is not considered further here.

In chapter 7 we will show how the Bogoliubov theory considered here may be modified to describe elementary excitations in a one-dimensional quasicondensate, where there is no single macroscopically occupied ground state. A quasi-condensate is a gas of bosons which experiences macroscopic phase fluctuations but only very small density fluctuations.
Chapter 3

Conservation laws and continuity equations

3.1 Fluid mechanics

Conserved quantities are of great interest in physics. They allow us to distinguish between processes which are physical and those which are not. For example, consider the total amount of matter in the universe. This must remain constant. A global conservation law like this is incomplete since it is possible to satisfy it with a particle disappearing at a point A and instantaneously reappearing at a point B, a macroscopic distance away. This is not a physical process and we thus require a local version of this law. Qualitatively we say that in any volume V a decrease in mass must be compensated for by a flow of mass out of the volume. We quantify this by writing [14]

$$\frac{\partial}{\partial t} \int_{V} \rho \mathrm{d}V = \int_{V} \mathrm{d}V \frac{\partial \rho}{\partial t} = -\oint_{A} \rho \boldsymbol{v} \cdot \mathrm{d}\boldsymbol{S}, \qquad (3.1)$$

where ρ is the density, \boldsymbol{v} is the flow velocity, A is the surface of V and $d\boldsymbol{S}$ is a unit vector normal to A. Figure 3.1 gives a pictorial representation of the situation. Gauss' theorem for a vector \boldsymbol{q} is given by

$$\oint_{A} \boldsymbol{q} \cdot \mathrm{d}\boldsymbol{S} = \int_{V} \mathrm{d}V \nabla \cdot \boldsymbol{q}$$
(3.2)



Figure 3.1: A pictorial representation of matter with density ρ and velocity v flowing through a volume V.

and upon using this in the local conservation equation we obtain

$$\int_{V} \mathrm{d}V \frac{\partial \rho}{\partial t} = -\int_{V} \mathrm{d}V \nabla \cdot (\rho \boldsymbol{v}). \tag{3.3}$$

This must hold for any volume V and so we can remove the integrals, giving the differential form of the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0. \tag{3.4}$$

We say that ρv describes the mass flux density of particles. Conserved densities other than the mass density satisfy equations similar to (3.4). Such quantities include the energy, momentum and angular momentum. The energy density is given by

$$w = \frac{\rho v^2}{2} + \rho \epsilon, \qquad (3.5)$$

where ϵ is the internal energy density of the fluid. This quantity satisfies a continuity equation given by

$$\frac{\partial w}{\partial t} + \nabla \cdot \left[\rho v \left(\frac{v^2}{2} + \epsilon + \frac{p}{\rho} \right) \right] = 0$$
(3.6)

where p is the pressure. In both of the cases mentioned the density is a scalar quantity and the flux density is a vector. We shall consider the case of the momentum of the fluid, which is a vector quantity, having a density given by

$$\boldsymbol{P} = \rho \boldsymbol{v}.\tag{3.7}$$

We introduce the component notation for vectors, wherein v_i is the *i*-th component of the vector v and the index *i* takes the values 1 to 3, corresponding to the *x*, *y* and *z* directions respectively. With this in mind, we introduce the summation convention [15] which will be assumed for the remainder of the thesis. In the summation convention, a repeated index is assumed to be summed over. Thus for example

$$a_i b_i \equiv \sum_{i=1}^3 a_i b_i = \boldsymbol{a} \cdot \boldsymbol{b}.$$
(3.8)

In order to find the continuity equation satisfied by the momentum density, we take the time derivative of the momentum density which is given by

$$\frac{\partial P_i}{\partial t} = v_i \frac{\partial \rho}{\partial t} + \rho \frac{\partial v_i}{\partial t}.$$
(3.9)

We use the mass continuity equation (3.4) and the fluid equation of motion known as Euler's equation [14], which is obtained from the force acting on a volume element due to its pressure. Euler's equation is

$$\frac{\partial v_i}{\partial t} + v_j \nabla_j v_i = -\frac{1}{\rho} \nabla_i p, \qquad (3.10)$$

where p is the pressure, and only holds for ideal fluids - ones where thermal conductivity and viscosity are negligible - in the absence of gravity. Thus we can write the momentum density in the form of a continuity equation. This is written as

$$\frac{\partial P_i}{\partial t} = -v_i \nabla_j (\rho v_j) - \rho v_k \nabla_k v_i - \nabla_i p
= -\nabla_j (\rho v_i v_j + \delta_{ij} p).$$
(3.11)

Thus the continuity equation which the momentum density satisfies is

$$\frac{\partial P_i}{\partial t} + \nabla_j \Pi_{ij} = 0, \qquad (3.12)$$

where Π_{ij} is the momentum flux density which is the rank 2 tensor quantity

$$\Pi_{ik} = p\delta_{ik} + \rho v_i v_k. \tag{3.13}$$

This specifies the flux in the k direction of the *i* component of the momentum. In general if the density is a rank n tensor the flux density is a rank n + 1 tensor.

3.2 Electromagnetic theory

We have seen that certain properties of fluids are conserved and thus obey continuity equations. Similarly we may write continuity equations for the charge, energy, momentum and angular momentum of electromagnetic waves. As these quantities are traditionally associated with solid bodies in mechanics, we will call them the mechanical properties. In order to find the continuity equations for the mechanical properties of electromagnetic waves, we use the Maxwell equations for the electromagnetic field in the presence of a continuous charge and current distribution, given by ρ and J respectively. The Maxwell equations are

$$\nabla_{i}E_{i} = \frac{\rho}{\epsilon_{0}}$$

$$\nabla_{i}B_{i} = 0$$

$$\epsilon_{ijk}\nabla_{j}B_{k} - \frac{1}{c^{2}}\frac{\partial E_{i}}{\partial t} = \mu_{0}J_{i}$$

$$\epsilon_{ijk}\nabla_{j}E_{k} + \frac{\partial B_{i}}{\partial t} = 0,$$
(3.14)

where E and B are the electric and magnetic field vectors respectively, ϵ_0 is the permittivity of free space and μ_0 is the permeability of free space. Here we have introduced the permutation symbol [15] ϵ_{ijk} which takes the value 1 if ijk is a cyclic permutation of 123, -1 if ijk is a cyclic permutation of 321 and zero otherwise. Thus

$$\epsilon_{ijk}a_ib_j \equiv \left(\boldsymbol{a} \times \boldsymbol{b}\right)_k. \tag{3.15}$$

By taking the time derivative of the first equation in (3.14)

$$\nabla_i \frac{\partial E_i}{\partial t} = \frac{1}{\epsilon_0} \frac{\partial \rho}{\partial t}, \qquad (3.16)$$

the divergence of the third

$$\nabla_i \frac{\partial E_i}{\partial t} = \frac{1}{\epsilon_0} \nabla_i J_i + c^2 \epsilon_{ijk} \nabla_i \nabla_j B_k, \qquad (3.17)$$

and using the cyclic property of ϵ_{ijk} , we obtain the well known charge conservation equation [16]

$$\frac{\partial \rho}{\partial t} + \nabla_i J_i = 0 \tag{3.18}$$

As well as the charge, we may consider continuity equations for each of energy, momentum and angular momentum. The electromagnetic energy density is given by

$$u = \frac{1}{2} \left(\epsilon_0 E_i E_i + \frac{1}{\mu_0} B_i B_i \right) \tag{3.19}$$

Upon using the Maxwell equations we may calculate the time derivative of the energy density and obtain

$$\frac{\partial u}{\partial t} + \frac{1}{\mu_0} \nabla_i \epsilon_{ijk} E_j B_k = -E_i J_i. \tag{3.20}$$

This has the form of a continuity equation, except that the term on the right hand side is non-zero. Equation (3.20) represents the generalisation of the continuity equation to situations in which there is a sink or source of the

quantity. In this case the fields do a total rate of work given by

$$\int_V E_i J_i \mathrm{d}V$$

which is why $E_i J_i$ appears as the source term in (3.20).

One can extend the same type of calculation to the momentum of the electromagnetic field. The momentum density is given by

$$P_i = \epsilon_0 \epsilon_{ijk} E_j B_k \tag{3.21}$$

and the continuity equation is

$$\frac{\partial P_i}{\partial t} + \nabla_i T_{ij} = -\left(\epsilon_{ijk} J_j B_k + \rho E_i\right). \tag{3.22}$$

Here we have defined the electromagnetic momentum flux density tensor

$$T_{ij} = \frac{1}{2} \delta_{ij} \left(\mu_0^{-1} B_k B_k + \epsilon_0 E_k E_k \right) - \epsilon_0 E_i E_j - \mu_0^{-1} B_i B_j, \qquad (3.23)$$

where δ_{ij} is the Krönecker delta function. The source term in (3.22) is simply the negative of the force per unit volume imparted by the electromagnetic field on a charged particle. A similar calculation is possible for the conservation of angular momentum [16, 17], but we will not discuss this further here.

It is worth noting that in this chapter we have defined the flux by finding an equation of the general form

$$\frac{\partial a}{\partial t} + \nabla_i b_i = c \tag{3.24}$$

where a is the density of interest. We then define b as the flux density of the given quantity and c as its source density. This definition of the flux density is not unique, however, since the divergence of the curl of any vector is zero. Thus the same equation may be satisfied by a quantity

$$b'_i = b_i + \epsilon_{ijk} \nabla_j d_k \tag{3.25}$$

where d is any vector field. For the energy density equation one may show from relativistic considerations that the Poynting vector

$$S_i = \frac{1}{\mu_0} \epsilon_{ijk} E_j B_k \tag{3.26}$$

satisfies (3.20) uniquely [16]. This is done by equating the derivative of the electromagnetic symmetric stress tensor $\Theta^{\alpha\beta}$ to zero, so that

$$\frac{\partial}{\partial x^{\alpha}}\Theta^{\alpha\beta} = 0. \tag{3.27}$$

Here the Greek indices take the values $0, \ldots, 3$. The components of the tensor $\Theta^{\alpha\beta}$ are given by

$$\Theta^{00} = \frac{1}{2} \left(\epsilon_0 E_k E_k + \frac{1}{\mu_0} B_k B_k \right)$$
(3.28)

$$\Theta^{0i} = \frac{1}{\mu_0} \epsilon_{ijk} E_j B_k \tag{3.29}$$

$$\Theta^{ij} = \frac{1}{2} \delta_{ij} \left(\mu_0^{-1} B_k B_k + \epsilon_0 E_k E_k \right) - \epsilon_0 E_i E_j - \mu_0^{-1} B_i B_j, \quad (3.30)$$

where the components i, j and k each take the values 1, 2, 3. Thus calculating (3.27) with $\beta = 0$ gives the Poynting vector uniquely as the electromagnetic flux density. Similarly, setting $\beta = i$ gives expression (3.23) as the unique electromagnetic momentum density tensor. It seems likely that this uniqueness extends to other quantities, or at least that the addition of a divergenceless term has no physical consequences.

Chapter 4

Mechanical properties of matter waves

4.1 Introduction

We have seen in the previous chapter that electromagnetic waves have properties analogous to fluids in that we can define flux densities for their mechanical properties. As experiments in matter waves are performed with ever more control and precision, with a view to the applications of matter waves, it will be important to calculate important mechanical properties such as energy, momentum and angular momentum at a local level. In this chapter we present the beginnings of a theory of the mechanical properties of matter waves. This will allow the calculation of such quantities. The work presented herein represents an original contribution to the literature and has been published in ref. [18].

4.2 Formalism

We turn our attention to the semiclassical description of matter waves. Consider an observable A having a corresponding Hermitian operator \hat{A} . If A is an observable which corresponds to a mechanical property and thus obeys a continuity equation of the form (3.24), then the operator representing its density $\hat{\mathcal{A}}(\boldsymbol{R})$ at a point \boldsymbol{R} will obey the generalised local continuity equation

$$\frac{\partial}{\partial t}\hat{\mathcal{A}}(\boldsymbol{R}) + \frac{\partial}{\partial X_{i}}\hat{T}_{i}^{(A)}(\boldsymbol{R}) = \hat{\mathcal{S}}^{(A)}(\boldsymbol{R}), \qquad (4.1)$$

where X_i are the components of \mathbf{R} , $\hat{T}_i^{(A)}$ is the flux density operator for the observable A and $\hat{S}^{(A)}$ is the source density operator. The particle density, for example, is described by the Dirac delta function operator $\delta(\hat{\mathbf{r}} - \mathbf{R})$. We can see this if we consider the position representation, in which its expectation value will be

$$\langle \delta(\hat{\boldsymbol{r}} - \boldsymbol{R}) \rangle = \int_{-\infty}^{\infty} d^3 \boldsymbol{r} \psi^*(\boldsymbol{r}, t) \delta(\boldsymbol{r} - \boldsymbol{R}) \psi(\boldsymbol{r}, t)$$

= $|\psi(\boldsymbol{R}, t)|^2$, (4.2)

which is the particle density at \mathbf{R} . Expanding on this, we expect that $\hat{\mathcal{A}}(\mathbf{R})$, which represents the density of a quantity A, to be proportional to product of the operator for A and the delta function operator:

$$\hat{\mathcal{A}}(\boldsymbol{R}) \propto \hat{A}\delta(\hat{\boldsymbol{r}} - \boldsymbol{R}).$$
 (4.3)

The product written above is not Hermitian, however, and so instead we define $\hat{\mathcal{A}}(\mathbf{R})$ to be

$$\hat{\mathcal{A}}(\mathbf{R}) = \frac{1}{2} \left[\hat{A}\delta(\hat{\mathbf{r}} - \mathbf{R}) + \left(\hat{A}\delta(\hat{\mathbf{r}} - \mathbf{R}) \right)^{\dagger} \right] \\ = \frac{1}{2} \left[\hat{A}\delta(\hat{\mathbf{r}} - \mathbf{R}) + \delta(\hat{\mathbf{r}} - \mathbf{R})\hat{A} \right], \qquad (4.4)$$

since both \hat{A} and $\delta(\hat{r} - R)$ are themselves Hermitian. We write this in the more compact form

$$\hat{\mathcal{A}}(\mathbf{R}) = \frac{1}{2} \left\{ \hat{A}, \delta(\hat{\mathbf{r}} - \mathbf{R}) \right\}, \qquad (4.5)$$

where $\{,\}$ denotes the anticommutator which is defined by

$$\left\{\hat{A},\hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A}.$$
(4.6)

From the Heisenberg equation of motion we can show that the density will evolve according to

$$\frac{\partial}{\partial t}\hat{\mathcal{A}}(\boldsymbol{R}) = \frac{i}{\hbar} \left[\hat{H}, \hat{\mathcal{A}}(\boldsymbol{R}) \right] \\
= \frac{i}{2\hbar} \left\{ \{ [H, A], \delta(\hat{\boldsymbol{r}} - \boldsymbol{R}) \} + \left\{ \hat{A}, [H, \delta(\hat{\boldsymbol{r}} - \boldsymbol{R})] \right\} \right) \quad (4.7)$$

If A is a conserved quantity, then its time derivative must vanish. From the Heisenberg equation this means that it will commute with the Hamiltonian. We see that the first term on the right hand side will vanish if A is conserved. It is therefore reasonable to associate this term with the source term in (4.1) and the last term with the flux density. In order to proceed with the calculation we move to the position representation and use the standard Hamiltonian (2.35) for a particle in a potential $V(\mathbf{r})$. Note that this simple Hamiltonian does not describe systems where particles are lost or gained. On evaluating the last term in (4.7) we find that the commutator can be calculated to be

$$\left[\hat{H},\delta(\boldsymbol{r}-\boldsymbol{R})\right] = \frac{-\hbar^2}{2m} \left[\nabla_i \nabla_i,\delta(\boldsymbol{r}-\boldsymbol{R})\right] + \left[V(\boldsymbol{r}),\delta(\boldsymbol{r}-\boldsymbol{R})\right].$$
(4.8)

The commutator of $\delta(\boldsymbol{r}-\boldsymbol{R})$ with $V(\boldsymbol{r})$ vanishes and we find that

$$\left[\hat{H},\delta(\boldsymbol{r}-\boldsymbol{R})\right] = \frac{-\hbar^2}{2m} \left\{\nabla_i, \left[\nabla_i\delta(\boldsymbol{r}-\boldsymbol{R})\right]\right\}.$$
(4.9)

Thus the last term of (4.7) becomes

$$\frac{-i\hbar}{4m}\left\{\hat{A},\left\{\nabla_{i},\left[\nabla_{i}\delta(\boldsymbol{r}-\boldsymbol{R})\right]\right\}\right\}.$$

We use a property of the Dirac delta function

$$\frac{\partial}{\partial x}\delta(x-y) = -\frac{\partial}{\partial y}\delta(x-y), \qquad (4.10)$$

which comes about from the definition of the delta function as the limit of a Gaussian. Since \hat{A} is independent of \mathbf{R} , this allows us to write

$$abla_{R,i}rac{i\hbar}{4m}\left\{\hat{A},\{
abla_i,\delta(m{r}-m{R})\}
ight\},$$

where

$$\nabla_{R,i} \equiv \frac{\partial}{\partial X_i}.$$
(4.11)

We now return from the position representation by identifying $\hat{p}_i = -i\hbar\nabla_i$ and so the last term in (4.7) can be written as

$$- \nabla_{R,i} \frac{1}{4} \left\{ \hat{A}, \left\{ \frac{\hat{p}_i}{m}, \delta(\hat{\boldsymbol{r}} - \boldsymbol{R}) \right\} \right\}.$$

Thus we can rewrite (4.7) as

$$\frac{1}{2}\frac{\partial}{\partial t}\left\{\hat{A},\delta(\hat{\boldsymbol{r}}-\boldsymbol{R})\right\} + \frac{1}{4}\nabla_{\boldsymbol{R},i}\left\{\hat{A},\left\{\frac{\hat{p}_{i}}{m},\delta(\hat{\boldsymbol{r}}-\boldsymbol{R})\right\}\right\}$$

$$= \frac{1}{2}\left\{\frac{\partial}{\partial t}\hat{A},\delta(\hat{\boldsymbol{r}}-\boldsymbol{R})\right\},$$
(4.12)

which takes the form of a conservation equation (4.1). This allows us to identify the flux density operator

$$\hat{T}_{i}^{(A)}(\boldsymbol{R}) = \frac{1}{4} \left\{ \hat{A}, \left\{ \frac{\hat{p}_{i}}{m}, \delta(\hat{\boldsymbol{r}} - \boldsymbol{R}) \right\} \right\}.$$
(4.13)

We can associate the operator $\{\hat{p}_i/m, \delta(\hat{r} - R)\}$ with the velocity density and hence see that $\hat{T}_i^{(A)}(R)$ is a suitably symmetrised product of the velocity density and the observable. This operator is the flow of the density of the observable, that is its flux density. The forms of the flux density and source density for the observable A will come from the expectation value of (4.12). In the Heisenberg picture and the position representation, the matter wave will be described by a wavefunction $\psi(r)$ at all times. The expectation value of the conservation equation for this state is

$$\frac{\partial}{\partial t}\mathcal{A}(\mathbf{R}) + \nabla_{\mathbf{R},i}\mathcal{T}_{i}^{(A)}(\mathbf{R}) = \mathcal{S}^{(A)}(\mathbf{R}), \qquad (4.14)$$

which is the continuity equation for the expectation values of the relevant operators. Here we have introduced the notation $\mathcal{A}(\mathbf{R}) \equiv \langle \hat{\mathcal{A}}(\mathbf{R}) \rangle$. The flux density expectation value is

$$\mathcal{T}_{i}^{(A)}(\boldsymbol{R}) = \int \mathrm{d}^{3}r\psi^{*}(\boldsymbol{r})\hat{\mathcal{T}}_{i}^{(A)}(\boldsymbol{R})\psi(\boldsymbol{r})$$

$$= \frac{i\hbar}{4m} \left[\psi\nabla_{i}(\hat{A}\psi)^{*} - (\hat{A}\psi)^{*}\nabla_{i}\psi + \hat{A}\psi(\nabla_{i}\psi^{*}) - \psi^{*}\nabla_{i}(\hat{A}\psi)\right]\Big|_{\boldsymbol{r}=\boldsymbol{R}}$$
(4.15)

and the source density expectation value is

$$\mathcal{S}^{(A)}(\boldsymbol{R}) = \frac{i}{2\hbar} \left\{ -\left(\left[\hat{H}, \hat{A} \right] \psi \right)^* \psi + \psi^* \left(\left[\hat{H}, \hat{A} \right] \psi \right) \right\} \Big|_{\boldsymbol{r} = \boldsymbol{R}}.$$
(4.16)

In the next section we will consider several quantities which may be conserved, specifically the particle number, energy, momentum and angular momentum.

4.3 Conserved Quantities

4.3.1 Particle Number

Following Landau [19], the operator corresponding to particle density in a semiclassical theory is represented by the Dirac delta function, so in (4.5) we put the operator \hat{A} equal to the identity operator $\hat{1}$. From (4.15) the flux density of particles at position \boldsymbol{r} can be calculated as

$$\begin{aligned} \mathcal{T}_{i}^{(\rho)}(\boldsymbol{R}) &= \frac{i\hbar}{4m} \left(\psi \nabla_{i}\psi^{*} - \psi^{*}\nabla_{i}\psi + \psi \nabla_{i}\psi^{*} - \psi^{*}\nabla_{i}\psi \right)|_{\boldsymbol{r}=\boldsymbol{R}} \\ &= \frac{i\hbar}{2m} \left(\psi \nabla_{i}\psi^{*} - \psi^{*}\nabla_{i}\psi \right)|_{\boldsymbol{r}=\boldsymbol{R}} \\ &= \frac{\hbar}{m} \operatorname{Im} \left\{ \psi^{*}\nabla_{i}\psi \right\}|_{\boldsymbol{r}=\boldsymbol{R}}, \end{aligned}$$

$$(4.17)$$

where Im indicates the imaginary part. This is the form of the well-known quantum mechanical probability flux J_i [20]. The source term vanishes as the identity operator commutes with the Hamiltonian. This is a reasonable result as there is no particle source present in the system.

4.3.2 Energy

Energy in quantum mechanics is represented by the Hamiltonian operator, so we can calculate the energy flux density from (4.15) to be

$$T_{i}^{(E)}(\mathbf{R}) = \frac{i\hbar}{4m} \left\{ \psi \nabla_{i} \left(\hat{H} \psi^{*} \right) - \psi^{*} \nabla_{i} \left(\hat{H} \psi \right) + \left(\hat{H} \psi \right) \nabla_{i} \psi^{*} - \left(\hat{H} \psi^{*} \right) \nabla_{i} \psi \right\} \Big|_{\mathbf{r} = \mathbf{R}}.$$
(4.18)

Upon using the Hamiltonian from (2.35), and performing the product derivatives, the expression given above can be simplified considerably to give

$$\mathcal{T}_{i}^{(E)}(\boldsymbol{R}) = \frac{\hbar^{3}}{4m^{2}} \operatorname{Im} \left\{ \psi \nabla^{2} \nabla_{i} \psi^{*} + (\nabla_{i} \psi^{*}) \nabla^{2} \psi \right\} \Big|_{\boldsymbol{r}=\boldsymbol{R}} + V(\boldsymbol{R}) \mathcal{T}_{i}^{(\rho)}(\boldsymbol{R}).$$
(4.19)

The source term for energy clearly vanishes as the Hamiltonian commutes with itself. This is reasonable as energy is conserved in this system.

4.3.3 Momentum

Momentum is represented by the spatial derivative operator $p_i = -i\hbar\nabla_i$, and we can calculate the momentum flux density from (4.15). Thus the *j* component of flux of the *i* component of momentum is

$$T_{ij}^{(p)}(\mathbf{R}) = \frac{\hbar^2}{4m} \{ -\psi \nabla_j \nabla_i \psi^* - \psi^* \nabla_j \nabla_i \psi + (\nabla_i \psi) (\nabla_j \psi^*) + (\nabla_i \psi^*) (\nabla_j \psi) \} |_{\mathbf{r}=\mathbf{R}}$$
$$= \frac{\hbar^2}{2m} \operatorname{Re} \{ (\nabla_i \psi) (\nabla_j \psi^*) - \psi \nabla_i \nabla_j \psi^* \} |_{\mathbf{r}=\mathbf{R}}.$$
(4.20)

The source term for momentum will not necessarily vanish as the potential term may contain a momentum source (such as gravity), which from (4.16) is given by

$$\mathcal{S}_{i}^{(p)}(\boldsymbol{R}) = \frac{1}{2} \left\{ \left(\left[H, \nabla_{i} \right] \psi^{*} \right) \psi + \psi^{*} \left(\left[H, \nabla_{i} \right] \psi \right) \right\} |_{\boldsymbol{r} = \boldsymbol{R}} \right\}.$$
(4.21)

By expanding the commutator and evaluating product derivatives, we arrive at the expression for momentum source

$$\mathcal{S}_{i}^{(p)}(\boldsymbol{R}) = -|\psi(\boldsymbol{R})|^{2} \nabla_{\boldsymbol{R},i} V(\boldsymbol{R}).$$
(4.22)

This is equivalent to a force term suitably weighted by the probability density. This is the form of a source density of momentum that we might have expected on the basis of Newton's second law of motion.

4.3.4 Angular Momentum

Angular momentum is represented by the cross product of position and momentum:

$$L_{i} = (\boldsymbol{x} \times \boldsymbol{p})_{i}$$
$$= \epsilon_{ijk} x_{j} p_{k}. \qquad (4.23)$$

Thus from (4.14), substituting \mathcal{P}_i for \mathcal{A} , we obtain

$$\frac{\partial}{\partial t}\mathcal{P}_{i}(\boldsymbol{R}) = -\nabla_{\boldsymbol{R},j}\mathcal{T}_{ij}^{(\boldsymbol{p})}(\boldsymbol{R}) + \mathcal{S}_{i}^{(\boldsymbol{p})}(\boldsymbol{R}).$$
(4.24)

To determine the flux and source terms for angular momentum density in terms of the momentum density, we simply take the time derivative of the angular momentum density

$$\frac{\partial}{\partial t} \mathcal{L}_{i}(\mathbf{R}) = \epsilon_{ijk} X_{j} \frac{\partial}{\partial t} \mathcal{P}_{k}(\mathbf{R})$$

$$= \epsilon_{ijk} X_{j} \nabla_{R,l} \mathcal{T}_{kl}^{(p)}(\mathbf{R}) + \epsilon_{ijk} X_{j} \mathcal{S}_{k}^{(p)}(\mathbf{R}).$$
(4.25)

Thus we expect that

$$\nabla_{R,l} \mathcal{T}_{il}^{(L)}(\boldsymbol{R}) = \epsilon_{ijk} X_j \nabla_{R,l} \mathcal{T}_{kl}^{(p)}(\boldsymbol{R})$$
(4.26)

$$S_i^{(L)}(\boldsymbol{R}) = \epsilon_{ijk} X_j S_k^{(\boldsymbol{p})}(\boldsymbol{R})$$
(4.27)

which, from (4.22) implies that the source will be a torque, suitably weighted with the probability density. This is as expected for the source of angular momentum.

Inserting (4.23) into (4.15), the *l* component of flux of the *i* component of angular momentum can be calculated as

$$\mathcal{T}_{il}^{(L)}(\boldsymbol{R}) = \frac{\hbar^2}{4m} \epsilon_{ijk} \left\{ -\psi \nabla_l \left(x_j \nabla_k \psi^* \right) - \psi^* \nabla_l \left(x_j \nabla_k \psi \right) \right. \\ \left. + \left. x_j \left(\nabla_k \psi \right) \left(\nabla_l \psi^* \right) + \left. x_j \left(\nabla_k \psi^* \right) \left(\nabla_l \psi \right) \right\} \right|_{\boldsymbol{r} = \boldsymbol{R}} \right.$$
(4.28)

Upon evaluating the product derivatives in the first line, we can show that the angular momentum flux density is given by

$$\mathcal{T}_{il}^{(L)}(\boldsymbol{R}) = \epsilon_{ijk} X_j \mathcal{T}_{kl}^{(p)}(\boldsymbol{R}) - \frac{\hbar^2}{4m} \epsilon_{ilk} \nabla_{R,k} |\psi(\boldsymbol{R})|^2.$$
(4.29)

It can be easily verified using the antisymmetric properties of the ϵ_{ijk} that this is consistent with (4.26). The source will not necessarily vanish, so from (4.16)

$$S_{i}^{(L)}(\mathbf{R}) = \frac{1}{2} \epsilon_{ijk} \left\{ \left([H, x_{j} \nabla_{k}] \psi^{*} \right) \psi + \psi^{*} \left([H, x_{j} \nabla_{k}] \psi \right) \right\} |_{\mathbf{r} = \mathbf{R}} .$$
(4.30)

Upon expanding the commutators and performing the product derivatives we arrive at the expression for the angular momentum source

$$S_i^{(L)}(\boldsymbol{R}) = -\left|\psi(\boldsymbol{R})\right|^2 \epsilon_{ijk} X_j \nabla_k V(\boldsymbol{R}), \qquad (4.31)$$

which is a torque density, and exactly that anticipated in (4.27).

4.4 Conclusion

In this chapter, we have derived general flux density and source density operators for conserved quantities in matter waves within the semiclassical description. This theory will be important when considering the deposition of these quantities during interactions of matter waves with other objects. An example of this is the detection of matter waves themselves, which requires one to consider the particle flux density [21] as we will see in the following chapters.

One problem is that, just as described in chapter 3, the flux density operator (4.13) might contain an arbitrary divergenceless operator in addition to the terms present. The angular momentum flux density shows this most clearly. The method used above involved taking the time derivative of the operator representing the density of the observable, identifying the flux-density operator and then taking expectation values. If instead we took the expectation values first and then the time derivative, the flux density we obtain for the angular momentum case is given by

$$\mathcal{T}_{il}^{(L)}(\boldsymbol{R}) = \frac{\hbar^2}{4m} \epsilon_{ijk} x_j \left\{ -\psi \nabla_l \nabla_k \psi^* - \psi^* \nabla_l \nabla_k \psi + (\nabla_k \psi) (\nabla_l \psi^*) + (\nabla_k \psi^*) (\nabla_l \psi) \right\}|_{\boldsymbol{r}=\boldsymbol{R}}$$

$$= \epsilon_{ijk} X_j \mathcal{T}_{kl}^{(\boldsymbol{p})}(\boldsymbol{R}).$$
(4.32)

This is just the flux density given in (4.28) and (4.29), without the divergenceless quantity

$$rac{\hbar^2}{4m}\epsilon_{ilk}
abla_{R,k}\,|\psi({m R})|^2\,.$$

As these methods are both equivalent and correct we deduce that this divergenceless quantity has no physical significance. It seems likely that this will be the case for all mechanical properties.

Chapter 5

Semiclassical theory of matter wave detection

5.1 Introduction

In a recent experiment, Robert *et al* [22] created a BEC of metastable triplet Helium atoms (He^{*}) and highlighted the ability to count single atoms falling from the trap after it was turned off (see figure 5.1 for a schematic representation of the experiment). This allows for the exciting possibility of more detailed investigation of the quantum statistical properties of matter waves.

As a first step into this field, we model the detection of matter waves falling under gravity. We will use a simplistic model, not including the effects of interactions which exist between atoms [23, 24]. This will allow the features specific to detection to be more readily illustrated. As we are considering matter waves, we can draw a direct analogy with the well known theory of the detection of light waves, or photo-detection [25], which will be outlined here. The work presented in this chapter is an original contribution and is published in ref. [21].



Figure 5.1: Schematic representation of the experiment which is being modelled here.

5.2 Semiclassical theory of photo-detection

The semiclassical theory of photo-detection is based on the assumption that the probability of an ionisation event occurring in the photo-detector in a time period dt is proportional to the cycle-averaged intensity $\bar{I}(t)$ of the incoming light:

$$p(t)dt = \xi \bar{I}(t)dt, \qquad (5.1)$$

where ξ is a constant of proportionality which represents the efficiency of the detector, including geometric factors such as its area, and dt is sufficiently small that the probability of more than one detection event occurring is negligible. For monochromatic light whose statistical properties are independent of time (stationary), the cycle-averaged intensity is taken to be

$$\bar{I}(t) = \frac{1}{2} \epsilon_0 c |E(t)|^2 \equiv c W(t),$$
(5.2)

pointing in the direction of beam propagation, where W(t) is the energy density. Under assumption (5.1), if we take a time interval from t to t + T, then the probability of m detection events occurring is

$$P_m(T) = \left\langle \frac{\bar{n}^m}{m!} e^{-\bar{n}} \right\rangle, \tag{5.3}$$

where

$$\bar{n} = \xi \int_{t}^{t+T} \mathrm{d}t' \bar{I}(t') \tag{5.4}$$

and the angled brackets indicate a statistical average. From (5.3) we can evaluate the mean number of detection events to be

$$\begin{array}{lll} \langle m \rangle & = & \sum_{m=0}^{\infty} m P_m(T) \\ & = & \sum_{m=0}^{\infty} m \left\langle \frac{\bar{n}^m}{m!} e^{-\bar{n}} \right\rangle \end{array}$$

$$= \sum_{m=1}^{\infty} \left\langle \bar{n} \frac{\bar{n}^{m-1}}{(m-1)!} e^{-\bar{n}} \right\rangle$$
(5.5)

and since we can take the sum inside the statistical average, we can write

$$\langle m \rangle = \langle \bar{n} \rangle \,.$$
 (5.6)

5.3 Matter waves

We wish to construct a semiclassical theory of matter wave detection by analogy with the theory of photo-detection presented above. A natural way to proceed is to replace the electric field $E(\mathbf{r}, t)$ with the particle wavefunction $\psi(\mathbf{r}, t)$. Thus the matter wave analogy to the expression for $\bar{I}(t)$ in (5.2) will be $|\psi(\mathbf{r}, t)|^2 \bar{\boldsymbol{v}}$, where we have included a characteristic velocity $\bar{\boldsymbol{v}}$. This is in direct analogy with the velocity of light c in the photo-detection theory and is of vectorial nature to allow for matter waves which are not travelling perpendicular to the detector. It is also required so that the equations have the correct dimensionality. In the analysis that follows, $\bar{\boldsymbol{v}}$ will be associated with the mean velocity of the wavepacket. The probability of detection over a time interval from t to t + T would again be given by (5.3) and the average number of counts $\langle m \rangle$ by (5.6) where instead of (5.4), we have

$$\bar{n} = \xi \int_{t}^{t+T} \mathrm{d}t' \int_{A} |\psi(\boldsymbol{r}, t')|^{2} \,\bar{\boldsymbol{v}} \cdot \mathrm{d}\boldsymbol{S}.$$
(5.7)

We have now explicitly included the area of the detector A, and dS is the infinitesimal area element normal to the surface of the detector. If we assume that the particle wavefunction is normalised so that it contains on average N particles, then for all times t

$$\int_{-\infty}^{\infty} \mathrm{d}^3 \boldsymbol{r} \, |\psi(\boldsymbol{r},t)|^2 = N.$$
(5.8)

If the detector is of perfect efficiency then we would expect that for a wavepacket falling under gravity, a sufficiently long detection window and large detection area would produce a mean of N detection events. This means that from (5.7) we might expect that as $T \to \infty$ and $t \to -\infty$,

$$\xi \int_{-\infty}^{\infty} \mathrm{d}t' \int_{A} |\psi(\boldsymbol{r}, t')|^{2} \, \bar{\boldsymbol{v}} \cdot \mathrm{d}\boldsymbol{S} = N, \qquad (5.9)$$

for the value of ξ corresponding to a perfectly efficient detector.

By drawing analogy with photo-detection of light waves, we have derived (5.7) which includes the characteristic velocity \bar{v} . As a first approximation we might expect that this will be the mean velocity of the wavepacket. This is not an approximation for light in free space because free space is not dispersive; at all frequencies light travels at c. For matter waves, however, free space is dispersive.

In order to take into account matter wave dispersion we ought to base our theory of detection on the flux-density of particles - the mean rate at which particles cross a unit area of the detector. As particle number is a conserved quantity its density ρ must satisfy an equation of continuity [19, 26]

$$\frac{\partial}{\partial t} |\psi(\boldsymbol{r},t)|^2 + \nabla \cdot \boldsymbol{J}(\boldsymbol{r},t) = 0, \qquad (5.10)$$

where J is the particle flux-density. This equation is of the same form as the one for local charge conservation in electromagnetic theory or, more relevantly for our purpose, relating particle density ρ and particle flux-density $J = \rho v$ in fluid mechanics [14]. The particle flux density is the same as that calculated in chapter 4, and is given by

$$\boldsymbol{J}(\boldsymbol{r},t) = \frac{\hbar}{m} \operatorname{Im} \left\{ \psi^*(\boldsymbol{r},t) \nabla \psi(\boldsymbol{r},t) \right\}.$$
 (5.11)

As this is analogous to the particle flux-density $J = \rho v$ from fluid mechanics, it seems reasonable that (5.7) should become

$$\bar{n} = \xi \int_{t}^{t+T} \mathrm{d}t' \int_{A} \boldsymbol{J}(\boldsymbol{r}, t') \cdot \mathrm{d}\boldsymbol{S}.$$
(5.12)

As we have seen in chapter 3, the energy density is related to the energy flux-density (the Poynting vector) [16, 27] by a continuity equation similar to (5.10). In a general situation, outwith the conditions which make (5.2) valid

(for example inside a dispersive and/or lossy dielectric), the cycle-averaged intensity in (5.2) must be replaced by the magnitude of the Poynting vector.

5.4 Single atom example

In order to illustrate fully the difference between the theories given by (5.7) and (5.12), it is instructive to evaluate both expressions in the case of the detection of a wavepacket falling in the -z direction under gravity onto a flat, large-area detector aligned parallel to the x-y plane. Such a system closely models the He^{*} experiment in [22], and it is one in which we would expect all particles to fall onto the detector, which will allow us to check the expression for $\langle m \rangle$.

In evaluating the probability of detection for a wavepacket falling under gravity we will need to calculate the form of the matter wavefunction. We consider a model BEC, released at time t = 0, described by a Gaussian wavefunction centred at r_0 with width parameter w,

$$\psi(\mathbf{r},0) = N^{1/2} (\pi w^2)^{-3/4} \exp\left\{-\frac{|\mathbf{r}-\mathbf{r}_0|^2}{2w^2}\right\}.$$
 (5.13)

The Hamiltonian for this system will be given by the standard position representation Hamiltonian (2.35) for particles in a potential $V(\hat{r})$, with the potential being the gravitational potential

$$V(\hat{\boldsymbol{r}}) = mg\hat{z}.\tag{5.14}$$

With this potential the Hamiltonian is written in the position representation as

$$\hat{H} = \frac{-\hbar^2}{2m} \nabla^2 + mgz, \qquad (5.15)$$

where we have taken the zero of gravitational potential energy to be at z = 0,

the plane of our detector. The Schrödinger equation is thus written

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = \frac{-\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r},t) + mgz\psi(\boldsymbol{r},t).$$
(5.16)

We simplify this by transforming to a frame rotating at frequency mgz/\hbar and writing

$$\psi(\mathbf{r},t) = \exp\left(\frac{-imgzt}{\hbar}\right)\phi(\mathbf{r},t).$$
(5.17)

Under this transformation the time derivative becomes

$$\frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial t} - \frac{imgz}{\hbar}$$
 (5.18)

and the spatial derivative is

$$\frac{\partial}{\partial z} \to \frac{\partial}{\partial z} - \frac{imgt}{\hbar}.$$
 (5.19)

The evolution equation for $\phi(\mathbf{r}, t)$ is thus written

$$i\hbar\frac{\partial}{\partial t}\phi(\boldsymbol{r},t) = \frac{-\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \left(\frac{\partial}{\partial z} - \frac{imgt}{\hbar}\right)^2\right]\phi(\boldsymbol{r},t).$$
(5.20)

If we introduce the Fourier transform $\tilde{\phi}(\boldsymbol{q},t)$ of $\phi(\boldsymbol{r},t)$ via the relation

$$\phi(\boldsymbol{r},t) = \left(\frac{1}{2\pi}\right)^{3/2} \int \mathrm{d}^3 q \exp\left(i\boldsymbol{q}\cdot\boldsymbol{r}\right) \tilde{\phi}(\boldsymbol{q},t), \tag{5.21}$$

then we may take the Fourier transform of the evolution equation (5.20). This gives

$$i\hbar\frac{\partial}{\partial t}\tilde{\phi}(\boldsymbol{q},t) = \frac{1}{2m} \left[\hbar^2 q_x^2 + \hbar^2 q_y^2 + (\hbar q_z - mgt)^2\right] \tilde{\phi}(\boldsymbol{q},t).$$
(5.22)

We then formally solve this equation for $\tilde{\phi}(\boldsymbol{q},t)$, invert the Fourier transform

and return to the lab frame to give the wavefunction at any time t:

$$\psi(\mathbf{r},t) = N^{1/2} \pi^{-3/4} \left(\frac{w}{w^2 + i\frac{\hbar t}{m}} \right)^{3/2} \exp\left\{ -\frac{|\mathbf{r} - \mathbf{R}(t)|^2}{2\left(w^2 + i\frac{\hbar t}{m}\right)} - \frac{itmg}{\hbar} \left(z + \frac{1}{6}gt^2\right) \right\}.$$
 (5.23)

Here we have defined the average "classical" position of the particle $\mathbf{R}(t) \equiv \langle \mathbf{r}(t) \rangle = \mathbf{r}_0 - \frac{1}{2}gt^2\hat{\mathbf{k}}$, where $\hat{\mathbf{k}}$ is the unit vector in the z direction. This gives the position of the centre of the wavepacket. As the wavepacket is accelerating from rest under gravity, the spatial integral in (5.7) will be given by

$$\int_{A} |\psi(\boldsymbol{r},t)|^{2} \, \bar{\boldsymbol{v}} \cdot \mathrm{d}\boldsymbol{S} = gt \iint |\psi(\boldsymbol{r},t)|^{2} \, \mathrm{d}x \mathrm{d}y.$$
(5.24)

It can be seen that the expression in (5.24) depends on $\exp\{-(z-z_0)^2\}$ and thus depends on the height that the wavepacket starts above the detection screen. With this taken into account, one can see that the integral of (5.24) over all time cannot give a constant value of N, and so the expression for N in (5.9) cannot hold for any ξ which is solely dependent on detector properties. This result can be verified numerically.

If we now use (5.11) to calculate the flux-density of particles for this system, we obtain an expression for the integral in (5.12)

$$\int_{A} \boldsymbol{J}(\boldsymbol{r},t) \cdot \mathrm{d}\boldsymbol{S} = \left[gt - \frac{z - z_0 + gt^2/2}{t + w^4 m^2/(\hbar^2 t)} \right] \iint |\psi(\boldsymbol{r},t)|^2 \,\mathrm{d}x \mathrm{d}y.$$
(5.25)

Upon performing the integral in this expression, we may rewrite equation (5.25) as

$$\int_{A} \boldsymbol{J}(\boldsymbol{r},t) \cdot \mathrm{d}\boldsymbol{S} = \left[gt - \frac{z - z_{0} + gt^{2}/2}{t + w^{4}m^{2}/(\hbar^{2}t)} \right] N\pi^{-1/2} \left(\frac{w^{2}}{w^{4} + \hbar^{2}t^{2}/m^{2}} \right)^{1/2} \\ \exp\left\{ \frac{-w^{2}(z - z_{0} + gt^{2}/2)^{2}}{w^{4} + \hbar^{2}t^{2}/m^{2}} \right\}.$$
(5.26)

If we define the quantity u to be

$$u = \frac{w(z - z_0 + gt^2/2)}{\sqrt{w^4 + \hbar^2 t^2/m^2}},$$
(5.27)

then we can simplify (5.26) to give

$$\int_{A} \boldsymbol{J}(\boldsymbol{r},t) \cdot \mathrm{d}\boldsymbol{S} = N\pi^{-1/2} \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} e^{-\boldsymbol{u}^{2}}.$$
(5.28)

The average number of detections \bar{n} is given by (5.12), and if we take a very long detection window such that $t \to -\infty$ and $t + T \to \infty$ then this gives

$$\bar{n} = \xi N \pi^{-1/2} \int_{-\infty}^{\infty} e^{-u^2} \frac{\mathrm{d}u}{\mathrm{d}t} \mathrm{d}t$$
$$= \xi N \pi^{-1/2} \int_{-\infty}^{\infty} e^{-u^2} \mathrm{d}u$$
$$= \xi N \qquad (5.29)$$

Thus we can see that the constant of proportionality ξ is in fact the efficiency of the detector which takes values between 0 and 1.

It is clear to see that the expression obtained in (5.25) is that from (5.24) plus an additional correction, which is a height-dependent velocity term. This additional velocity term is a direct consequence of the dispersive nature of free space for matter waves. From (5.23) it is clear that the wave undergoes dispersion as it falls under gravity. The detection theory based on (5.24) assumes that this dispersed wavepacket propagates through the detection plane at the mean packet velocity. The detection formula in (5.25) based on particle flux does not make this assumption and the factor \hbar/m which quantifies the dispersion of the wave in (5.23) also appears in the detection formula. If this factor is taken to zero either by taking $\hbar \to 0$ or $m \to \infty$, then the dispersion in (5.23) disappears, as does the additional velocity term in (5.25). The time variation of the integrals given by the two different theories are plotted in figure 5.2. For ease of calculation we have used the dimensionless variables $\mathbf{Q} = w\mathbf{r}$ and $T = \hbar t/(mw^2)$, and we have

shows the dimensionless rate $mw^2/\hbar \int \mathbf{J} \cdot d\mathbf{S}$ for the correct theory and the corresponding quantity $mw^2/\hbar \int |\psi(\mathbf{r},t)|^2 \bar{\boldsymbol{v}} \cdot d\mathbf{S}$ for the incorrect theory. It can be seen that the differences in the expressions are quite pronounced: in a detection theory which takes account of dispersion the majority of particles will arrive earlier than they would in a detection theory in which dispersion is not correctly accounted for. In order to see this we consider the case of a wavepacket in the absence of gravity. The average velocity of the wavepacket $(\bar{\boldsymbol{v}} \text{ in } (5.24))$ would remain zero at all times. Because the incorrect theory predicts a detection rate proportional to $\bar{\boldsymbol{v}}$, we would have a zero detection rate at all times. Due to dispersion, however, the bosons would pass the detection plane at some time and so the detection rate would be non-zero. We would expect in this case that a perfect detector with an infinite time window would detect half of the particles. Clearly the incorrect theory does not predict this result. Thus we conclude that the atoms would arrive earlier in a theory in which dispersion is correctly accounted for.

From (5.23) we can see that if the factor $\hbar t/(mw^2)$ is greater than unity, the wavepacket becomes significantly wider (due to dispersion), and this dispersion ought to be taken account of in detection theory. As an example of how important dispersion is in the system under consideration, we take values from the He^{*} experiment presented in [22]. The time of flight of atoms here is 0.1s and the mass of a He^{*} atom is 6.68×10^{-27} kg. We thus find that the dispersion factor will be important for any wavepacket with an initial width of less than 0.1mm. The size of the He^{*} condensate in the z direction is 6μ m and so dispersion will indeed be important in this situation.

5.5 Conclusion

We have described in this chapter the construction of a semiclassical theory of matter wave detection, drawing on the well known theory of photoelectron detection. It is the intrinsically dispersive nature of matter waves which prevents the direct analogy from working. We must instead consider the flux-density of particles, which gives an additional velocity term. Indeed if light passes through and is detected in a dispersive medium, the magnitude



Figure 5.2: Comparison of detection rate for the correct and incorrect detection theories, as a function of time. The plots are taken at the detector surface $Q_z = 0$ and we have chosen the initial centre of the wavepacket to be at $Q_z = 3$. The solid line shows the correct theory (5.25) and the dotted line shows the incorrect theory (5.24).

of the Poynting vector, which represents the flux-density of energy, must be used in place of (5.2).

In the next chapter we derive the link between the detection rate and the flux density through the detector from microscopic considerations. In order to do this we quantise the matter wave field and start from the fact that the detector responds to the field density, not its flux.

Chapter 6

Quantum theory of matter wave detection

6.1 Introduction

In the previous chapter, we saw that the detection probability was explicitly related to the flux through the detector surface. Here we derive a quantum theory of matter wave detection, starting from a microscopic description of detection and progressing to the description of a bulk detector of finite extent. We calculate the detection rate using perturbation theory, which does not take account of the back-action of detection on the atomic wavefunction. We then modify this using a Langevin-type description to give an exact result. In order to illustrate the difference between the methods, we present an example involving a single atom falling under gravity onto a flat detector. This chapter represents an original contribution and is currently in preparation for publication.

6.2 Formalism

The He^{*} experiment of Robert, *et al* [22] uses a microchannel plate (MCP) placed below the trap to detect the falling atoms. MCPs can detect either UV photons or charged particles. As there are no charged particles present in

the system, we conclude that the electric field of the detector atoms disturbs the symmetry of the He^{*} wavefunction. This causes the atom to decay to its ground state and release a UV photon which induces the creation of an ion-electron pair in the detector.

In this chapter we will use second quantised operators to describe the matter wave field. As we have seen in chapter 2, the field is represented by the operator $\hat{\psi}^{\dagger}(\mathbf{r})$, which creates a condensate atom at position \mathbf{r} , and its hermitian conjugate $\hat{\psi}(\mathbf{r})$, which annihilates an atom. We will work in the interaction picture in section 6.3 and the Heisenberg picture in section 6.4. Both of these involve time varying operators, and the equal time commutation relation between the field creation operator and its conjugate is given by

$$\left[\hat{\psi}(\boldsymbol{r},t),\hat{\psi}^{\dagger}(\boldsymbol{r}',t)\right] = \delta(\boldsymbol{r}-\boldsymbol{r}'), \qquad (6.1)$$

where $\delta(\mathbf{r} - \mathbf{r'})$ is the Dirac delta function. In general the matter wave field operator should be a spinor field, which includes a spin quantum number, rather than a scalar one. In the case of He^{*}, however, the condensate is a spin polarised gas of atoms, so that a scalar field contains sufficient information.

We can construct a model for the process described above in which the Hamiltonian has terms describing the matter wave field, the detector and the interactions between them. For a matter wave field in a (possibly nonlinear) potential $V(\mathbf{r})$ and with internal electronic energy E_e , the Hamiltonian is given by

$$\hat{H}_{MW} = \int_{-\infty}^{\infty} \mathrm{d}^3 \boldsymbol{r} \left\{ \frac{\hbar^2}{2m} \left[\nabla \hat{\psi}^{\dagger}(\boldsymbol{r}) \right] \cdot \left[\nabla \hat{\psi}(\boldsymbol{r}) \right] + \hat{\psi}^{\dagger}(\boldsymbol{r}) \left[V(\boldsymbol{r}) + E_e \right] \hat{\psi}(\boldsymbol{r}) \right\}.$$
(6.2)

Because the field is second quantised we must also introduce a second quantised description of the detector. The detection process involves the creation of an ion-electron pair inside the detector. We therefore introduce the operator $\hat{\sigma}^{\dagger}(\mathbf{r}, E)$ which creates such a pair with total energy E at position \mathbf{r} . The position considered here is in fact an element of a set of discrete positions, due to the construction of the detector. In the situation of interest however, the distance between detector atoms will be very small compared with the width of the matter wavepacket and the associated de Broglie wavelength. Thus we treat r as a continuum of possible points in space. Any single detector atom will never be doubly excited and hence we are free to choose the detection event creation operator to be either bosonic or fermionic in nature. For ease of calculation, however, we choose it to be bosonic and thus obey equal-time commutation relations given by

$$\left[\hat{\sigma}(\boldsymbol{r}, \boldsymbol{E}, t), \hat{\sigma}^{\dagger}(\boldsymbol{r}', \boldsymbol{E}', t)\right] = \delta(\boldsymbol{r} - \boldsymbol{r}')\delta(\boldsymbol{E} - \boldsymbol{E}').$$
(6.3)

When the detector creation operator acts on the ground state of the detector $|0\rangle_D$, we obtain the continuum detector states

$$\hat{\sigma}^{\dagger}(\boldsymbol{r}, E)|0\rangle_{D} = |\boldsymbol{r}, E\rangle_{D} \tag{6.4}$$

which obey the normalisation condition

$$\langle \mathbf{r}', E' | \mathbf{r}, E \rangle = \delta(\mathbf{r} - \mathbf{r}') \delta(E - E').$$
 (6.5)

With this in mind, the detector Hamiltonian is constructed to be

$$\hat{H}_D = \int_{-\infty}^{\infty} \mathrm{d}^3 r \int_0^{\infty} \mathrm{d}EED(\boldsymbol{r})\hat{\sigma}^{\dagger}(\boldsymbol{r}, E)\hat{\sigma}(\boldsymbol{r}, E), \qquad (6.6)$$

where D(r) is a function which is unity for values of r which are inside the detector and zero for those which are outside.

The interaction between the detector and the matter wave is described by the interaction Hamiltonian

$$\hat{V} = \int_{-\infty}^{\infty} \mathrm{d}^3 r \int_{-\infty}^{\infty} \mathrm{d}^3 r' \int_{0}^{\infty} \mathrm{d}ED(\mathbf{r}') \left[\xi(\mathbf{r} - \mathbf{r}', E)\hat{\sigma}^{\dagger}(\mathbf{r}', E)\hat{\psi}(\mathbf{r}) + H.C. \right]. (6.7)$$

Here we have introduced the function $\xi(\mathbf{r} - \mathbf{r}', E)$ which describes the separation of the boson and the detector atom and also contains the detector response as a function of energy and *H.C.* represents the Hermitian conjugate of the first term.

The total Hamiltonian for the system of matter wave and detector may be written as

$$\hat{H} = \hat{H}_{MW} + \hat{H}_D + \hat{V}.$$
 (6.8)

In the following sections we calculate the matter wave detection rate using this formalism.

6.3 Perturbation theoretic approach

In this section we use perturbation theory to first order to calculate the short-time detection rate. Given an initial state $|i\rangle$ and a final state $|f\rangle$ in the Schrödinger picture the probability of transition within a time window $t_0 \rightarrow t$ is given by

$$P_{fi}(t_0,t) = \frac{1}{\hbar^2} \left| \int_{t_0}^t \mathrm{d}t' \langle f | \exp\left[\frac{i(t'-t)}{\hbar} \hat{H}_0\right] \hat{V} \exp\left[-\frac{it'}{\hbar} \hat{H}_0\right] |i\rangle \right|^2.$$
(6.9)

In the case where $|i\rangle$ and $|f\rangle$ are eigenstates of \hat{H}_0 , (6.9) gives

$$P_{fi}(0,t) = \frac{1}{\hbar^2} \left| \int_0^t \mathrm{d}t' \exp\left[\frac{it'(E_f - E_i)}{\hbar}\right] \langle f|\hat{V}|i\rangle \right|^2, \tag{6.10}$$

where we have replaced t_0 with 0. If \hat{V} is independent of time, we may take it outside the integral and write

$$P_{fi}(0,t) = \frac{\left|\langle f|\hat{V}|i\rangle\right|^{2}}{\hbar^{2}} \left|\int_{0}^{t} dt' \exp\left[\frac{it'(E_{f}-E_{i})}{\hbar}\right]\right|^{2}$$
$$= \frac{\left|\langle f|\hat{V}|i\rangle\right|^{2}}{(E_{f}-E_{i})^{2}} \left|\exp\left[\frac{it'(E_{f}-E_{i})}{\hbar}\right] - 1\right|^{2}$$
$$= \frac{\left|\langle f|\hat{V}|i\rangle\right|^{2}}{(E_{f}-E_{i})^{2}} 4\sin^{2}\left[\frac{t'(E_{f}-E_{i})}{2\hbar}\right].$$
(6.11)

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This is a sharply peaked function of $(E_f - E_i)$, with a peak width of $2\pi/t$. If the Hamiltonian \hat{H}_0 has a continuum of states with a number density per unit energy of $\rho(E)$, then the transition probability will be given by

$$\mathcal{P}_{fi} = \int dE_f \rho(E_f) P_{fi}(0,t)$$

=
$$\int dE_f \rho(E_f) \frac{\left|\langle f|\hat{V}|i\rangle\right|^2}{(E_f - E_i)^2} 4\sin^2\left[\frac{t'(E_f - E_i)}{2\hbar}\right]. \quad (6.12)$$

As the sinc function is sharply peaked at $E_f = E_i$, we can take the slowly varying functions of E_f out of the integral. This leaves us with

$$\mathcal{P}_{fi} = \left\{ \rho(E_f) \left| \langle f | \hat{V} | i \rangle \right|^2 \right\}_{E_f = E_i} \int \mathrm{d}E_f \frac{4}{(E_f - E_i)^2} \sin^2 \left[\frac{t'(E_f - E_i)}{2\hbar} \right]$$
$$= \left\{ \rho(E_f) \left| \langle f | \hat{V} | i \rangle \right|^2 \right\}_{E_f = E_i} \frac{2\pi t}{\hbar}.$$
(6.13)

The transition rate is given by the time rate of change of the transition probability, which is

$$\mathcal{R}_{fi} = \frac{2\pi}{\hbar} \left[\left| \langle f | \hat{V} | i \rangle \right|^2 \rho(E_f) \right]_{E_f = E_i}.$$
(6.14)

This expression is known as Fermi's Golden Rule.

For the case of matter wave detection, we define the initial and final states to be

$$|i\rangle = |I\rangle_{MW} \otimes |0\rangle_D \tag{6.15}$$

$$|f\rangle = |F\rangle_{MW} \otimes |\mathbf{r}_0, E_0\rangle_D. \tag{6.16}$$

The operator expression in equation (6.9) may be written in the expanded form

$$\exp\left[rac{it'\hat{H}_{MW}}{\hbar}
ight]\exp\left[rac{it'\hat{H}_D}{\hbar}
ight]\hat{V}\exp\left[rac{-it'\hat{H}_D}{\hbar}
ight]\exp\left[rac{-it'\hat{H}_{MW}}{\hbar}
ight],$$

where we have omitted the term proportional to t. The middle three terms

of this expression become, upon substituting expression (6.7) for \hat{V}

$$\int_{-\infty}^{\infty} \mathrm{d}^{3}r \int_{-\infty}^{\infty} \mathrm{d}^{3}r' \int_{0}^{\infty} \mathrm{d}ED(\mathbf{r}')$$
$$\exp\left[\frac{it'\hat{H}_{D}}{\hbar}\right] \left[\xi(\mathbf{r}-\mathbf{r}',E)\hat{\sigma}^{\dagger}(\mathbf{r}',E)\hat{\psi}(\mathbf{r}) + H.C.\right] \exp\left[\frac{-it'\hat{H}_{D}}{\hbar}\right]$$

We will concentrate only on the term

$$I \equiv D(\mathbf{r}') \exp\left[\frac{it'\hat{H}_D}{\hbar}\right] \hat{\sigma}^{\dagger}(\mathbf{r}', E) \exp\left[\frac{-it'\hat{H}_D}{\hbar}\right].$$
 (6.17)

In order to simplify this we will calculate the commutator

$$C \equiv \left[\hat{H}_D, \hat{\sigma}^{\dagger}(\boldsymbol{r}', E)\right].$$

Upon substituting expression (6.6) for \hat{H}_D we obtain

$$C = \left[\int_{-\infty}^{\infty} d^3 r_1 \int_{0}^{\infty} dE_1 E_1 D(\boldsymbol{r}_1) \hat{\sigma}^{\dagger}(\boldsymbol{r}_1, E_1) \hat{\sigma}(\boldsymbol{r}_1, E_1), \hat{\sigma}^{\dagger}(\boldsymbol{r}', E) \right]$$

$$= \int_{-\infty}^{\infty} d^3 r_1 \int_{0}^{\infty} dE_1 E_1 D(\boldsymbol{r}_1) \hat{\sigma}^{\dagger}(\boldsymbol{r}_1, E_1) \left[\hat{\sigma}(\boldsymbol{r}_1, E_1), \hat{\sigma}^{\dagger}(\boldsymbol{r}', E) \right]$$

$$= D(\boldsymbol{r}') E \hat{\sigma}^{\dagger}(\boldsymbol{r}', E).$$
(6.18)

If we expand the left exponential in (6.17) then we obtain

$$I = D(\mathbf{r}') \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{it'}{\hbar}\right)^n \hat{H}_D^n \hat{\sigma}^{\dagger}(\mathbf{r}', E) \exp\left[\frac{-it'\hat{H}_D}{\hbar}\right], \qquad (6.19)$$

and by using the expression for C above, we can simplify this to

$$I = D(\mathbf{r}') \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{it'}{\hbar}\right)^n \hat{\sigma}^{\dagger}(\mathbf{r}', E) \left[\hat{H}_D + D(\mathbf{r}')E\right]^n \exp\left[\frac{-it'\hat{H}_D}{\hbar}\right]$$
$$= D(\mathbf{r}')\hat{\sigma}^{\dagger}(\mathbf{r}', E) \exp\left[\frac{it'E}{\hbar}\right].$$
(6.20)

Therefore we can write detector part of the expectation value in (6.9) as

$$\langle \boldsymbol{r}_{0}, E_{0} | \hat{\sigma}^{\dagger}(\boldsymbol{r}', E) | 0 \rangle \exp\left[\frac{-i(t-t')E}{\hbar}\right]$$

= $\delta(\boldsymbol{r}_{0} - \boldsymbol{r}')\delta(E_{0} - E) \exp\left[\frac{-i(t-t')E}{\hbar}\right].$ (6.21)

In order to calculate the remainder of the transition probability, we assume that the detector material is dense enough that the UV photon travels a distance much smaller than the size of the matter wavepacket. We quantify this by writing

$$\xi(\boldsymbol{r} - \boldsymbol{r}', E) \simeq \chi(E)\delta(\boldsymbol{r} - \boldsymbol{r}'), \qquad (6.22)$$

where $\chi(E)$ now represents the detector response as a function of energy.

The internal energy of a He^{*} atom is about 20 eV, which greatly exceeds its motional energy and it is the internal energy that will determine the energy of the excited ion-electron pair. For this reason it is convenient to split the matter wave Hamiltonian \hat{H}_{MW} into its electronic part

$$\hat{H}_{\boldsymbol{e}} = \int_{-\infty}^{\infty} \mathrm{d}^{3} r \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}) E_{\boldsymbol{e}}$$
(6.23)

and its motional part $\hat{H}_M = \hat{H}_{MW} - \hat{H}_e$. We may then consider the calculation in terms of the field operator evolved under \hat{H}_M alone, which we define as

$$\hat{\psi}_0(\boldsymbol{r},t) = \exp\left[\frac{it\hat{H}_M}{\hbar}\right]\hat{\psi}(\boldsymbol{r})\exp\left[\frac{-it\hat{H}_M}{\hbar}\right].$$
 (6.24)

After substituting all of the above into (6.9) we obtain

$$P_{\boldsymbol{r},E,i}(t_0,t) \mathrm{d}^3 r \mathrm{d}E = \sum_F \frac{1}{\hbar^2} \left| \int_{t_0}^t \mathrm{d}t' D(\boldsymbol{r}) \exp\left[\frac{it'(E-E_e)}{\hbar}\right] \chi(E) \right| \langle F| \exp\left[\frac{-it\hat{H}_{MW}}{\hbar}\right] \hat{\psi}_0(\boldsymbol{r},t') |I\rangle \right|^2 \mathrm{d}^3 r \mathrm{d}E, \quad (6.25)$$

where $P_{\mathbf{r},E,i}(t_0,t)$ is the probability per unit detector volume per unit ionelectron pair energy of a detection taking place between t_0 and t. If we assume that $\langle F | \exp \left[-it\hat{H}_0/\hbar \right] \hat{\psi}_0(\mathbf{r},t') | I \rangle$ varies much more slowly with t'than $\exp[it'(E - E_e)/\hbar]$ then we can take this matrix element outside the time integral and evaluate that integral explicitly.

After the detection event, the electron which is released causes an avalanche process similar to that occurring in photoelectron detection. This means that the detector does not resolve the energy imparted to it during detection. For this reason we integrate (6.25) over all possible ion-electron pair energies. We also integrate over a volume $(\Delta r)^3$ with one corner at r, giving the total probability of detection over the volume $r \to r + \Delta r$ within a time window $t \to t + \Delta t$ as

$$\mathcal{P}(t,\Delta t; \boldsymbol{r},\Delta \boldsymbol{r}) = \int_{0}^{\infty} dE_{0} \int_{\boldsymbol{r}}^{\boldsymbol{r}+\Delta \boldsymbol{r}} d^{3}\boldsymbol{r}' P_{\boldsymbol{r}',E_{0},i}(t,t+\Delta t)$$

$$= 4 \int_{\boldsymbol{r}}^{\boldsymbol{r}+\Delta \boldsymbol{r}} d^{3}\boldsymbol{r}' D(\boldsymbol{r}') \langle \hat{\psi}_{0}^{\dagger}(\boldsymbol{r}',t) \hat{\psi}_{0}(\boldsymbol{r}',t) \rangle$$

$$\int_{-E_{e}}^{\infty} dE' \frac{|\chi(E'+E_{e})|^{2}}{E'^{2}} \sin^{2} \left[\frac{\Delta t}{2\hbar}E'\right], \quad (6.26)$$

where we have used the completeness relation for the states $|F\rangle$. It is interesting to note that the normal ordering of the field operators in this expression has appeared naturally from the derivation. This ensures that detection does not occur when there are no matter waves present. The function $E^{-2}\sin^2(aE)$ is sharply peaked at E = 0 with a central peak of width π/a . We assume that $|\chi(E' + E_e)|^2$ is slowly varying near E' = 0 so that it can be taken out of the energy integral and replaced with its value at E' = 0. If $E_e \gg 2\pi\hbar/\Delta t$, we may extend the lower limit of the energy integral to infinity without changing the result. The total probability may therefore be written in the form

$$\mathcal{P}(t,\Delta t; \boldsymbol{r},\Delta \boldsymbol{r}) = 2\Gamma \Delta t \int_{\boldsymbol{r}}^{\boldsymbol{r}+\Delta \boldsymbol{r}} \mathrm{d}^{3} \boldsymbol{r}' D(\boldsymbol{r}') \langle \hat{\psi}_{0}^{\dagger}(\boldsymbol{r}',t) \hat{\psi}_{0}(\boldsymbol{r}',t) \rangle, \quad (6.27)$$

where we have defined the rate constant

$$\Gamma = \frac{\pi \left| \chi(E_e) \right|^2}{\hbar}.$$
(6.28)
Equation (6.27) is the small-time-window approximation to the probability of detection in a region $\mathbf{r} \to \mathbf{r} + \Delta \mathbf{r}$ in a time window $t \to t + \Delta t$, and is linear in the time-window size. It is also proportional to the mean number of condensate atoms in the detection volume during the detection time. The detection rate is the change in probability with time and in this case will be given by

$$\mathcal{R}(t, \boldsymbol{r}, \Delta \boldsymbol{r}) = \frac{\partial}{\partial \Delta t} \mathcal{P}(t, \Delta t; \boldsymbol{r}, \Delta \boldsymbol{r})$$

= $2\Gamma \int_{\boldsymbol{r}}^{\boldsymbol{r}+\Delta \boldsymbol{r}} \mathrm{d}^{3} \boldsymbol{r}' D(\boldsymbol{r}') \langle \hat{\psi}_{0}^{\dagger}(\boldsymbol{r}', t) \hat{\psi}_{0}(\boldsymbol{r}', t) \rangle.$ (6.29)

This is the instantaneous rate of particle detection at time t in a volume $r \rightarrow r + \Delta r$. We can relate the number of atoms present now to the number which were present earlier by writing

$$\int_{\mathbf{r}}^{\mathbf{r}+\Delta\mathbf{r}} \mathrm{d}^{3}\mathbf{r}' D(\mathbf{r}') \langle \hat{\psi}_{0}^{\dagger}(\mathbf{r}',t) \hat{\psi}_{0}(\mathbf{r}',t) \rangle$$

=
$$\int_{-\infty}^{t} \frac{\partial}{\partial t'} \int_{\mathbf{r}}^{\mathbf{r}+\Delta\mathbf{r}} \mathrm{d}^{3}\mathbf{r}' D(\mathbf{r}') \langle \hat{\psi}_{0}^{\dagger}(\mathbf{r}',t') \hat{\psi}_{0}(\mathbf{r}',t') \rangle.$$
(6.30)

If there were initially no atoms present (as would normally be the case in an experiment), then (6.29) may be rewritten as

$$\mathcal{R}(t, \boldsymbol{r}, \Delta \boldsymbol{r}) = 2\Gamma \int_{\boldsymbol{r}}^{\boldsymbol{r}+\Delta \boldsymbol{r}} \mathrm{d}^{3} \boldsymbol{r}' D(\boldsymbol{r}') \int_{-\infty}^{t} \mathrm{d}t' \frac{\partial}{\partial t'} \langle \hat{\psi}_{0}^{\dagger}(\boldsymbol{r}', t') \hat{\psi}_{0}(\boldsymbol{r}', t') \rangle. \quad (6.31)$$

As we have seen in chapter 4, we may relate this to the flux density of matter waves. We will show this here using Heisenberg's equation of motion to write the time derivative in the above as

$$\frac{\partial}{\partial t}\hat{\psi}_{0}^{\dagger}(\boldsymbol{r},t)\hat{\psi}_{0}(\boldsymbol{r},t) = \frac{1}{i\hbar}\left[\hat{H}_{M},\hat{\psi}_{0}^{\dagger}(\boldsymbol{r},t)\hat{\psi}_{0}(\boldsymbol{r},t)\right].$$
(6.32)

The commutator in (6.32) may be evaluated using the form of \hat{H}_M and the delta function property

$$\int_{-\infty}^{\infty} d^3r' f(\boldsymbol{r}') \left[\nabla' \delta(\boldsymbol{r} - \boldsymbol{r}') \right] = - \int_{-\infty}^{\infty} d^3r' \left[\nabla' f(\boldsymbol{r}') \right] \delta(\boldsymbol{r} - \boldsymbol{r}')$$

$$= -\nabla f(\boldsymbol{r}), \tag{6.33}$$

which holds so long as $f(\mathbf{r})$ vanishes at $|\mathbf{r}| = \pm \infty$. The result of this calculation is

$$\left[\hat{H}_{M},\hat{\psi}_{0}^{\dagger}(\boldsymbol{r})\hat{\psi}_{0}(\boldsymbol{r})\right] = \frac{\hbar^{2}}{2m}\nabla\cdot\left\{\left[\nabla\hat{\psi}_{0}^{\dagger}(\boldsymbol{r})\right]\hat{\psi}_{0}(\boldsymbol{r}) - \hat{\psi}_{0}^{\dagger}(\boldsymbol{r})\left[\nabla\hat{\psi}_{0}(\boldsymbol{r})\right]\right\}.$$
 (6.34)

Thus we may write the time derivative in (6.31) as

$$\frac{\partial}{\partial t}\hat{\psi}_{0}^{\dagger}(\boldsymbol{r},t)\hat{\psi}_{0}(\boldsymbol{r},t) = -\nabla \cdot \frac{\hbar}{2im} \left\{ \hat{\psi}_{0}^{\dagger}(\boldsymbol{r},t) \left[\nabla \hat{\psi}_{0}(\boldsymbol{r},t) \right] - \left[\nabla \hat{\psi}_{0}^{\dagger}(\boldsymbol{r},t) \right] \hat{\psi}_{0}(\boldsymbol{r},t) \right\}, \quad (6.35)$$

which has the form of a continuity equation with a flux density operator given by

$$\hat{\boldsymbol{J}}_{0}(\boldsymbol{r},t) = \frac{\hbar}{2im} \left\{ \hat{\psi}_{0}^{\dagger}(\boldsymbol{r},t) \left[\nabla \hat{\psi}_{0}(\boldsymbol{r},t) \right] - \left[\nabla \hat{\psi}_{0}^{\dagger}(\boldsymbol{r},t) \right] \hat{\psi}_{0}(\boldsymbol{r},t) \right\}.$$
(6.36)

We may therefore write equation (6.35) in the more compact form

$$\frac{\partial}{\partial t}\hat{\psi}_{0}^{\dagger}(\boldsymbol{r},t)\hat{\psi}_{0}(\boldsymbol{r},t) = -\nabla \cdot \hat{\boldsymbol{J}}_{0}(\boldsymbol{r},t).$$
(6.37)

Analogy may be drawn with the continuity equations from fluid mechanics [14]. By using Gauss' Theorem

$$\int_{V} \mathrm{d}V \nabla \cdot \hat{\boldsymbol{J}}_{0} = \int_{A} \hat{\boldsymbol{J}}_{0} \mathrm{d}\boldsymbol{S}, \qquad (6.38)$$

we can write the detection rate as

L

$$\mathcal{R}(t,\boldsymbol{r},\Delta\boldsymbol{r}) = -2\Gamma \int_{-\infty}^{t} \mathrm{d}t' \left\langle \int_{A'} \hat{\boldsymbol{J}}_0(\boldsymbol{r}',t') \cdot \mathrm{d}\boldsymbol{S} \right\rangle, \tag{6.39}$$

where A' is the surface of that part of the volume $r \to r + \Delta r$ which is inside the detector and dS is an infinitesimal area element normal to A'. Equation (6.39) gives the small-time-window approximation to the detection rate for bosons, which depends on the boson probability flux-density through the surface of the detector. If the integral in \mathcal{R} includes the entire detector volume then we find that the total detection rate depends on the time-integrated flux of atoms across the surface of the detector. The obvious limitation of this is that it takes no account of the fact that the bosons are absorbed within the detector. They simply pass into the detector, and out of it, and the rate is proportional to the number within it at any one time. In the next section we will remedy this by providing a correction to (6.39) which accounts for the removal of atoms from the condensate.

6.4 Langevin type approach

As the wave travels through the detector, we expect that the detection rate should drop due to the finite probability of detection already having occurred. This is not included in (6.39) as only the free space field operator appears in that expression. In order to quantify this decay we use a Langevin type calculation. The atom and electron-ion pair annihilation operators in the Heisenberg picture

$$\hat{\psi}(\boldsymbol{r},t) = \exp\left(\frac{it\hat{H}}{\hbar}\right)\hat{\psi}(\boldsymbol{r})\exp\left(\frac{-it\hat{H}}{\hbar}\right)$$
 (6.40)

$$\hat{\sigma}(\mathbf{r}, E, t) = \exp\left(\frac{it\hat{H}}{\hbar}\right)\hat{\sigma}(\mathbf{r}, E)\exp\left(\frac{-it\hat{H}}{\hbar}\right),$$
 (6.41)

will be used, where \hat{H} is the full Hamiltonian for the system, given in (6.8). Consider a detector volume which contains condensate atoms. As time evolves these can do one of three things. They can remain in the volume, they can flow out of the surface of the volume or they can be detected. Thus the rate at which atoms are detected in the volume is the rate of decrease of particles in the volume, less the rate of flow of particles out of the volume. Upon defining the particle flux-density operator

$$\hat{J}(\boldsymbol{r},t) = \frac{\hbar}{2im} \left\{ \hat{\psi}^{\dagger}(\boldsymbol{r},t) \left[\nabla \hat{\psi}(\boldsymbol{r},t) \right] - \left[\nabla \hat{\psi}^{\dagger}(\boldsymbol{r},t) \right] \hat{\psi}(\boldsymbol{r},t) \right\}, \qquad (6.42)$$

we may write the detection rate as

$$\mathcal{R}(t, \boldsymbol{r}, \Delta \boldsymbol{r}) = -\frac{\partial}{\partial t} \int_{\boldsymbol{r}}^{\boldsymbol{r}+\Delta \boldsymbol{r}} \mathrm{d}^{3} \boldsymbol{r}_{0} \left\langle \hat{\psi}^{\dagger}(\boldsymbol{r}_{0}, t) \hat{\psi}(\boldsymbol{r}_{0}, t) \right\rangle \\ - \left\langle \int_{A} \hat{\boldsymbol{J}}(\boldsymbol{r}_{0}, t) \cdot \mathrm{d} \boldsymbol{S} \right\rangle.$$
(6.43)

In order to calculate this we need to know the time derivative of the field operator. It is possible to draw analogy between this system and the lossy harmonic oscillator [28]. In our case the reservoir will be the detector atoms, while the matter wave field is analogous to the harmonic oscillator itself.

We use the Heisenberg equation of motion to calculate the evolution of the boson field operator, which is given by

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, t) = \left[\frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + E_e \right] \hat{\psi}(\mathbf{r}, t) \\ + \int_{-\infty}^{\infty} \mathrm{d}^3 \mathbf{r}' \int_0^{\infty} \mathrm{d}E D(\mathbf{r}') \xi^*(\mathbf{r} - \mathbf{r}', E) \hat{\sigma}(\mathbf{r}', E, t). \quad (6.44)$$

The evolution of the detector operator $\hat{\sigma}$ can also be calculated, with the result being

$$i\hbar \frac{\partial}{\partial t} \hat{\sigma}(\mathbf{r}, E, t) = D(\mathbf{r}) E \hat{\sigma}(\mathbf{r}, E, t) + D(\mathbf{r}) \int_{-\infty}^{\infty} \mathrm{d}^{3} \mathbf{r}' \xi(\mathbf{r} - \mathbf{r}', E) \hat{\psi}(\mathbf{r}', t).$$
(6.45)

In order to proceed we formally integrate (6.45) and substitute the result into (6.44). Just as in the previous section, we assume that the UV photons involved in the detection travel a distance much smaller than the wavepacket size before it is detected and write $\xi(\mathbf{r} - \mathbf{r}', E)$ in the form (6.22). The detector response function $\chi(E)$ is assumed to be a slowly varying function of E. We also use the fact that the internal energy E_e is large. This leads us to write the time derivative of the boson field operator as

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(\boldsymbol{r},t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) + E_e - i\hbar\Gamma D(\boldsymbol{r})\right]\hat{\psi}(\boldsymbol{r},t) - i\hbar\hat{F}(\boldsymbol{r},t), (6.46)$$

where we have defined

$$\hat{F}(\boldsymbol{r},t) = \frac{i}{\hbar} D(\boldsymbol{r}) \chi^*(E_e) \int_{-\infty}^{\infty} \mathrm{d}E \exp\left(\frac{-iEt}{\hbar}\right) \hat{\sigma}(\boldsymbol{r},E,0)$$
(6.47)

after the Langevin force in the lossy harmonic oscillator problem. We see that Γ is the decay rate for the field operator while inside the detector. In order to be consistent the commutator must remain constant under this evolution. We can show this by formally integrating (6.46) and using the fact that the initial matter wave and detector operators commute. The commutator of the Langevin force operator with its conjugate is also needed and this can be shown to be

$$\left[\hat{F}(\boldsymbol{r},t),\hat{F}^{\dagger}(\boldsymbol{r}',t')\right] = 2\Gamma D(\boldsymbol{r})D(\boldsymbol{r}')\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t').$$
(6.48)

This leads us to recover the equal time commutator for the matter wave field operator inside the detector:

$$\left[\hat{\psi}(\boldsymbol{r},t),\hat{\psi}^{\dagger}(\boldsymbol{r}',t)\right] = \delta(\boldsymbol{r}-\boldsymbol{r}'), \qquad (6.49)$$

which demonstrates the consistency of our approximations.

In order to obtain the correction to the detection rate in (6.39) we use equation (6.46) to calculate the rate of increase of particles in a volume $r \rightarrow r + \Delta r$, which is given by

$$\frac{\partial}{\partial t} \int_{\mathbf{r}}^{\mathbf{r}+\Delta\mathbf{r}} \mathrm{d}^{3}r_{0} \left\langle \hat{\psi}^{\dagger}(\mathbf{r}_{0},t)\hat{\psi}(\mathbf{r}_{0},t) \right\rangle \\
= \int_{\mathbf{r}}^{\mathbf{r}+\Delta\mathbf{r}} \mathrm{d}^{3}r_{0} \left\langle -\nabla \cdot \hat{\boldsymbol{J}}(\mathbf{r}_{0},t) - 2\Gamma D(\mathbf{r}_{0})\hat{\psi}^{\dagger}(\mathbf{r}_{0},t)\hat{\psi}(\mathbf{r}_{0},t) \right. \\
\left. -\hat{F}^{\dagger}(\mathbf{r}_{0},t)\hat{\psi}(\mathbf{r}_{0},t) - \hat{\psi}^{\dagger}(\mathbf{r}_{0},t)\hat{F}(\mathbf{r}_{0},t) \right\rangle.$$
(6.50)

As the state used to evaluate the expectation value is the initial state (6.15), which contains only the unexcited detector state, the terms involving $\hat{F}(\mathbf{r}_0, t)$ and its Hermitian conjugate vanish exactly as $\hat{F}(\mathbf{r}_0, t) \propto \hat{\sigma}(\mathbf{r}_0, E, 0)$. Upon

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using Gauss' theorem on the flux term we find

$$\frac{\partial}{\partial t} \int_{\mathbf{r}}^{\mathbf{r}+\Delta\mathbf{r}} \mathrm{d}^{3}r_{0} \left\langle \hat{\psi}^{\dagger}(\mathbf{r}_{0},t)\hat{\psi}(\mathbf{r}_{0},t) \right\rangle
= -\left\langle \int_{A} \hat{J}(\mathbf{r}_{0},t) \cdot \mathrm{d}\mathbf{S} \right\rangle
-2\Gamma \int_{\mathbf{r}}^{\mathbf{r}+\Delta\mathbf{r}} \mathrm{d}^{3}r_{0}D(\mathbf{r}_{0}) \left\langle \hat{\psi}^{\dagger}(\mathbf{r}_{0},t)\hat{\psi}(\mathbf{r}_{0},t) \right\rangle,$$
(6.51)

where A is the surface of the volume of interest and dS is an infinitesimal area element normal to this surface. This allows the atom detection rate to be expressed as

$$\mathcal{R}(t, \boldsymbol{r}, \Delta \boldsymbol{r}) = 2\Gamma \int_{\boldsymbol{r}}^{\boldsymbol{r}+\Delta \boldsymbol{r}} \mathrm{d}^{3} r_{0} D(\boldsymbol{r}_{0}) \left\langle \hat{\psi}^{\dagger}(\boldsymbol{r}_{0}, t) \hat{\psi}(\boldsymbol{r}_{0}, t) \right\rangle, \qquad (6.52)$$

which has the same form as the perturbative rate (6.29), but with the fullyevolved matter wave operators replacing the free evolution operators. In order to express the detection rate in terms of the flux operator alone, we once again consider the case in which no helium atoms were present in the detector at $t = -\infty$. This allows us to rewrite the detection rate as

$$\mathcal{R}(t,\boldsymbol{r},\Delta\boldsymbol{r}) = 2\Gamma \int_{\boldsymbol{r}}^{\boldsymbol{r}+\Delta\boldsymbol{r}} \mathrm{d}^{3}\boldsymbol{r}_{0}D(\boldsymbol{r}_{0}) \int_{-\infty}^{t} \mathrm{d}t' \frac{\partial}{\partial t'} \left\langle \hat{\psi}^{\dagger}(\boldsymbol{r}_{0},t')\hat{\psi}(\boldsymbol{r}_{0},t')\right\rangle.$$
(6.53)

In order to proceed we must explicitly solve the differential equation in (6.51). The resulting expression for the rate is

$$\mathcal{R}(t, \boldsymbol{r}, \Delta \boldsymbol{r}) = -2\Gamma \int_{-\infty}^{t} \mathrm{d}t' \left\langle \int_{A'} \hat{\boldsymbol{J}}(\boldsymbol{r}_0, t') \cdot \mathrm{d}\boldsymbol{S} \right\rangle \exp\left[-2\Gamma(t - t')\right], \quad (6.54)$$

where A' is the surface of that part of the volume $\mathbf{r} \to \mathbf{r} + \Delta \mathbf{r}$ which is inside the detector and $d\mathbf{S}$ is an infinitesimal area element normal to A'. The rate of detection is dependent on the flux through the detector surface at all previous times, weighted by a factor which decays exponentially with time.

6.5 Single atom example

As an example we will consider a single atom wavepacket falling under gravity onto a flat detector which is much larger than the width of the wavepacket. In the direction of acceleration of the wavepacket, the detector is large enough for the probability of the wavepacket exiting through the bottom surface to be negligible. We quantify this by considering the direction of acceleration to be -z, with the detector being infinite in the x and y dimensions and semi-infinite in the z dimension. The top of the detector is set at z = 0. We will use the initial state from (6.15) with the initial matter wave state given by the single particle state

$$|\phi\rangle_{MW} = \int_{-\infty}^{\infty} d^3 r \hat{\psi}^{\dagger}(\boldsymbol{r}) \phi(\boldsymbol{r}) |0\rangle_{MW}$$
(6.55)

where $\phi(\mathbf{r})$ is the single particle wavefunction. For the sake of simplicity we choose $\phi(\mathbf{r})$ to be a Gaussian with the normalised form

$$\phi(\mathbf{r}) = (\pi w^2)^{-3/4} \exp\left[\frac{-|\mathbf{r} - \mathbf{r}_0|^2}{2w^2}\right].$$
 (6.56)

Here w is the width of the Gaussian and r_0 is the initial position of the centre of the wavepacket. In order to calculate the rate given in (6.54) we must solve (6.46) with $V(\mathbf{r}) = mgz$. Thus the equation of motion for the field operator is

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(\boldsymbol{r},t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + mgz + E_e - i\hbar\Gamma D(z)\right]\hat{\psi}(\boldsymbol{r},t) - i\hbar\hat{F}(\boldsymbol{r},t).$$
(6.57)

We do not need to solve (6.57) explicitly in order to find the detection rate. What we do need is the action of $\hat{\psi}$ on the initial state vector. In order to find this we act (6.57) on $|i\rangle$, noting that \hat{F} depends only on the initial value of $\hat{\sigma}$:

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(\boldsymbol{r},t)|\phi\rangle_{MW} = \left[\frac{-\hbar^2}{2m}\nabla^2 + mgz + E_e - i\hbar\Gamma D(z)\right]\hat{\psi}(\boldsymbol{r},t)|\phi\rangle_{MW}.$$
(6.58)

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The conditions that we would like to impose at the boundary are those of continuity of the operator and of its first spatial derivative. If we were to insist on continuity of the derivative then we would have to include reflections in our model. In making the decay rate Γ small we make the reflections negligible. This allows us to neglect the derivative continuity and make the *ansatz*

$$\hat{\psi}(\boldsymbol{r},t) = A(z,t)\hat{\psi}_f(\boldsymbol{r},t) \tag{6.59}$$

where $\hat{\psi}_f$ is the free space field operator which satisfies

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}_f(\boldsymbol{r},t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + mgz + E_e\right]\hat{\psi}_f(\boldsymbol{r},t).$$
(6.60)

If we substitute (6.59) into (6.58) we obtain

$$i\hbar\frac{\partial A}{\partial t}\hat{\psi}_{f}|\phi\rangle_{MW} = \left[\frac{-\hbar^{2}}{2m}\frac{\partial^{2}A}{\partial z^{2}} - \frac{\hbar^{2}}{m}\frac{\partial A}{\partial z}\frac{\partial}{\partial z} - i\hbar\Gamma D(z)A\right]\hat{\psi}_{f}|\phi\rangle_{MW}.$$
 (6.61)

As we have neglected reflections in this calculation, it is also necessary to neglect the contribution of $\frac{\partial^2 A}{\partial z^2}$ to the evolution of A. In doing this we obtain the first order differential equation

$$i\hbar\frac{\partial A}{\partial t}\hat{\psi}_{f}|\phi\rangle_{MW} = \left[\frac{-\hbar^{2}}{m}\frac{\partial A}{\partial z}\frac{\partial}{\partial z} - i\hbar\Gamma D(z)A\right]\hat{\psi}_{f}|\phi\rangle_{MW}.$$
 (6.62)

It is a straightforward but lengthy calculation to solve this for A using the method of characteristics. The result obtained is

$$A(z,t) = \exp\left\{-\Gamma D(z)t - \Gamma D(z)\left[\frac{-(z-z_0)}{g(t-imw^2/\hbar)} - \frac{(t+imw^2/\hbar)}{2} - \sqrt{\frac{(z-z_0)^2}{g^2(t-imw^2/\hbar)^2} + \frac{(t-imw^2/\hbar)^2}{4} + \frac{z+z_0}{g}}\right]\right\}.$$
 (6.63)

For simplicity in plotting we have used dimensionless variables

$$Q = \frac{r}{w}$$
(6.64)

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$$T = \frac{\hbar t}{mw^2} \tag{6.65}$$

$$\gamma = \frac{\Gamma m w^2}{\hbar} \tag{6.66}$$

and we have used a system of units such that

$$\frac{gm^2w^3}{\hbar^2} = 1.$$
 (6.67)

In figure 6.1 we have plotted both $w \iint \langle \hat{\psi}_0^{\dagger}(\boldsymbol{r},t) \hat{\psi}_0(\boldsymbol{r},t) \rangle dxdy$ from section 6.3 and $w \iint \langle \hat{\psi}^{\dagger}(\boldsymbol{r},t) \hat{\psi}(\boldsymbol{r},t) \rangle dxdy$ from section 6.4 as functions of Q_z , with the decay constant being $\gamma = 0.1$. The initial centre of the wavepacket is at $Q_z = 4$ which is sufficiently high above the detector for the probability of finding the atom inside the detector to be negligible. These snapshots are taken at T = 4 which corresponds to a time at which most of the wavepacket has entered the detector. Here we see the effect of the detector on the probability density, with the probability of the atom being present decaying exponentially with distance travelled through the detector. Figure 6.2 shows the form of the dimensionless rate $mw^2 \mathcal{R}(t, \boldsymbol{r}, \Delta \boldsymbol{r})/\hbar$ as a function of T, with the perturbative solution and the exact solution both plotted. Here the volume under consideration contains the entire detector. From this graph the effect of the detector presence on the detector rate is quite clear, with an exponential decay in time being seen.

6.6 Conclusions

With a microscopic description of detection as a starting point, we have derived a rate for quantum matter wave detection. This detection rate depends upon the flux-density of the matter waves through the detector surface at all earlier times, with an exponentially decaying weight factor.

It is probable that this theory could be extended to photo-detection. The electromagnetic energy density is given by

$$\hat{W}(\boldsymbol{r},t) = \frac{1}{2} \left\{ \hat{\boldsymbol{E}}(\boldsymbol{r},t) \cdot \hat{\boldsymbol{D}}(\boldsymbol{r},t) + \hat{\boldsymbol{B}}(\boldsymbol{r},t) \cdot \hat{\boldsymbol{H}}(\boldsymbol{r},t) \right\}.$$
(6.68)

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Figure 6.1: $w \iint \langle \hat{\psi}^{\dagger}(\mathbf{r},t) \hat{\psi}(\mathbf{r},t) \rangle dxdy$ as a function of Q in the single atom example. The solid line is the Langevin solution and the dot-dash line is the short-time-window approximation. The horizontal line indicates the position of the detector top surface.

This energy density obeys a continuity equation of the form

$$\frac{\partial}{\partial t}\hat{W}(\boldsymbol{r},t) + \nabla \cdot \hat{\boldsymbol{S}}(\boldsymbol{r},t) = -\hat{\boldsymbol{E}}(\boldsymbol{r},t) \cdot \hat{\boldsymbol{J}}(\boldsymbol{r},t), \qquad (6.69)$$

where the electromagnetic energy flux density is given by the Poynting vector operator

$$\hat{\boldsymbol{S}}(\boldsymbol{r},t) = \left\{ \hat{\boldsymbol{E}}(\boldsymbol{r},t) \times \hat{\boldsymbol{H}}(\boldsymbol{r},t) \right\}$$
(6.70)

and \hat{J} is the current operator [16]. One may show, using Fermi's Golden Rule, that the photo-detection rate is proportional to $\langle \hat{E}^{-}(\mathbf{r},t) \cdot \hat{E}^{+}(\mathbf{r},t) \rangle$, where the superscripts + and - refer to the positive and negative frequency components, or the annihilation and creation operator components, respectively. In the case of polarised parallel light beams this can be shown to be equal to the normal ordered Poynting vector operator [25]. However in



Figure 6.2: $mw^2 \mathcal{R}/\hbar$ as a function of T in the single atom example. The solid line is the Langevin solution and the dashed line is the short-time-window approximation.

general we would expect to use a similar method to that in section 6.3 to relate the detection rate to \hat{S} .

The relationship between detection rate and flux arises, at least in the perturbative calculation, from the continuity equation which states that the number of particles is conserved. In the Langevin calculation particles are not conserved as loss due to detection is included, however equation (6.50) is a form of the continuity equation in the presence of a sink. As we have seen in chapter 4, there are other quantities apart from particle number which are conserved. These include energy, momentum and angular momentum and it would be interesting to investigate the transfer of these quantities in terms of their flux-densities.

Chapter 7

Phase fluctuations of two coupled one-dimensional condensates

7.1 Introduction

We turn our attention to trapped condensates. In such situations, the interactions between atoms, which we have ignored up until this point, become important. This chapter is concerned with trapped condensates which can be approximated by a one-dimensional (1D) gas. This means that the trapping in one dimension is much weaker than that in the transverse dimensions. This chapter represents an original contribution to the literature and is published in ref. [29].

7.2 Background

Recently, longitudinal phase fluctuations in very elongated Bose-Einstein condensates have been observed experimentally [30, 31]. Such phase fluctuations are characteristic of 1D Bose gases and appear in the small interaction regime where $\rho \gg \sqrt{m\rho g}/\hbar$, ρ being the linear density of atoms, g the interaction between atoms and m their mass. The opposite limit, called the

Tonks regime [32], where strong correlations between atoms appear is not investigated in this chapter. For 1D Bose gases, at temperatures T much smaller than $T_{\rho} = \hbar \rho \sqrt{\rho g/m}/k_B$, fluctuations of density are suppressed and one has a quasi-condensate [33, 34, 35, 36, 37]. However fluctuations of phase are still present [33] and with normal experimental parameters these phase fluctuations are produced by the thermal population of collective modes.

In this chapter we are interested in the case of two elongated condensates coupled along their whole extension by a single-atom interaction which enables local transfer of atoms from one condensate to the other. Such a situation could be achieved using a Raman or RF coupling between different internal states. It could also model the case of condensates in two very elongated traps coupled by a tunnelling effect. The physics of two coupled condensates, which contains the Josephson oscillations, has been studied in a two-mode model [38, 39, 40]. In particular the many body ground state [39] and the thermal equilibrium state [40] have been computed. Within the two-mode model the excitation spectrum of two-component condensates coupled by a local single-atom coupling has been calculated using Bogoliubov theory [41]. In the case of two elongated condensates, two effects act in opposite directions. Longitudinal phase fluctuations in each condensate tend to smear out the relative phase between the two condensates, while the coupling between the condensates energetically favours the case of identical local relative phase. The goal of this chapter is to determine the relative phase of the two condensates at thermal equilibrium as a function of the strength of the coupling.

7.3 Formalism

We are interested in cylindrical condensates where the temperature k_BT , the interaction energy $g\rho$ and the coupling strength γ are all much smaller than the transverse confinement energy $\hbar\omega_{\perp}$, which is the strength of the trap in the dimensions perpendicular to the condensate axis. In this case we can treat the BECs as 1D objects. Figure 7.1 gives a pictorial representation of the situation studied here. The BECs are labelled a and b, and we write the



Figure 7.1: Situation studied in this chapter. Two elongated condensates are coupled by a interaction which enables local transfer of atoms from one condensate to the other.

Hamiltonian in the form

$$\begin{split} H_{0} &= \int_{-\infty}^{\infty} \mathrm{d}z \left\{ \frac{-\hbar^{2}}{2m} \left[\hat{\psi}_{a}^{\dagger}(z,t) \frac{\partial^{2}}{\partial z^{2}} \hat{\psi}_{a}(z,t) + \hat{\psi}_{b}^{\dagger}(z,t) \frac{\partial^{2}}{\partial z^{2}} \hat{\psi}_{b}(z,t) \right] \\ &+ U(z) \left[\hat{\psi}_{a}^{\dagger}(z,t) \hat{\psi}_{a}(z,t) + \hat{\psi}_{b}^{\dagger}(z,t) \hat{\psi}_{b}(z,t) \right] \\ &+ \frac{g}{2} \left[\hat{\psi}_{a}^{\dagger}(z,t) \hat{\psi}_{a}^{\dagger}(z,t) \hat{\psi}_{a}(z,t) + \hat{\psi}_{b}^{\dagger}(z,t) + \hat{\psi}_{b}^{\dagger}(z,t) \hat{\psi}_{b}^{\dagger}(z,t) \hat{\psi}_{b}(z,t) \right] \\ &- \gamma \left[\hat{\psi}_{a}^{\dagger}(z,t) \hat{\psi}_{b}(z,t) + \hat{\psi}_{b}^{\dagger}(z,t) \hat{\psi}_{a}(z,t) \right] \right\}, \end{split}$$
(7.1)

where U(z) is the trapping potential in the axial direction. Here we can see the kinetic energy term, the trapping potential and the interaction terms on the first three lines respectively, and the last line represents the coupling between the condensates. As we wish to conserve the number of particles on average, the Hamiltonian we use is in fact $\hat{H} = \hat{H}_0 - \mu \hat{N}$, where μ is the chemical potential. Assuming that the size of the transverse ground state $a_{\perp} = \sqrt{2\hbar/m\omega_{\perp}}$ is much larger than the s-wave scattering length a, the effective coupling constant is simply $g = (2\hbar^2/m)(2a/a_{\perp}^2)$.

The bosonic field operators for different condensates commute and so we write the equal time commutation relations as

$$\left[\hat{\psi}_i(z,t),\hat{\psi}_j^{\dagger}(z',t)\right] = \delta(z-z')\delta_{ij}.$$
(7.2)

Upon calculating the Heisenberg equation of motion (2.29) for the bosonic

field operators, we obtain their evolution

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}_{a,b}(z,t) = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \hat{\psi}_{a,b}(z,t) + [U(z) - \mu] \hat{\psi}_{a,b}(z,t) + g \hat{\psi}^{\dagger}_{a,b}(z,t) \hat{\psi}_{a,b}(z,t) \hat{\psi}_{a,b}(z,t) - \gamma \hat{\psi}_{b,a}(z,t)$$
(7.3)

For quasi-condensates the Bogoliubov theory cannot be used in the same form as presented in chapter 2. This is due to the fact that there is not a single macroscopically occupied quantum state. Instead we must expand the operator $\hat{\psi}(z,t)$ in terms of its density operator $\hat{\rho}$ and phase operator $\hat{\theta}$. The field operator thus becomes [33, 37]

$$\hat{\psi}(z,t) = \exp\left[i\hat{\theta}(z,t)\right]\sqrt{\hat{\rho}(z,t)},$$
(7.4)

where the commutator of the density and phase operators is given by

$$\left[\hat{\rho}_i(z,t),\hat{\theta}_j(z',t)\right] = i\delta(z-z')\delta_{i,j}.$$
(7.5)

We must be very careful with the definition of the phase operator. In quantum optics the phase operator is not a simple quantity to define, due to the its periodicity. Pegg and Barnett [42, 43, 44] give a detailed description of an interpretation of the phase operator in quantum optics. It is only permissible to write the field operator in the form in (7.4) if the state in question has a large amplitude and the fluctuations in the phase and density operators are small. This is indeed the situation in quasi-condensates.

Upon expanding the field operator as suggested in (7.4), we obtain a complex differential equation. If we equate the real and imaginary parts, the resulting coupled evolution equations are given by

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$$-g\hat{\rho}_{a,b} + \gamma \cos\left(\hat{\theta}_{a,b} - \hat{\theta}_{b,a}\right) \frac{\sqrt{\hat{\rho}_{a,b}}}{\sqrt{\hat{\rho}_{b,a}}}$$
(7.7)

The approximation of small density fluctuations together with equation (7.6) implies that the phase gradient will also be small. We make the *a priori* assumption that the phase difference between the condensates at a given position will be small, so that

$$\left|\Delta\hat{\theta}(z)\right| = \left|\hat{\theta}_a(z) - \hat{\theta}_b(z)\right| \ll 1.$$
(7.8)

The small density fluctuations are quantified by splitting the density operator into a mean field (stationary solution) and a fluctuating part

$$\hat{\rho}_{a,b}(z,t) = \rho_0(z) + \delta \hat{\rho}_{a,b}(z,t)$$
(7.9)

where $\delta \hat{\rho}_{a,b} \ll \rho_0$. The coupled evolution equations above may be expanded in terms of the small parameters $\delta \hat{\rho}_{a,b}/\rho_0$, $\Delta \hat{\theta}$ and $\partial \hat{\theta}_{a,b}/\partial z$. To the lowest order in these parameters we obtain the equations

$$\frac{\partial \rho_0}{\partial t} = 0 \tag{7.10}$$

$$0 = \frac{\hbar^2}{2m\sqrt{\rho_0}} \frac{\partial^2 \sqrt{\rho_0}}{\partial z^2} - U + \mu - g\rho_0 + \gamma.$$
 (7.11)

The first of these gives the stationarity of ρ_0 and the second is the timeindependent Gross-Pitaevskii equation for $\sqrt{\rho_0}$, with the chemical potential modified by taking $\mu \to \mu + \gamma$. The first order terms give us the evolution equations

$$\hbar \frac{\partial}{\partial t} \left(\hat{\theta}_{a,b} \sqrt{\rho_0} \right) = - \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + U + 3g\rho_0 - \mu \right) \left(\frac{\delta \hat{\rho}_{a,b}}{2\sqrt{\rho_0}} \right)
 + \gamma \left(\frac{\delta \hat{\rho}_{b,a}}{2\sqrt{\rho_0}} \right)$$

$$\hbar \frac{\partial}{\partial t} \left(\frac{\delta \hat{\rho}_{a,b}}{2\sqrt{\rho_0}} \right) = \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + U + g\rho_0 - \mu \right) \left(\hat{\theta}_{a,b} \sqrt{\rho_0} \right)$$

$$(7.12)$$

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$$- \gamma \left(\hat{\theta}_{b,a} \sqrt{\rho_0} \right). \tag{7.13}$$

We can see that these are identical to the single 1D condensate equations, with coupling terms added. In order to begin to solve these equations, we perform a transformation to new operators $\hat{B}_{a,b}$ given by

$$\hat{B}_{a,b} = \frac{\delta \hat{\rho}_{a,b}}{2\sqrt{\rho_0}} + i\hat{\theta}_{a,b}\sqrt{\rho_0}.$$
(7.14)

By using the commutator (7.5) we can evaluate the equal time commutator

$$\begin{bmatrix} \hat{B}_{i}(z,t), \hat{B}_{j}^{\dagger}(z',t) \end{bmatrix} = \begin{bmatrix} \frac{\delta \hat{\rho}_{i}(z,t)}{2\sqrt{\rho_{0}(z)}} + i\hat{\theta}_{i}\sqrt{\rho_{0}(z')}, \frac{\delta \hat{\rho}_{j}(z',t)}{2\sqrt{\rho_{0}(z')}} - i\hat{\theta}_{j}(z',t)\sqrt{\rho_{0}(z')} \end{bmatrix}$$

$$= \frac{i\sqrt{\rho_{0}(z')}}{2\sqrt{\rho_{0}(z)}} \left\{ \begin{bmatrix} \delta \hat{\rho}_{i}(z,t), \hat{\theta}_{j}(z',t) \end{bmatrix} - \begin{bmatrix} \hat{\theta}_{i}(z,t), \delta \hat{\rho}_{j}(z',t) \end{bmatrix} \right\}$$

$$= \delta(z-z')\delta_{ij},$$
(7.15)

with all other combinations being zero. Thus the \hat{B} are bosonic operators and they evolve according to

$$i\hbar \frac{\partial}{\partial t} \hat{B}_{a,b}(z,t) = \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + U + 2g\rho_0 - \mu\right) \hat{B}_{a,b}(z,t) + g\rho_0 \hat{B}_{a,b}^{\dagger}(z,t) - \gamma \hat{B}_{b,a}(z,t).$$
(7.16)

With the help of the matrices

$$\mathcal{L}(\alpha) = \begin{pmatrix} \frac{-\hbar^2}{2m}\Delta + U - \alpha + 2g\rho_0 & g\rho_0 \\ -g\rho_0 & \frac{\hbar^2}{2m}\Delta - U + \alpha - 2g\rho_0 \end{pmatrix}$$
(7.17)

$$\Gamma = \begin{pmatrix} -\gamma & 0 \\ 0 & \gamma \end{pmatrix}, \tag{7.18}$$

we can write the evolution of the \hat{B} operators as a matrix equation

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} B_a \\ B_a^{\dagger} \\ B_b \\ B_b^{\dagger} \end{pmatrix} = \begin{pmatrix} \mathcal{L}(\mu) & \Gamma \\ \Gamma & \mathcal{L}(\mu) \end{pmatrix} \begin{pmatrix} B_a \\ B_a^{\dagger} \\ B_b \\ B_b^{\dagger} \end{pmatrix}.$$
 (7.19)

Such an evolution is the same as the one given by standard Bogoliubov theory. This has been calculated before for the case of a multicomponent condensate with a single particle coupling [41].

We wish to transform these equations into a decoupled set of equations, which means transforming the matrix in (7.19) into a block diagonal one. In order to do this we write the \hat{B} operators in terms of their decomposition into quasi-particle modes, just as we did in chapter 2. Thus we write

$$\hat{B}_{a}(z,t) = \sum_{k} \left[\hat{b}_{sk}(t) u_{sk}(z) + \hat{b}_{sk}^{\dagger}(t) v_{sk}^{*}(z) + \hat{b}_{nk}(t) u_{nk}(z) + \hat{b}_{nk}^{\dagger}(t) v_{nk}^{*}(z) \right]$$
(7.20)

$$\hat{B}_{b}(z,t) = \sum_{k} \left[\hat{b}_{sk}(t) u_{sk}(z) + \hat{b}^{\dagger}_{sk}(t) v^{*}_{sk}(z) - \hat{b}_{nk}(t) u_{nk}(z) - \hat{b}^{\dagger}_{nk}(t) v^{*}_{nk}(z) \right]$$
(7.21)

and the inverse transformation equations are

$$\hat{b}_{sk}(t) = \int_{-\infty}^{\infty} dz \left\{ u_{sk}^{*}(z) \left[\hat{B}_{a}(z,t) + \hat{B}_{b}(z,t) \right] - v_{sk}^{*}(z) \left[\hat{B}_{a}^{\dagger}(z,t) + \hat{B}_{b}^{\dagger}(z,t) \right] \right\}$$
(7.22)

$$\hat{b}_{nk}(t) = \int_{-\infty}^{\infty} dz \left\{ u_{nk}^{*}(z) \left[\hat{B}_{a}(z,t) - \hat{B}_{b}(z,t) \right] - v_{nk}^{*}(z) \left[\hat{B}_{a}^{\dagger}(z,t) - \hat{B}_{b}^{\dagger}(z,t) \right] \right\}.$$
(7.23)

The meaning of the subscripts is shown by equations (7.22) and (7.23). The subscript s indicates a symmetric combination of the two \hat{B} operators, where n indicates an antisymmetric combination. The quasi-particle mode opera-

tors obey the bosonic commutation relations

$$\left[\hat{b}_{ik},\hat{b}^{\dagger}_{jk'}\right] = \delta_{i,j}\delta_{k,k'}, \qquad (7.24)$$

where i and j take on the values s or n. This is valid so long as the mode functions labelled u and v obey the orthonormality rules

$$\int_{-\infty}^{\infty} \left[u_{ik}(z) u_{jk'}^{*}(z) - v_{ik}(z) v_{jk'}^{*}(z) \right] = \frac{1}{2} \delta_{i,j} \delta_{k,k'}.$$
 (7.25)

In linear algebra terms, this transformation diagonalises the matrix in (7.19) if the vectors $(u_{sk}, v_{sk}, u_{sk}, v_{sk})^T$, $(v_{sk}^*, u_{sk}^*, v_{sk}^*, u_{sk}^*)^T$, $(u_{nk}, v_{nk}, -u_{nk}, -v_{nk})^T$ and $(v_{nk}^*, u_{nk}^*, -v_{nk}^*, -u_{nk}^*)^T$ are its eigenvectors. We label the corresponding eigenvalues as ϵ_{sk} , $-\epsilon_{sk}$, ϵ_{nk} and $-\epsilon_{nk}$ respectively. The evolution equation (7.19) thus reduces to the decoupled equation

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} b_{sk} \\ b_{sk}^{\dagger} \\ b_{nk} \\ b_{nk}^{\dagger} \end{pmatrix} = \begin{pmatrix} \epsilon_{sk} & 0 & 0 & 0 \\ 0 & -\epsilon_{sk} & 0 & 0 \\ 0 & 0 & \epsilon_{nk} & 0 \\ 0 & 0 & 0 & -\epsilon_{nk} \end{pmatrix} \begin{pmatrix} b_{sk} \\ b_{sk}^{\dagger} \\ b_{nk} \\ b_{nk}^{\dagger} \end{pmatrix}.$$
(7.26)

As for the standard Bogoliubov theory, the Hamiltonian is then written as a sum of independent bosonic excitations (cf. equation (2.110))

$$\hat{H} - H_0 = \sum_i \sum_k \epsilon_{ik} \hat{b}_{ik}^{\dagger} \hat{b}_{ik}, \qquad (7.27)$$

where *i* takes on the values *s* and *n*, H_0 is the ground state energy and the sums are done only on the eigenvectors normalised as in (7.25).

In terms of the \hat{B} operators, the phase operator is written as

$$\hat{\theta}_{a,b} = \frac{1}{2i\sqrt{\rho_0}} \left(\hat{B}_{a,b} - \hat{B}_{a,b}^{\dagger} \right) \tag{7.28}$$

and in terms of the \hat{b} operators this becomes

$$\hat{\theta}_{a,b} = \frac{1}{2i\sqrt{\rho_0}} \sum_{k} \left\{ \left[\hat{b}_{sk}(u_{sk} - v_{sk}) - \hat{b}_{sk}^{\dagger}(u_{sk}^* - v_{sk}^*) \right] \right\}$$

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$$\pm \left[\hat{b}_{nk}(u_{nk} - v_{nk}) - \hat{b}_{nk}^{\dagger}(u_{nk}^{*} - v_{nk}^{*}) \right] \right\}, \qquad (7.29)$$

where the sum and difference refer to $\hat{\theta}_a$ and $\hat{\theta}_b$, respectively. We are interested in the correlation function of the phase difference $\Delta \hat{\theta}$ which is written, after commuting the \hat{B} operators to normal order, as

$$\langle \Delta \hat{\theta}(z) \Delta \hat{\theta}(z') \rangle = \langle : \Delta \hat{\theta}(z) \Delta \hat{\theta}(z') : \rangle + \frac{\delta(z-z')}{2\rho_0}.$$
(7.30)

The second term merely accounts for the phase fluctuations in a coherent state with linear density ρ_0 for each condensate. We are only interested here in the anomalous fluctuations, and thus we will consider only the normal ordered expectation value. If we expand this in terms of the \hat{b} operators and consider thermal equilibrium, so that no correlations between different excitations exist, we obtain

$$\langle : \Delta \hat{\theta}(z) \Delta \hat{\theta}(z') : \rangle = \frac{1}{\rho_0} \sum_k \left\{ \langle \hat{b}_{nk}^{\dagger} \hat{b}_{nk} \rangle \left[f_{nk}(z) f_{nk}^*(z') + f_{nk}(z') f_{nk}^*(z) \right] - v_{nk}^* f_{nk}(z') - v_{nk} f_{nk}^*(z') \right\},$$

$$(7.31)$$

where $f_{nk}(z) = u_{nk}(z) - v_{nk}(z)$. As expected only the antisymmetric modes contribute because we are interested in phase difference. This expression, which gives the relative phase fluctuations once the spectrum of antisymmetric modes has been calculated, is the main result of this chapter. In the following section we will give explicit results in the case of a homogeneous gas.

7.4 Results for homogeneous condensates

We now consider a homogeneous gas with periodic boundary conditions in a box of size L, which is a 1D version of the method presented in section 2.3. We set the potential U to zero and the density is uniform. Thus the Gross-Pitaevskii equation gives

$$\mu = g\rho_0 - \gamma. \tag{7.32}$$

The Bogoliubov functions can be looked for in the form

$$u_{sk} = (2L)^{-\frac{1}{2}} \exp(ikz) U_{sk}$$
$$v_{sk} = (2L)^{-\frac{1}{2}} \exp(ikz) V_{sk}$$
(7.33)

where the functions U and V are real and $U_{sk}^2 - V_{sk}^2 = 1$. A similar equation holds for the antisymmetric modes, given by

$$u_{nk} = (2L)^{-\frac{1}{2}} \exp(ikz) U_{nk}$$

$$v_{nk} = (2L)^{-\frac{1}{2}} \exp(ikz) V_{nk}.$$
(7.34)

The eigenvalue equation for the symmetric modes then reduces to the equation

$$\begin{pmatrix} \frac{\hbar^2 k^2}{2m} + g\rho_0 & g\rho_0 \\ -g\rho_0 & \frac{-\hbar^2 k^2}{2m} - g\rho_0 \end{pmatrix} \begin{pmatrix} U_{sk} \\ V_{sk} \end{pmatrix} = \epsilon_{sk} \begin{pmatrix} U_{sk} \\ V_{sk} \end{pmatrix}, \quad (7.35)$$

with eigenvalues given by

$$\epsilon_{sk} = \sqrt{\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2g\rho_0\right)}.$$
(7.36)

This is exactly the spectrum for the standard Bogoliubov calculation given in section 2.3. This time we find the values of U and V in a slightly different way, by defining them as the eigenvector components above. Upon expanding the eigenvalue equation, we obtain two coupled equations given by

$$\left(\frac{\hbar^2 k^2}{2m} + g\rho_0\right) U_{sk} + g\rho_0 V_{sk} = \epsilon_{sk} U_{sk}$$
(7.37)

$$-g\rho_0 U_{sk} - \left(\frac{\hbar^2 k^2}{2m} + g\rho_0\right) V_{sk} = \epsilon_{sk} V_{sk}$$
(7.38)

If we then add and subtract these equations and multiply the resulting simultaneous equations for $U_{sk} + V_{sk}$ and $U_{sk} - V_{sk}$, we obtain the equation

$$\left(\frac{U_{sk} + V_{sk}}{U_{sk} - V_{sk}}\right)^2 = \frac{\frac{\hbar^2 k^2}{2m}}{\frac{\hbar^2 k^2}{2m} + 2g\rho_0}.$$
(7.39)

Combining this with the normalisation condition

$$(U_{sk} + V_{sk})^2 (U_{sk} - V_{sk})^2 = 1$$
(7.40)

leads to the sum and difference of the mode functions:

$$U_{sk} + V_{sk} = \left(\frac{\frac{\hbar^2 k^2}{2m}}{\frac{\hbar^2 k^2}{2m} + 2g\rho_0}\right)^{1/4}$$
(7.41)

$$U_{sk} - V_{sk} = \left(\frac{\frac{\hbar^2 k^2}{2m}}{\frac{\hbar^2 k^2}{2m} + 2g\rho_0}\right)^{-1/4}.$$
 (7.42)

For the antisymmetric modes the eigenvalue equation becomes

$$\begin{pmatrix} \frac{\hbar^2 k^2}{2m} + g\rho_0 + 2\gamma & g\rho_0 \\ -g\rho_0 & \frac{-\hbar^2 k^2}{2m} - g\rho_0 - 2\gamma \end{pmatrix} \begin{pmatrix} U_{nk} \\ V_{nk} \end{pmatrix} = \epsilon_{nk} \begin{pmatrix} U_{nk} \\ V_{nk} \end{pmatrix}$$
(7.43)

which is simply the same as the symmetric case, with the kinetic energy shifted by 2γ . Thus the eigenvalues and eigenvector components are

$$\epsilon_{nk} = \sqrt{\left(\frac{\hbar^2 k^2}{2m} + 2\gamma\right) \left(\frac{\hbar^2 k^2}{2m} + 2\gamma + 2g\rho_0\right)}$$
(7.44)

$$U_{nk} + V_{nk} = \left(\frac{\frac{\hbar^2 k^2}{2m} + 2\gamma}{\frac{\hbar^2 k^2}{2m} + 2\gamma + 2g\rho_0}\right)^{1/4}$$
(7.45)

$$U_{nk} - V_{nk} = \left(\frac{\frac{\hbar^2 k^2}{2m} + 2\gamma}{\frac{\hbar^2 k^2}{2m} + 2\gamma + 2g\rho_0}\right)^{-1/4}.$$
 (7.46)

The behaviour of the symmetric and antisymmetric spectra as a function of wavenumber is plotted in figure 7.2. This two-branch spectrum was obtained for the case of a two-component condensate in [41]. In the strong coupling



Figure 7.2: The two-branch spectrum of excitations. The dashed line shows the symmetric spectrum ϵ_{sk} and the solid line shows the antisymmetric one ϵ_{nk} . We have used the dimensionless wavenumber $K = \hbar k / \sqrt{mg\rho_0}$ and the dimensionless energy $E = \epsilon / g\rho_0$. The dimensionless quantity $\gamma / g\rho_0$ is set to 10 here in order to illustrate the nature of the spectrum. A typical value of ϵ/\hbar can be found by taking the reasonable experimental parameters $\gamma/\hbar =$ 50Hz and $g\rho_0/\hbar = 3kHz$, giving a value of ϵ_{nk}/\hbar at k = 0 on the order of 400Hz.

case where $\gamma \gg g\rho_0$, we find that $V_{nk} \ll U_{nk}$ for any k. From (7.23) we see that this means the excitations will be in the form of particles in a superposition of the two condensates and their energy is simply $\hbar^2 k^2/2m + 2\gamma$. In the opposite case (weak coupling) where $\gamma \ll g\rho_0$, three zones can be identified. For $k \ll 2\sqrt{m\gamma}/\hbar$ we obtain collective excitations with $|V| \simeq$ |U| and with energy $2\sqrt{\gamma g\rho_0}$. For $2\sqrt{m\gamma}/\hbar \ll k \ll 2\sqrt{mg\rho_0}/\hbar$ we still have collective excitations with $|V| \simeq |U|$ but their energy is given by the normal Bogoliubov dispersion law $\hbar k \sqrt{g\rho_0/m}$. Finally for $k \gg 2\sqrt{mg\rho_0}/\hbar$ excitations are just particles with energy $\hbar^2 k^2/2m$.

Using the plane wave expansion (7.34) and the normalisation condition $U_{nk}^2 - V_{nk}^2 = 1$, the correlation function (7.31) of the relative phase fluctuation is written

$$\langle : \Delta \hat{\theta}(z) \Delta \hat{\theta}(z') : \rangle = \frac{1}{2\rho_0 L} \sum_k \left\{ (U_{nk} - V_{nk})^2 (2n_{nk} + 1) - 1 \right\} \cos[k(z - z')],$$
 (7.47)

where $n_{nk} = 1/(e^{\epsilon_{nk}/k_BT} - 1)$ is the occupation number for the state with energy ϵ_{nk} . Using the expression (7.46) this correlation function can be computed numerically. In the following we analytically compute the phase fluctuations using some approximations.

The terms which do not involve n_k correspond to the zero temperature contribution. As the function $V_{nk}^2 - U_{nk}V_{nk}$ is always smaller than the corresponding function for a single condensate, the relative phase fluctuations will be smaller than the phase fluctuations of a single condensate. These fluctuations can be calculated by a similar method to that given here, but without the presence of the coupling term γ . The result is that the phase fluctuations of a single condensate are given by

$$\langle (\hat{\theta}(0) - \hat{\theta}(r))^2 \rangle \simeq \frac{\sqrt{m\rho g}}{\pi \hbar \rho} \ln(\sqrt{mg\rho} r/\hbar) + \frac{mk_B Tr}{\hbar^2 \rho}.$$
 (7.48)

Thus the relative phase fluctuations will be bounded via

$$\langle : \Delta \hat{\theta}^2 : \rangle < \frac{\sqrt{mg\rho_0}}{\hbar\rho_0} \ln\left(\frac{L\sqrt{mg\rho_0}}{\hbar}\right). \tag{7.49}$$

The whole theory is valid only for large density so that $\sqrt{mg\rho_0}/(\hbar\rho_0) \ll 1$ and in the experiments accessible until now the size of the condensate is not large enough to produce noticeable phase fluctuations at zero temperature.

Phase fluctuations are thus due to thermal excitation of the collective modes and we will give a simplified expression by making several approximations. First we will approximate the Bose factor by

$$n_{nk} = \frac{k_B T}{\epsilon_{nk}}.\tag{7.50}$$

This is justified as this expression deviates in a significant way from the Bose occupation factor only when n_k becomes smaller than 1, i.e. when $\epsilon_{nk} < k_B T$, and the contribution to phase fluctuations of those modes is small even with the previous expression which overestimates their population. Let us now consider separately the case where $\gamma \gg g\rho_0$ and the case $\gamma \ll g\rho_0$.

If the coupling strength is much stronger than the interparticle interaction, so $\gamma \gg g\rho_0$, then $(U_{nk} - V_{nk})^2 \simeq 1$ for all k and $\epsilon_k \simeq \hbar^2 k^2/2m + 2\gamma$. This gives, approximating the discrete sum by an integral,

$$\langle : \Delta \hat{\theta}(z) \Delta \hat{\theta}(z') : \rangle = \frac{2k_B T}{2\pi\rho_0} \int_{-\infty}^{\infty} dk \frac{\cos[k(z-z')]}{\hbar^2 k^2/m + 4\gamma}$$
(7.51)

$$= \frac{k_B T}{2\hbar\rho_0} \sqrt{\frac{m}{\gamma}} e^{-2|z-z'|\sqrt{m\gamma}/\hbar}.$$
 (7.52)

As we are in the quasi-condensate regime, we consider only temperatures lower than $\hbar \rho_0 \sqrt{g\rho_0/m}/k_B$ and therefore these phase fluctuations are always very small. This is physically reasonable because for strong coupling we expect the phases of the two condensates to be locked and thus fluctuations will be negligible.

Let us now consider the case where the coupling is much weaker than the interparticle interaction, so $\gamma \ll g\rho_0$. We expect the modes with high wavevectors, such that $|k| \gg k_0 = \sqrt{mg\rho_0}/\hbar$, to give a negligible contribution to the phase fluctuations. Indeed for those terms $(U_{nk} - V_{nk})^2 \simeq 1$ and $\epsilon_k \simeq \hbar^2 k^2/2m$ so that their contribution to the phase fluctuation is

$$\frac{mk_BT}{\pi\hbar^2\rho_0}\int_{k_0}^{\infty} dk \frac{1}{k^2} = \frac{k_BT\sqrt{m}}{\pi\hbar\rho_0\sqrt{g\rho_0}},$$
(7.53)

which is always small in the regime of quasi-condensates. Thus only the low wavevector modes $|k| \ll 2\sqrt{g\rho_0 m}/\hbar$ are considered for which

$$(U_{nk} - V_{nk})^2 \simeq \frac{2\sqrt{g\rho_0}}{\sqrt{\hbar^2 k^2/m + 4\gamma}}$$
 (7.54)

and the correlation function then becomes

$$\langle : \Delta \hat{\theta}(z) \Delta \hat{\theta}(z') : \rangle \simeq \frac{2k_B T}{\rho_0 \pi} \int_0^{k_0} \frac{dk}{\frac{\hbar^2 k^2}{m} + 4\gamma} \cos[k(z - z')]. \tag{7.55}$$

The integral can be extended to infinity as higher k values give negligible contributions and we find

$$\langle : \Delta \hat{\theta}(z) \Delta \hat{\theta}(z') : \rangle = \frac{k_B T}{2\rho_0 \hbar} \sqrt{\frac{m}{\gamma}} \exp\left[\frac{-2\sqrt{m\gamma}|z-z'|}{\hbar}\right].$$
(7.56)

Note that this expression is the same as (7.52), which was not expected a *priori*. This formula, which gives the amplitude of the relative phase fluctuations as well as their correlation length $\hbar/(2\sqrt{m\gamma})$ agrees well with the numerical calculation of equation (7.47), and these are plotted in figure 7.3. Phase fluctuations are small only if

$$k_B T \ll \rho_0 \hbar \sqrt{\frac{\gamma}{m}}.$$
 (7.57)

Note that as we assume small relative phase difference, this is also the limit of validity of our calculation. The phase diagram in figure 7.4 summarises these results.



Figure 7.3: Correlation function of the relative phase fluctuations. The solid line is the numerical calculation of equation (7.47) with $\gamma = g\rho_0/10$, $T = \hbar\rho_0\sqrt{\gamma}/(2\sqrt{m}k_B)$ and $L = 100\hbar/\sqrt{mg\rho_0}$. The dotted line is the analytical expression equation (7.56) which only differs from the numerical expression at small separations.

7.5 Discussion

In conclusion we have shown that as long as the temperature is small enough to fulfil equation (7.57), although there might exist large phase fluctuations along each condensate, the local relative phase between the two condensates stays small. In the opposite case there are large fluctuations of the relative phase whose correlation length is $l_c = \hbar/2\sqrt{m\gamma}$. As an example let us consider the case of two Rubidium condensates of 10^4 atoms elongated over $L = 200 \,\mu\text{m}$, confined transversely with an oscillation frequency $\omega_{\perp}/2\pi = 1 \,\text{kHz}$ and coupled using $\gamma/\hbar = 50 \,\text{Hz}$. The phase of each condensate changes by about 2π from one end of the condensate to the other as soon as $T > T_{\phi} = \hbar^2 \rho_0/(mLk_B) = 1.8 \,\text{nK}$. However the local relative phase between the two condensates stays very small if $T \ll \hbar \rho_0 \sqrt{\gamma}/(k_B \sqrt{m}) =$



Figure 7.4: Phase diagram for the fluctuations of the relative phase between the two condensates. Only temperatures much smaller than $\hbar\rho_0\sqrt{g\rho_0}/(k_B\sqrt{m})$ are relevant as for larger temperatures one does not have a quasi-condensate anymore. For temperatures larger than $\hbar^2\rho_0/(k_BLm)$, each condensate has longitudinal phase fluctuations. Below the curve, which corresponds to equation (7.57), the coupling between the condensates is large enough to suppress local relative phase fluctuations between the two condensates. Above this curve, there are local relative phase fluctuations between the two condensates.

180 nK. The calculations made here for homogeneous condensates could be used to describe a trapped inhomogeneous gas via a local density approximation similar to that used in [45] as long as both the healing length $l_h = \hbar/\sqrt{mg\rho_0}$ - the length over which, after being subject to a localised perturbation, the condensate wave function tends to its bulk value - and the correlation length of the phase fluctuations are both much smaller than the extension of the condensate. In the above example, $l_h = 0.6 \,\mu\text{m}$ and $l_c = 2 \,\mu\text{m}$ are indeed much smaller than L.

To measure experimentally the relative phase fluctuations and their correlation length, one should perform an interference experiment. In the case where the two states are internal states, an intense $\pi/2$ pulse has to be applied. Measurement of the local density of atoms in the states $|a\rangle$ and $|b\rangle$ then gives access to the local relative phase of the two condensates. In the case where $|a\rangle$ and $|b\rangle$ are confined in the wells of a double well potential, the interference measurement is performed via a fast release of the confining potential followed by a time of flight long enough for the two clouds to overlap. Indeed, the total intensity presents fringes in the direction orthogonal to z [46] and, at a given z, the position of the central fringe gives the value of the local relative phase.

Chapter 8

Summary and Conclusion

In this thesis we have studied matter waves and Bose-Einstein condensates. In particular, we have derived a theory of matter wave detection. This was done semiclassically in chapter 5, where we revealed the failure of analogy with photoelectron detection, and quantum mechanically in chapter 6 through a microscopic description of the detection process. As experiments performed in this area progress towards the counting of single atoms incident on a detector surface, this theory will become increasingly important. The conclusions we have drawn are that due to the dispersive nature of matter waves in free space one must consider the flux density of particles through the detector rather than simply the particle density. Now that the theory of matter wave detection is laid out clearly, there are many possible applications to consider. Some of these include calculating correlations between detection of matter waves at different point on the detector surface and correlations between subsequent detections in a matter wave beam.

In terms of the properties of BECs themselves, we have calculated in chapter 7 the fluctuations in the relative phase between two very elongated condensates which are connected via a localised coupling. This has given a regime in which experiments should be performed in order to see the relative phase fluctuations, and this occurs between the true condensate temperature $\hbar\rho_0/(Lmk_B)$ and the quasi-condensate temperature $\hbar\rho_0\sqrt{g\rho_0/m}/k_B$. There are several potential elaborations on this theory which are possible. The calculation is only done here in terms of a uniform (square-well) trap. In an experiment it is more likely that the trapping potential will be harmonic and so the theory will need to be modified to predict the fluctuations in that situation. Also there is the more ambitious problem which involves coupled 3D condensates as opposed to the 1D ones used here.

Finally, we have shown in chapter 4 that matter waves should in principle be subject to conservation laws and have given some examples for a very simple particle conserving system in a linear potential. This work has great potential for further development. In particular the second quantised version of this theory should be developed, and then realistic situations could be considered including those where particles are created or annihilated.

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