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Josephson Effects within Atomic Bose-Einstein Condensates

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Abstract

When dilute atomic gases are cooled down to a fraction above absolute zero, we observe the formation of Bose-Einstein condensates. In this state, all particles behave identically, and display quantum behaviour on a macroscopic scale. By weakly coupling two such condensates within a double-well potential trap (a bosonic Josephson junction), we may observe dynamical systems of atomic oscillations between the condensates, collectively known as the Josephson Effects. In this report, we discuss the Josephson relations, which define these oscillations, and observe how such dynamics may be caused by an initial imbalance in atomic population, or by a phase difference between the two condensates. By altering the magnitude of the potential barrier separating the condensates, we observe two distinct Josephson Effects: Josephson oscillations, and macroscopic quantum self-trapping. We also qualitatively compare these simulated results to experimental data.

Chapter 1

Introduction to Bose-Einstein Condensates

Throughout this report, we shall be discussing Josephson Effects within dilute atomic Bose-Einstein condensates, so first we must discuss the question: what is a Bose-Einstein condensate? A Bose-Einstein condensate (BEC) is a state of matter which can only form under very specific conditions of temperature and density. We shall primarily be considering the case of a dilute atomic gas, for which the temperature required is of the order of 500nK, 5×10^{-7} degrees above absolute zero. Other examples of Bose-Einstein condensation are superfluid helium and superconductors, although the temperatures required here are much higher (around 2.2K). A BEC is a quantum phenomenon, in which all of the paritcles are indistinguishable from one another, and the particles within the condensate act identically. Due to this behaviour, they form a macroscopic wave of matter, and they allow us to observe quantum effects on a macroscopic scale. Before discussing them further, we shall first consider some results from quantum theory which are relevant to the formation of BECs.

1.1 Important Quantum Results

1.1.1 Wave Particle Duality

Classically, waves and particles were considered distinct from one another. For example, massive bodies such as electrons were described as particles, each particle discrete from others, with motion completely specified by the properties of position, velocity, and mass; electromagnetic radiation was described as a wave, a continuous transfer of energy, without mass. This interpretation is reasonable on a macroscopic scale, but once experiments began taking place on the atomic (and smaller) scale, where the laws of quantum mechanics take over, it became apparent that this was not the case. In the early 20th century, experimental evidence showed that electrons could diffract (like a wave), whereas light was necessarily transferred in quantised packages (light particles called photons). Hence, we cannot consider particles and waves as separate from one another under quantum mechanics; this is known as wave-particle duality. The position and velocity of a particle can no longer be known with certainty, but are described by a probability distribution.

Since we now consider particles as waves, we can ask what the wavelength of a particle is. In 1924, Louis de Broglie postulated that the wavelength of an electron could be written as $\lambda = h/p$ [1], where h is Planck's constant, and p is the electron's momentum. In fact, this is true for all forms of matter, and the (thermal) de Broglie wavelength is defined as [2]

$$\lambda_T = \left(\frac{2\pi\hbar^2}{mkT}\right)^{1/2},\tag{1.1}$$

where m is the mass of the particle, T is the temperature, and k, \hbar are the Boltzmann constant and Planck's reduced constant respectively. Hence we can see that the de Broglie wavelength increases inversely proportional to \sqrt{T} ; as the temperature decreases, we see an increase in the particle's wavelength. This concept is key to the formation of BECs, and we shall discuss further the effect of an increasing de Broglie wavelength as $T \to 0$.

1.1.2 The Schrödinger Equation (SE)

Since we can no longer describe a particle by its classical properties of position and momentum, we need a new way to define it. We introduce the wavefunction, $\Psi(\mathbf{r}, t)$, a complex-valued function (in general), which defines the probability of finding the particle at position \mathbf{r} , at time t, by

$$P(\boldsymbol{r},t) = |\Psi(\boldsymbol{r},t)|^2, \qquad (1.2)$$

$$\int |\Psi(\boldsymbol{r},t)|^2 d^3 \boldsymbol{r} = 1.$$
(1.3)

Note that Equation (1.3) gives the normalisation condition; since we are dealing with a probability, we must normalise Ψ such that the total probability is 1. In 1926, Erwin Scrödinger postulated the Schrödinger Equation (SE) [3]:

$$i\hbar \frac{\partial \Psi(\boldsymbol{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right)\Psi(\boldsymbol{r},t), \qquad (1.4)$$

where $\hbar \approx 1.055 \times 10^{-34}$ is Planck's reduced constant. This linear partial differential equation describes how the wavefunction Ψ evolves through space and time. The quantity within the brackets on the right hand side of the SE, called the Hamiltonian operator, \hat{H} , defines the total energy of the particle; when operating on Ψ , $(-\hbar^2/2m)\nabla^2$ corresponds the kinetic energy of the particle, and $V(\mathbf{r})$ to the potential energy.

1.1.3 Bosons and Fermions

We may group all particles in nature into two categories based on their spin value, an intrinsic property of a particle which is a form of angular momentum. The two categories are bosons, which have integer spin, and fermions, which have half integer spin [2]. Quarks and leptons, essentially the building blocks of matter, are all fermions; for example, an electron is a type of lepton, while protons and neutrons are both made up of three quarks. The spin of combined particles is simply added, so for example, protons and neutrons, consisting of 3 quarks, each with spin 1/2, have to a spin 1/2 + 1/2 + 1/2 = 3/2, hence are fermions. More generally, as neutral atoms have equal numbers of protons and electrons, the classification of the atom depends on the number of neutrons within the nucleus; if there is an even number of neutrons, the atom has integer spin and is a boson, else it is a fermion. For this reason, different isotopes of the same element will often have a different classification. For example, helium has two stable isotopes, ³He and ⁴He, which have 1 and 2 neutrons respectively; ³He is a fermion, while ⁴He is a boson.

The key difference between bosons and fermions is that no two fermions may occupy the same quantum state, due to the Pauli Exclusion Principle [4], whereas many bosons may. This property of sharing a quantum state is hugely important for Bose-Einstein Condensation, and as the name may suggest, we shall be focussing solely on bosons for the rest of the report.

1.2 Bose-Einstein Condensates (BECs)

Bose-Einstein condensation was first predicted to occur in photons in 1924 by Indian physicist, Satyendra Bose [5]. Later that year, Einstein, whom Bose had contacted to help publish his results, generalised the phenomenon to particles [6]. We shall now consider the underlying idea of why such condensation should occur, and look at the first experiments which succeeded in creating them.

1.2.1 Underlying Concept

As discussed earlier, the thermal form of the de Broglie wavelength tells us that λ_{dB} of a particle increases proportionally with $1/\sqrt{T}$, with T the temperature. So as T decreases, λ_{dB} increases. Define a length D as the typical distance between atoms within a dilute atomic gas [7]. At normal human temperatures, of order 300K, the de Broglie wavelength is much smaller than D; the atoms have more kinetic energy (note that temperature is a measure of the average kinetic energy of particles in a system), and hence occupy a range of different quantum energy states. However, if we decrease the temperature such that λ_{dB} increases to be of the same order of magnitude as D, then the "wavepackets" of the atoms, the area of space over which they are distributed by their wavefunction Ψ , begin to overlap. The temperature when $\lambda_{dB} = D$ is the critical temperature, T_C , as it is at about this point that we see the beginnings of Bose-Einstein condensation.

For atomic gases, we are now dealing with very low temperatures, $T \ll 1$ K, and so the atoms have very little kinetic energy, and as T decreases further, more and more of the atoms fall into the ground energy state. It is at this stage that the distinction between bosons and fermions becomes important; because we are dealing with bosons, the atoms may occupy the same quantum state. By decreasing the temperature further still, we arrive in the region of true Bose-Einstein condensation, where $\lambda_{dB} > D$. The temperature is now so low that almost all atoms are in the ground state, and as the wavelengths are now greater than the distance between atoms, their wavepackets overlap significantly, and the atoms become indistinguishable from one another. The sharing of the ground energy state, and the indistinguishability of the atoms is what causes all of the atoms in the condensate to behave identically, and hence for the condensate as a whole to demonstrate quantum behaviour on a much larger scale than normal.

1.2.2 Experimental Observation

The first gaseous BEC was created in 1995 by Eric Cornell and Carl Wieman at the JILA lab at the University of Colorado; they cooled a trapped gas of around 2000 rubidium-87 atoms to around 2×10^{-7} K [8]. Only a few months later, Wolfgang Ketterle and his team at MIT succeeded in creating a condensate of sodium-23 atoms containing hundreds of thousands of atoms [9], allowing a more detailed study of the behaviour of the condensate. For their work, the three shared the Nobel prize for Physics in 2001. Figure (1.1) shows the velocity distribution of the atoms after expanding for 1/20 of a second. The figure shows the distribution before condensation (left), just after (middle), and after further evaporative cooling has taken place (right). We can clearly see the well-defined peak in the centre of the image after condensation (sharper at the lower temperature), which represents particles with almost zero velocity. As there is a very high number of particles with close-to-zero velocity (and hence kinetic energy), initially all held near to the centre of the trap, this corresponds to a very high density of particles which have remained very close to the centre of the trap; this is the condensate. This is in stark contrast to the shot before condensation has occurred; although there is still a marginally higher density in the centre, there is a much more even distribution of velocities (and hence of atoms).



Figure 1.1: The velocity distribution (corresponding to how far the atoms have moved) of trapped rubidium-87 atoms in a condensate at: $T > T_C$), $T \approx T_C$ (middle), $T < T_C$ (right). The colour corresponds to the number of atoms at each velocity, from red (fewest) to white (most) [10].

The gap of 70 years between Bose's and Einstein's predictions, and the physical formation of BECs, was largely due to the problem of lowering the temperature to the miniscule values required. The liquefaction of helium was achieved in 1914, before Bose had even made his serendipitous discovery; in 1938, Fritz London attributed the phenomenon of superfluidity in liquid

helium to Bose-Einstein condensation, and predicted the critical temperature of superfluidity with remarkable accuracy [11]. However, it was not until 1992 that laser cooling allowed experiments to get below 1K [12] to create a pure, dilute gaseous BEC. Both the Cornell/Wieman and Ketterle experiments used a combination of laser cooling, followed by evaporative cooling (allowing the atoms with the highest energy to escape the trap in order to lower the average energy) to attain their condensates.

1.3 The Gross-Pitaevskii Equation (GPE)

The fundamental equation for modelling BECs, which will be used throughout this report, is the Gross-Pitaevskii equation (GPE), named after Eugene P. Gross, and Lev P. Pitaevskii. It describes how the wavefunction Ψ of a condensate evolves through time [13], and can be written:

$$i\hbar \frac{\partial \Psi(\boldsymbol{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) + g|\Psi(\boldsymbol{r},t)|^2\right)\Psi(\boldsymbol{r},t).$$
(1.5)

So the left-hand side of the GPE describes the time-evolution of the system, while the quantity in brackets on the right-hand side again describes the Hamiltonian operator, H, of the system. The GPE is also known as the Non-Linear Schrödinger Equation, and we can see that it is simply a generalisation of the SE discussed earlier. In the GPE, the $\nabla^2 \Psi$ term corresponds the kinetic energy, and the V term corresponds to the external potential as in the SE; the key difference between the equations is that the SE describes the time-evolution of a single particle, whereas the GPE describes the evolution of many particles in a system. The $q|\Psi|^2$ term, absent from the SE, describes the interactions between particles within a system, and it is this term that gives rise to the inherent non-linearity of the GPE. The coefficient g is a characteristic of the system, which defines how strong the effective interactions between particles are; if q > 0, these interactions are repulsive, if q < 0 they are attractive. If we set q = 0, the case with no interactions between particles, we recover the Schrödinger Equation. In this report, we shall consider only the repulsive case of q > 0.

The GPE is an excellent model for studying BECs, as it can accurately model their characteristics, whilst also being computationally inexpensive. It is a relatively poor model for other systems such as superfluid helium, due to their relatively strong long-range inter-particle interactions, and it also fails to take into account finite temperature effects (i.e. being above absolute zero). However, given the dilute nature and exceedingly low temperatures of typical BECs, these effects are negligible, and so the GPE provides a good model.

In this report, we shall be considering the GPE in one dimension only; that is $\Psi = \Psi(x,t)$, and $\nabla^2 = \frac{\partial^2}{\partial x^2}$, and henceforth we shall drop the x and t dependence from Ψ unless explicitly required. Thus the 1D GPE we are considering is given by

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi + g|\Psi|^2\Psi.$$
(1.6)

1.4 The Dimensionless GPE

Because we are dealing with a quantum phenomenon, many quantities involved are very small, and it is inconvenient to work in terms of coefficients such as \hbar all the time. It is also computationally inefficient; \hbar for example, is of the order 10^{-34} , and this can affect the precision of numerical computations. Hence it is convenient to define a new set of dimensionless variables to work with [7]:

$$\Psi = \Psi_{\infty} \Psi' \tag{1.7}$$

$$x = \xi x' \tag{1.8}$$

$$t = \frac{\hbar}{\mu} t' \tag{1.9}$$

$$V = \mu V' \tag{1.10}$$

where Ψ_{∞} , the wavefunction a long way from the boundary in an infinite potential well (explained in the next subsection), $n_{\infty} = |\Psi_{\infty}|^2$, and μ , the chemical potential of the system, are all dimensional constants. We also define the "healing length", $\xi = \hbar/\sqrt{mgn_{\infty}}$, the dimensional constant in the xtransformation. ξ corresponds to the distance required by a condensate in an infinite potential well to reach its asymptotic value, and will be discussed more in Chapter 3. By substituting these transformations into the 1D GPE, we find:

$$i\frac{\partial\Psi'}{\partial t'} = -\frac{1}{2}\frac{\partial^2\Psi'}{\partial x'^2} + V'\Psi' + |\Psi'|^2\Psi', \qquad (1.11)$$

from which we subsequently drop the primes. Note that all units shown on graphs are in these dimensionless units, unless stated otherwise.

Chapter 2

Josephson Effects

2.1 What Are Josephson Effects?

The term "Josephson Effects" cumulatively describes a set of macroscopic quantum phenomena, most commonly used to refer to a supercurrent (a current that flows indefinitely, without dissipation) flowing across a Josephson junction, which consists of two superconductors separated by a thin insulating barrier. It involves a flow of particles which tunnel through the barrier (impossible classically), when a difference in chemical potential is applied across the system. The effect is named after Brian David Josephson, who in 1962 predicted the equations for current and voltage across this barrier [14]. The effects were first discovered experimentally the following year, by Philip Anderson and John Rowell [15]. Josephson received the Nobel prize in physics in 1973 for this work. The Josephson effect has several applications, the most widely used of which is the superconducting quantum interference device (SQUID), which is a very sensitive magnetometer, used for a variety of purposes in engineering [16].

Analogous results have been discovered in both superfluid helium [17], and in dilute trapped Bose-Einstein condensates [18-21]. BECs in particular, when held in an optical trap, offer the opportunity to investigate some dynamical regimes not possible with superconductors or superfluids, in part due to the very low concentration of particles. They are also much more controllable than superfluids or superconductors; by simply altering the geometry of the trap in real time, one can observe several different effects with a single sample. Rather than a physical barrier, a potential barrier is introduced to split the condensate into two distinct parts. The dynamics of these systems are caused by two competing energy terms: E_J is the Josephson coupling energy, which dictates the tunnelling through the barrier; E_C describes the interactions between particles within a single condensate [22].

In order to intiate Josephson dynamics, an imbalance of some sort must be introduced between the two condensates. This can involve a population imbalance, in which one condensate contains a higher proportion of the particles than the other; an imbalance in chemical potential between the wells; or a difference in phase between the two condensates.

2.2 Origin of the Josephson Relations

Considering a condensate in a double well potential, we can view this condensate as two separate, interacting condensates. We can therefore write the wavefunction $\Psi(x, t)$ as a superposition of two states,

$$\Psi(x,t) = \psi_1(t)\Phi_1(x) + \psi_2(t)\Phi_2(x), \qquad (2.1)$$

where Φ_1 and Φ_2 are the time-independent eigenstates for the spearated condenstates. This is an approximation, as the nonlinear interaction term in the GPE affects such a superposition. However, since we are considering only a weakly linked pair of condensates, the density within the tunnelling region is low, and hence interactions are negligible. The dimensionless governing equations for two interacting condensates inside a double-well potential are given by [18]:

$$i\frac{\partial\psi_1(x,t)}{\partial t} = (E_1^0 + U_1|\psi_1|^2)\psi_1(x,t) - \kappa\psi_2(x,t), \qquad (2.2)$$

$$i\frac{\partial\psi_2(x,t)}{\partial t} = (E_2^0 + U_2|\psi_2|^2)\psi_2(x,t) - \kappa\psi_1(x,t).$$
(2.3)

The terms E_i^0, U_i , and κ denote respectively the zero point energy of each condensate, the atomic self-interaction energies, and the amplitude of tunnelling between the condensates. To maintain consistency with the earlier derivation of the dimensionless GPE, these three energy terms are also dimensionless. To derive the Josephson relations, we first apply the Madelung Transformation:

$$\psi_i(x,t) = \sqrt{N_i(x,t)} e^{i\theta_i(x,t)}, \qquad (2.4)$$

where $N_i(x,t) = |\psi_i|^2$ is the atom density of the condensate, and $\theta_i(x,t)$

represents the arbitrary phase, defined as

$$\theta_i = \arctan\left(\frac{\Im(\psi_i)}{\Re(\psi_i)}\right).$$
(2.5)

The phase of a single condensate does not have have any real physical effect; however, a difference in phase between two interacting condensates is of huge importance, as it can initiate Josephson effects.

Differentiating equation 2.2, the chain rule gives us

$$i\frac{\partial\sqrt{N_1}}{\partial t}e^{i\theta_1} - \sqrt{N_1}\frac{\partial\theta_1}{\partial t}e^{i\theta_1} = \left(E_1^0\sqrt{N_1} + U_1N_1\right)e^{i\theta_1} - \kappa\sqrt{N_2}e^{i\theta_2}$$

Rearranging, and applying $e^{i\theta} = \cos\theta + i\sin\theta$, we can separate real and imaginary parts to give

$$\frac{\partial N_1}{\partial t} = -2\kappa \sin(\theta_2 - \theta_1), \qquad (2.6)$$

$$\frac{\partial \theta_1}{\partial t} = \kappa \sqrt{\frac{N_2}{N_1}} \cos(\theta_2 - \theta_1) - (E_1^0 + U_1 N_1)$$
(2.7)

Analagously, by differentiating 2.3, we find

$$\frac{\partial N_2}{\partial t} = 2\kappa \sin(\theta_2 - \theta_1), \qquad (2.8)$$

$$\frac{\partial \theta_2}{\partial t} = \kappa \sqrt{\frac{N_1}{N_2}} \cos(\theta_2 - \theta_1) - (E_2^0 + U_2 N_2)$$
(2.9)

Now introduce the variables

$$z(t) = \frac{N_1 - N_2}{N_T},\tag{2.10}$$

$$\phi = \theta_2 - \theta_1, \tag{2.11}$$

where $N_T = N_1 + N_2$; z(t) is the fractional difference in atomic population of the two condensates, and ϕ is the relative difference in phase. By subtracting (2.6) - (2.8), and (2.9) - (2.7), we can find expressions for dz/dt and $d\phi/dt$:

$$\frac{dz}{dt} = -\frac{4\kappa\sqrt{N_1N_2}\sin\phi}{N_T}$$

$$\frac{d\phi}{dt} = (E_1^0 - E_2^0) + \kappa \left(\sqrt{\frac{N_1}{N_2}} - \sqrt{\frac{N_2}{N_1}}\right) \cos\phi + (U_1 N_1 - U_2 N_2)$$

By noting that we can rewrite $\sqrt{N_1N_2}$ as $\frac{1}{2}N_T\sqrt{1-z^2}$, and that for small $z, U_1 \approx U_2 = U$, and by rescaling time (dimensionlessly) by $2\kappa t \to t$, these equations become

$$\frac{dz}{dt} = -\sqrt{1-z^2}\sin\phi \tag{2.12}$$

$$\frac{d\phi}{dt} = \Delta E + \frac{z}{\sqrt{1-z^2}}\cos\phi + \Lambda z.$$
(2.13)

These are the Josephson relations, with the dimensionless constants ΔE and Λ defined as

$$\Delta E = \frac{E_1^0 - E_2^0}{2\kappa},$$
(2.14)

$$\Lambda = \frac{UN_T}{2\kappa} \tag{2.15}$$

Primarily, this report focusses on values of $z \ll 1$, within a symmetric doublewell trap, hence the difference in zero point energies is negligible, $\Delta E \approx 0$. Of much greater importance is the second parameter, Λ , which essentially describes the ratio between the atomic self-interaction energies of the condensates, U, and the tunnelling amplitude, κ . Going back to the self-interaction and coupling energy terms discussed in Chapter (2.1), by setting $E_C = UN_T$ and $E_J = 2\kappa$, we can define Λ as the ratio between these two terms,

$$\Lambda = \frac{E_C}{E_J}.\tag{2.16}$$

It is the value of this constant which dictates the dynamics of the Josephson effects within the condensates.

2.3 Selected Josephson Effects

We can separate the dynamical systems described by the Josephson relations into two primary regimes, based on the value of Λ : the critical value of Λ is defined as [19]

$$\Lambda_C = 2\left(\frac{1+\sqrt{1-z(0)^2}\cos[\phi(0)]}{z(0)^2}\right),\tag{2.17}$$

which can be derived from the Hamiltonian of the system and the constraint of energy conservation. If $\Lambda < \Lambda_C$, then the tunnelling effects dominate the intra-condensate interactions, and we see Josephson oscillations, as demonstrated in Figure 2.1 (a), (b).



Figure 2.1: The different regimes due to different population imbalances: (a) $\Lambda \ll \Lambda_C$; (b) $\Lambda < \Lambda_C$; (c) $\Lambda \to \Lambda_C^-$; (d) $\Lambda = \Lambda_C$; and (e) $\Lambda > \Lambda_C$ [19].

Here, we see that the population imbalance, z(t) oscillates about zero, between maxima and minima of $\pm z(0)$, where z(0) is the initial poulation imbalance. If the reverse is true, with $\Lambda > \Lambda_C$, then we see instead macroscopic quantum self trapping, shown in Figure ?? (e). In this case, z(t)still oscillates, but it no longer oscillates about zero; the condensate with the largest initial population remains the larger. Figure 2.1 (c) shows the case $\Lambda \to \Lambda_C$ from below; the population difference still oscillates about zero, but the shape of oscillations are no longer the smooth, sinusoidal shape as in cases (a) and (b), indicating the increasing effect of the atomic self-interaction energy term, E_C . Figure 2.1 (d) shows the special case of $\Lambda = \Lambda_C$; we can see that there are no oscillations whatsoever in this case, instead the population is critically damped, and so tends exponentially to zero. We shall now examine the two main cases in more detail: Josephson oscillations, and macroscopic quantum self-trapping.

2.3.1 Josephson Oscillations (JO)

Let us first consider the case of Josephson oscillations; when Λ is suitably small, we see oscillations in both population and phase differences, about a mean value of zero. We can derive this oscillatory behaviour analytically, by taking the Josephson relations derived in Section 2.1, and taking the second time derivative:

$$\frac{d^2z}{dt^2} = 2\kappa \frac{d}{dt} \left[-\sqrt{1-z^2} \sin \phi \right]$$

Note that the factor of 2κ appears because we are differentiating with respect to t for a second time; the transformation $2\kappa t \to t$ implies that $d/dt \to 2\kappa t$, $d^2/dt^2 \to (2\kappa)^2$. Calculating this derivative gives us the second order ODE:

$$\frac{d^2z}{dt^2} = -2\kappa(\Lambda+1)z.$$

Similarly, we can derive

$$\frac{d^2\phi}{dt^2} = -2\kappa \left(\frac{\Lambda}{\sqrt{1-z^2}}\sin\phi + \frac{1}{2}\sqrt{1-z^2}\sin 2\phi\right).$$
(2.18)

As opposed to our ODE for z, here we have non-linear terms, which makes finding a solution more difficult. However, for "small" values of z, ϕ , we can linearise this: $z^2 \approx 0, \sin \phi \approx \phi$. Hence, we obtain:

$$\frac{d^2\phi}{dt^2} = -2\kappa(\Lambda+1)\phi \tag{2.19}$$

From these ODEs, we can obtain solutions for z(t) and $\phi(t)$:

$$z(t) = z_{max} \cos\left(2\kappa\sqrt{\Lambda+1}\,t + \alpha\right),\tag{2.20}$$

$$\phi(t) = \phi_{max} \sin\left(2\kappa\sqrt{\Lambda+1}\,t + \alpha\right),\tag{2.21}$$

where z_{max} and ϕ_{max} are the maximum population and phase differences, and the value of α depends upon the initial conditions z(0) and $\phi(0)$. Hence we expect to see oscillations in both z(t) and $\phi(t)$, with frequency ω , where

$$\omega = \left(2\kappa\sqrt{\Lambda+1}\right) = \sqrt{E_C E_J + E_J^2} \tag{2.22}$$

The definition of "small" values of z, ϕ is somewhat arbitrary: in my results, z_{max} is no larger than 0.06, and hence linearisation is reasonable; whereas I observed phase differences of over 0.7π , well outside the values normally considered appropriate for linearisation, which still followed such an oscillatory solution.

2.3.2 Macroscopic Quantum Self Trapping (MQST)

If we instead look at the case in which $\Lambda > \Lambda_C$, we see drastically different behaviour in both population and phase differences. The most dramatic change is in $\phi(t)$, the phase difference. If we consider again the 2nd order PDE for ϕ :

$$\frac{d^2\phi}{dt^2} = -2\kappa \left(\frac{\Lambda}{\sqrt{1-z^2}}\sin\phi + \frac{1}{2}\sqrt{1-z^2}\sin 2\phi\right),\,$$

although we are still considering small z, we can no longer linearise the $\sin \phi$, $\sin 2\phi$ terms; rather than oscillating, the phase increases continually in the self-trapping regime, known as a "running" phase. The population difference, z(t) still exhibits oscillatory behaviour, as $d^2z/dt^2 = -2\kappa(\Lambda + 1)z$ without any linearisation in ϕ , but rather than oscillating between positive and negative, now whichever well has the higher initial population retains it. This is due primarily to the decrease in the tunnelling energy term, E_J ; in this regime, far fewer atoms have the energy to tunnel through the potential barrier, and so we see only smaller oscillations in z(t) which never reach zero.

2.4 Results

Plots of my results for both regimes are shown in Figure 2.2, with the time evolution of z(t) (top) and $\phi(t)$ (bottom) for Josephson oscillations shown on the left, and corresponding plots for MQST on the right. Figure 2.3 shows the experimental solutions obtained by Albiez, Gati et al [20], and, although the parameters used are different, we can see a good qualitative agreement



between the experimental plots, and my simulated results.

Figure 2.2: Population (top) and phase difference (bottom) plots for Josephson oscillations (left) and macroscopic quantum self-trapping (right) regimes.



Figure 2.3: Population (top) and phase difference (bottom) plots for Josephson oscillations (left) and macroscopic quantum self-trapping (right) regimes from experimental results [ref]. Solid lines represent numerically integrated GPE solution, points show experimental data [20].

For the Josephson oscillations regime, we can see the expected oscillations in both the population and phase differences, about an average value of zero, as predicted by the sinusoidal form of z and ϕ .

In contrast, the MQST plots show the oscillations in z confined to positive values, as quantum tunnelling is effectively blocked off. The phase plots show the running phase characteristic to MQST, as the phase continually increases with time (in my graph of the self-trapping phase, ϕ is constantly increasing, but has been bounded within $[-\pi, \pi]$, which is why it jumps from π to $-\pi$).

The main difference between my results and those from the Albiez experiment is the amplitude of oscillation; this is due to the methodology of initiating the different Josephson effects. The method used by Albiez et al was to alter the initial population imbalance; below a critical value, $z(0) < z_C$ to observe Josephson oscillations, or above, $z(0) > z_C$ for MQST. This method necessarily requires a large population imbalance for self-trapping. My method involved altering the self-interaction and tunnelling, E_C and E_J , by increasing the height of the potential barrier which separates the two condensates, which has very little imact on the value of z(0). We shall discuss this method in more detail in Chapter 4.

Chapter 3

Numerics

Having derived the dimensionless Gross-Pitaevskii Equation, we now need to introduce some numerical methods in order to create simulations of how a condensate would evolve. We require numerical schemes in order to simulate the two derivative terms, $\partial^2 \psi / \partial x^2$, and $\partial \psi / \partial t$. The first two subsections discuss the methods used to approximate these two terms.

3.1 Numerical Methods

3.1.1 The Central Difference Approximation

The Central Difference Approximation is a method for calculating the second derivative of a function f(x) at a point x_i to accuracy of $O[h^2]$, where h is the distance between adjacent x points [23]. To derive this result, we start by taking the forward and backward differences of f(x) at x_i . This involves taking the Taylor series of f about $x_i + h/2$ for the forward difference, and about $x_i - h/2$ for the backward difference:

$$f_{i+\frac{1}{2}} = f\left(x_i + \frac{h}{2}\right) = f(x_i) + \frac{h}{2}f'(x_i) + \frac{\left(\frac{h}{2}\right)^2}{2!}f''(x_i) + \frac{\left(\frac{h}{2}\right)^3}{3!}f'''(x_i) + \dots; \quad (3.1)$$

$$f_{i-\frac{1}{2}} = f(x_i - \frac{h}{2}) = f(x_i) - \frac{h}{2}f'(x_i) + \frac{\left(\frac{h}{2}\right)^2}{2!}f''(x_i) - \frac{\left(\frac{h}{2}\right)^3}{3!}f'''(x_i) + \dots (3.2)$$

By subtracting (1) - (2), we see that

$$f'(x_i) = \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{h} + O[h^3]$$
(3.3)

Now let g(x) = f'(x), and substitute into (3):

$$f_i'' = g_i' \approx \frac{g_{i+\frac{1}{2}} - g_{i-\frac{1}{2}}}{h} = \frac{\frac{f_{i+1} - f_i}{h} - \frac{f_i - f_{i-1}}{h}}{h} = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

This gives us the result

$$\left. \frac{d^2 f}{dx^2} \right|_{x=x_i} = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O[h^3]$$
(3.4)

However, because we are using this approximation at N different points, where $N_{-}(1/h)$, the error becomes of $O[h^3/h] = O[h^2]$.

3.1.2 Runge-Kutta 4th Order Method

In order to implement the time evolution of my numerical simulation, I used the 4th Order Runge Kutta Method, which as the name may suggest, is accurate to $O[\delta^4]$, where δ is the step between successive time points [23]. It works in a similar manner to Euler's method, but, as opposed to making a single straight line approximation to a curve over a single timestep, the RK4 method simply uses this approximation as an initial guess, and then improves upon it by taking two further estimates at the midpoint of the timestep, and another at the end. Supposing we are approximating a first order ODE:

$$\frac{dy}{dt} = f(y,t),\tag{3.5}$$

with initial conditions $y(0) = y_0, t(0) = t_0$. Then over a timestep of size δ , the approximation of the next step y_{i+1} is given by

$$y_{i+1} = y_i + \frac{\delta}{6}(k_1 + 2k_2 + 2k_3 + k_4), \qquad (3.6)$$

where the k_j which give the different approximations are defined by

$$k_1 = f(t_i, y_i) \tag{3.7}$$

$$k_2 = f\left(t_i + \frac{\delta}{2}, y_i + \frac{\delta}{2}k_1\right) \tag{3.8}$$

$$k_3 = f\left(t_i + \frac{\delta}{2}, y_i + \frac{\delta}{2}k_2\right) \tag{3.9}$$

$$k_4 = f(t_i + \delta, y_i + \delta k_3) \tag{3.10}$$

The weighting of the different k_j in the approximation of y_{i+1} are calculated in order to cancel terms in the Taylor series expansion to ensure the high order error term associated with this method. By using the RK4 method alongside the Central Difference Approximation in nested 'for loops' in Fortran, I was able to create a grid of t vs x, in which the full form of the wavefunction for each timestep would be calculated across the x-range, before updating each point of the wavefunction in time. It should also be noted that, for a stable solution, the Central Difference Approximation requires that the ratio

$$r = \frac{\delta}{h^2} < \frac{1}{2},\tag{3.11}$$

else the solution diverges.

3.1.3 Imaginary Time Propagation

Before attempting to run a simulation of the Gross-Pitaevskii Equation, one should first obtain the ground state of the condensate for the geometry of the system. A simple and reliable way to do this is by initially propagating through imaginary time [24]; that is, transform

$$\delta \to -i\delta.$$
 (3.12)

By directly integrating the Schrödinger equation:

$$i\frac{\partial\Psi}{\partial t} = \hat{H}\Psi,\tag{3.13}$$

we obtain

$$\Psi(x,t+\delta) = \Psi(x,t)e^{-i\hat{H}\delta}$$
(3.14)

We can write the wavefunction $\Psi(x,t)$ as a superposition of eigenstates, $\Phi_n(x)$, with corresponding amplitudes $\psi_n(t)$ and eigenenergies $E_n(t)$, that is,

$$\Psi(x,t) = \sum_{n} \psi_n(t) \Phi_n(x).$$
(3.15)

By combining Equations 3.14 and 3.15, and applying transformation 3.12, we obtain

$$\Psi(x,t+\delta) = \sum_{n} \psi_n(t) \Phi_n(x) e^{-E_n \delta}.$$
(3.16)

Hence, the larger the energy of the eigenstate, the more quickly it decays, and so as t increases, the eigenstate with the lowest energy, the ground state, dominates the solution. Thus, by starting with an initial guess at the equilibrium solution, and by renormalising the wavefunction after each timestep (in order to account for the decay of the ground state solution), we can equilibrate to the ground state of the system. We can generalise this approach to other Schrödinger-like equations, including the GPE.

3.2 Equilibrium Solutions

3.2.1 Infinite Potential Well

The most simple version of the GPE we shall discuss is that of the infinite potential well. In this geometry, the condensate is contained entirely within a well, with zero potential inside, and infinite potential outside. This requires that we set the condensate at the boundaries of the well to have zero density, as we must have continuity, and the condensate cannot have density in the infinite potential outside the well. One might expect that having an equal (zero) potential throughout the well would produce an entirely equally distributed condensate; however, these zero boundaries mean that this is not quite the case. Instead, the condensate "heals" form the zero boundary conditions to its asymptotic value n_{∞} . The distance required for the condensate to reach this value is the healing length, ξ , which we introduced in the derivation of the dimensionless GPE. In order to observe this healing length properly, the well must be much larger than ξ itself; my well is set over the range [-30, 30], and is shown below in Figure 3.1.

As well as my numerical solution, Figure 3.1 also shows the analytic solution to the GPE in a zero-potential infinite well [7]:

$$\psi = \psi_{\infty} \tanh(x), \tag{3.17}$$

shown by the blue points. By examining the subgraph, we can see that the analytic solution overlies my numeric solution very well. It should also be noted that decreasing the discretisation units, h and δ , did not give an improved convergence with the analytic tanh soultion.



Figure 3.1: Plot of the ground state of the GPE within an infinite potential well: simulated solution (red line), analytical tanh solution (blue points). Window plot shows the solution close to the boundary, as the condensate "heals".

3.2.2 Harmonic Trap

The next step in simulating the GPE is to add in a potential within the infinite well; initially I added a simple harmonic trap, that is, $V = \frac{1}{2}\Omega^2 x^2$. The potential increases away from the midpoint x = 0, and rather than an approximately constant density as in the infinite well, the condensate forms a Gaussian-like curve, with its peak at zero. The potentials and atom densities for two different values of Ω are shown in Figure 3.2. We can see that using a higher value of Ω (blue line) has the effect of "tightening" the trap; the potential increases more rapidly, and the condensate is contained within a smaller x-range, with a slightly higher peak density.



Figure 3.2: Plots showing the potential V(x) of a simple harmonic trap (left), and atomic density n(x) of the trapped condensate (right) for $\Omega = 2.0$ (red line) and $\Omega = 2.2$ (blue line).

In order to ascertain that my code was working correctly before attempting to simulate the Josephson effect, I simulated a simple harmonic step: this involves running imaginary time propagation with the harmonic potential set slightly higher than normal (in this case $\frac{1}{2}(1.1\Omega)^2 x^2$), and then, on the switch to real time propagation, dropping back to the standard harmonic potential, $\frac{1}{2}\Omega^2 x^2$. This causes the condensate to oscillate between the equilibrium solutions for the two different potentials without any damping. To demonstrate this effect, Figure 3.3 shows the oscillating density of the midpoint of the well, as well as the total energy of the condensate (we will consider energy in more detail at the end of this section).



Figure 3.3: Time-evolution of the density at the midpoint of a condensate (left) and energy (right) in a simple harmonic trap after a small perturbation in the potential.

In these figures, t < 0 corresponds to the equilibration stage during "imaginary time propagation", and show the convergence of density and energy to a constant, equilibrium value. Once running in real time, the density of the midpoint of the condesate oscillates perfectly, without damping, whilst the energy remains at a constant value, after an initial jump. This was a good sign that my code was working correctly. The idea of energy conservation will be further discussed at the end of this section.

3.2.3 Double-well Trap

In order to create the Josephson effect, I needed to split my condensate from the harmonic trap into two separate, interacting parts. To do this, I added a potential barrier in the form of a Gaussian term onto my harmonic potential:

$$V = \frac{1}{2}\Omega^2 x^2 + V_0 e^{-\frac{x^2}{2}}$$
(3.18)

For my master calculations, I used a value of $V_0 = 1.5$, as this created a significant barrier in the middle of the condensate, splitting it into two parts, whilst also still allowing quantum tunnelling of atoms through the barrier. The equilibrium density solution, and potential for $V_0 = 1.5$ is shown below in Figure 3.4. Altering the value of V_0 will be discussed in more detail in the Numerical Analysis section.



Figure 3.4: Plot showing the potential V(x) of a doublewell (blue line), and atomic density N(x) of the condensate within (red line).

3.3 Creating Imbalance in the Condensates

In order to initiate the Josephson effect, I first needed to imprint my condensates with an imbalance between the left and right wells. Initially I introduced a population imbalance by adding a linear imbalance to the external potential during imaginary time propagation, which led to an equilibrium solution with a non-zero z(0). At the switch to real time propagation, I then removed this imbalance to leave a symmetric trap:

$$V_{Im} = \frac{1}{2}\Omega x^2 + V_0 e^{-\frac{x^2}{2}} + \gamma x, \qquad (3.19)$$

$$V_{Re} = \frac{1}{2}\Omega x^2 + V_0 e^{-\frac{x^2}{2}}.$$
(3.20)

Figure 3.5 shows how the potential changes in the transition from imaginary to real time propagation.



Figure 3.5: The transition from asymmetric potential in imaginary time propagation (left), to the symmetric potential in real time (right).

The plot of the equilibrium solution under the imbalanced potential (i.e. the distribution of the condensate at the beginning of real time propagation) is shown in Figure 3.6.

The alternative method I used was to imprint an initial phase imbalance onto the condensates, by multiplying the left well by a constant $e^{i\theta}$, while leaving the right well unchanged. This made no difference during imaginary time propagation (when we are, in practice, considering a real-valued equation), but once running in real time, this imbalance in phase created the oscillations predicted by the Josephson relations. We shall discuss the results from both





Figure 3.6: Initial profile (after imaginary time propagation) of the atomic density within the doublewell, using potential parameters $\Omega = 2, V_0 = 1.5, \gamma = 0.5$.

3.4 Numerical Issues

3.4.1 The Phase Jump Problem

Calculating the phase difference between the two condensates turned out to be non-straightforward, in large part due to the jump in phase which occurs at $\pm \pi$. Recalling that the phase is defined as $\theta = \arctan(\Im(\psi)/\Re(\psi))$, and the range of arctan is $(-\pi/2, \pi/2)$, so by calculating the phase difference $\phi = \theta_2 - \theta_1$, ϕ is therefore defined on the range $(-\pi, \pi)$. Figure (3.7) (left) shows a typical plot of the phase of the wavefunction against its position in the trap. One can see that the phase follows a trend within the range -7 < x < 7, and appears random elsewhwere. This is due to the distribution of the wavefunction within the trap; the condensate only exists within the range [-7.0, 7.0], and hence the only meaningful phase values are those which fall within this range. Figure (3.7) (right) shows the phase plot for this range, along with the analytic arctan solution.



Figure 3.7: Plot of how the phase of the condensate varies across the trap; full range of well (left), and within the range [-7.0, 7.0] where the condensate is non-zero. Red points show simulated values, blue dashed line gives analytic arctan solution.

Initially, I calculated θ_1 and θ_2 , the phases in the left and right wells respectively, by averaging the phase value, over [-6.0, -2.0] for θ_1 , and over [2.0, 6.0] for θ_1 . I chose these regions specifically because they were well within the range in which the phase followed the arctan solution, whilst also avoiding the region around zero where the gradient is steeper. By subtracting $\phi = \theta_2 - \theta_1$, I was able to plot how the phase difference between the two condensates changed with time, and this initial plot is shown in Figure 3.8.



Figure 3.8: Time-evolution of phase difference using average phase values for $\theta_{1,2}$: simulated values (rep points), analytic solution (blue dashed line).

Although the general trend is correct, as shown by the fitted solution (using the same period of oscillation as calculated for the population difference), one can see that there are many anomalous points which do not fit the trend. Since several of the anomalies appeared to occur near minima and maxima of the oscillations, I looked at how the phase changed in snapshots over small timesteps around the first minimum, as shown in Figure 3.9. These snapshots show how the phase can jump by 2π at the boundary value of $-\pi$, and display how the position of the phase jump changes over time .



Figure 3.9: Snapshots of the phase of the condensate changes with position

Whilst defining θ_1, θ_2 as the average values across a range of points, it was particularly difficult to overcome this issue of phase jump, as the jump occurs at a different x-value each time, making it hard to know when to implement a correction of 2π . Instead, I solved the issue by defining θ_1, θ_2 as the phase at a single point, at the values x = -4.0, x = 4.0 respectively. This is not a perfect solution, as we lose some accuracy in the values of the phases. However, for the Josephson effect, we are only interested in ϕ , the difference in phase between the two condensates, and the trend it displays through time. Thus, as long as we define ϕ consistently, the trend should not be noticeably affected, even if the exact value is not quite the same as the integrated average. Also, by taking the phase at ± 4.0 , we are taking the midpoint of the region used initially, and hence should find a reasonable approximation of ϕ . By defining ϕ in this way, and adding a compensatory factor of 2π to θ_1 in the case when θ_2 had made the jump from $-\pi$ to π , but θ_1 had not, I was able to produce clear oscillations, shown in Figure 3.10.



Figure 3.10: Time-evolution of phase difference using single point values for $\theta_{1,2}$: simulated values (red solid line), analytic solution (blue dashed line).

3.4.2 Energy Drift

Ideally, when running a simulation of the time evolution of the condensates to observe the Josephson effect, all oscillations in population, phase, etc., would be perfect sinusoids, with constant period and amplitude. However, in many of my simulations, I discovered that as time increased, there would be some discrepancies in amplitude, generally in the form of weak damping. To investigate the cause of this damping effect, I plotted how energy of the system evolved with time. The dimensionless energy functional (in units of , $E(\psi)$, is given by [25]

$$E(\psi) = \int \left[\frac{1}{2} \left|\frac{\partial\psi}{\partial x}\right|^2 + V|\psi|^2 + \frac{1}{2}|\psi|^4\right] dx \qquad (3.21)$$

Unlike in the case of the simple harmonic trap in Section (3.6), I found that the energy of the system did not remain completely constant, or even oscillate continuously about a fixed value. Instead, I discovered a small amount of energy drift within the system; that is, after the initial energy jump at the start of real time propagation, the value of $E(\psi)$ gradually increased with time. In order to correct this, I investigated how decreasing the values of δ and h within the RK4 timestep and CDA methods discussed in Chapter 3 would affect this energy drift. The results are shown in Figure 3.11.



Figure 3.11: Time evolution of the energy of the system for different values of h and δ : $h = 0.1, \delta = 0.00001$ (solid red line); $h = 0.05, \delta = 0.000001$ (dashed green line); $h = 0.1, \delta = 0.000001$ (dotted blue line). Window graph shows the same plots for real time propagation only.

As we can see the value of energy drift is very small in each case; my initial parameters of $\delta = 0.00001$, h = 0.1 gives an energy drift of approximately 0.1%, whereas by decreasing both δ and h, this could be lowered to 0.02%. However, in order to check, I also looked at how the different numerical parameters h and δ affected the oscillations within the measurements of the Josephson effect; Figure 3.12 shows the plot of the time-evolution of z(t) for the three different pairs of (δ, h) values I tried.

All three solutions overlie each other so closely that is hard to distinguish

them. Due to the negligible effect that decreasing the timestep and x-step had upon my results, combined with the computaional expense involved with implementing them, I decided to continue using my initial numerical parameters, h = 0.1, $\delta = 0.00001$.



Figure 3.12: Plot of the time-evolution of population difference for the different values of δx and δt : $\delta x = 0.1, \delta t = 0.00001$ (solid red line); $\delta x = 0.05, \delta t = 0.000001$ (dashed green line); $\delta x = 0.1, \delta t = 0.000001$ (dotted blue line).

Chapter 4

Numerical Josephson Effects

In this Chapter, we shall examine the simulations produced by my code, and analyse them with respect to theoretical results.

4.1 Josephson Oscillations

4.1.1 Initial Population Imbalance

In order to simplify the Josephson relations discussed in Chapter 2, I decided to look primarily at the case in which the equations could be linearised in z(t); for this reason, I chose a relatively small potential imbalance of $\gamma = 0.5$ to run in imaginary time, which in turn created a small initial population difference, i.e. $|z(t)| \ll 1$. Due to this, we can use the linearised Josephson relations from Chapter 2:

$$z(t) = z_{max} \cos\left(\omega t + \phi(0)\right), \qquad (4.1)$$

$$\phi(t) = \phi_{max} \sin\left(\omega t + \phi(0)\right), \qquad (4.2)$$

In order to ascertain that the oscillations produced were indeed sinusoidal, I used the "fit" function on gnuplot to a sine curve of best fit to my data via the frequency parameter, ω . Recall Equation 2.22:

$$\omega = 2\kappa\sqrt{\Lambda + 1} = \sqrt{E_C E_J + E_J^2}$$

The results are shown in Figure 4.1. The sine wave solution overlies the simulated values very well; there are small discrepancies in amplitude at minima



and maxima, but the two sets of data oscillate with the same period.

Figure 4.1: Population difference z(t): simulated Josephson population oscillations denoted by red line, analytical cosine wave by blue points ($\omega = 1.635$).

Since, within the Josephson oscillation regime, the population and phase differences should oscillate with the same frequency, as discussed in Section 2.2, it is useful to plot the time evolution of $\phi(t)$. This is shown in Figure 4.2, with a sine wave of the same frequency, $\omega = 1.635$ overlaying my simulated values. We can see that the oscillations have a frequency which matches that of the sine wave, and hence the phase and population differences oscillate with the same frequency. It is also worth noting that z(t) and $\phi(t)$ oscillate $\pi/2$ radians out of phase with one another, which is what we should expect as, in the Josephson oscillations case, $z(t) = \cos(\omega t + \alpha)$, and $\phi(t) = \sin(\omega t + \alpha)$. Another plot of interest is that of z vs ϕ , shown in Figure 4.3: we have $z(t) = z_{max} \cos(\omega t + \phi(0)), \ \phi(t) = \phi_{max} \sin(\omega t + \phi(0))$. If we divide z by z_{max} , and ϕ by ϕ_{max} , then square both expressions, we see

$$\frac{z^2}{z_{max}^2} + \frac{\phi^2}{\phi_{max}^2} = \cos^2(\omega t + \phi(0)) + \sin^2(\omega t + \phi(0)).$$
(4.3)

That is,

$$\left(\frac{z}{z_{max}}\right)^2 + \left(\frac{\phi}{\phi_{max}}\right)^2 = 1.$$
(4.4)



This is the equation of an ellipse.

Figure 4.2: Phase difference, $\phi(t)$: simulated Josephson phase oscillations denoted by red line, analytical sine wave by blue points ($\omega = 1.635$).



Figure 4.3: Plot of z vs ϕ for Josephson oscillations, exhibiting an elliptical trajectory.

Although the plot shown in Figure 4.3 does not quite have the perfect, full, closed ellipse that the analytics suggest we should see, it captures the essence of what we expect to see; an ellipse with minimum and maximum zvalues of $\pm z_{max}$, and similarly for ϕ at $\pm \phi_{max}$.

4.1.2 Initial Phase Imbalance

As mentioned in Chapter 2, alternatively to starting with an imbalance in population, we can instead introduce a phase difference between the two condensates. In experiments, this can be done by firing a very brief, very tightly focussed pulse of energy at one condensate, and not at the other. In my simulations, I simply multiplied the left hand condensate by a coefficient of $e^{i\theta}$, with θ an adjustable parameter, to introduce an arbitrary phase difference to the two condensates. By setting my initial phase difference to be equal to the maximum phase difference observed when starting with a population imbalance, I was able to confirm that the frequency of Josephson oscillation was the same in both cases. This provided a good consistency check for my code; by altering the initial phase difference to its maximum value. The population and phase differences for $V_0 = 1.5$, $\phi(0) = 0.7\pi$ are shown below in Figures 4.4 and 4.5.



Figure 4.4: Population difference when applying: $\phi(0) = 0.7\pi$, z(0) = 0 (red solid), compared to $\phi(0) = 0$, z(0) = 0.05.



Figure 4.5: Phase difference when applying: $\phi(0) = 0.7\pi, z(0) = 0$ (red solid), compared to $\phi(0) = 0, z(0) = 0.05$.

4.2 Dependendence of Josephson Effects on Separation Barrier

We shall now look at how changing the height of the potential barrier, V_0 , affects the Josephson effect. As Figure 4.6 shows, increasing the coefficient of the Gaussian term within the external potential increases the barrier between the two wells. This increase in potential barrier causes the frequency of Josephson oscillations to change. Increasing V_0 causes a decrease in E_J , due to the higher energy required for particles to tunnel through the barrier, and an increase in E_C , due to a higher proportion of atoms being held in their respective well; Figure 4.6 shows that, for $V_0 = 2.75$, although the region of the condensate is marginally larger than when $V_0 = 1.5$ or 0.25, this does not compensate for the loss of the central tunnelling area, which relatively few atoms can now occupy. Within the JO regime, E_J dominates E_C ($\Lambda \ll 1$), and hence

$$\omega = E_J \sqrt{\Lambda + 1} \approx E_J. \tag{4.5}$$



Figure 4.6: Potentials (top) and densities (bottom) for equilibrium solutions of doublewells, using different values of V_0 : $V_0 = 0.25$ (left), $V_0 = 1.5$ (middle), $V_0 = 2.75$ (right).

So increasing the height of the separation barrier V_0 decreases the tunnelling energy, and hence causes the frequency of Josephson oscillations to decrease. This effect is shown in Figure 4.7, for which I used the "fit" function on GnuPlot to estimate ω for a range of values of V_0 .



Figure 4.7: Frequency change with varying height of potential barrier, V_0 , in the Josephson oscillations regime

The figure shows that, as expected, increasing the height of the separation barrier, V_0 , causes the frequency of oscillations to decrease. The main region of interest from this plot is $V_0 \ge 1$; if $V_0 < 1$, the barrier is not large enough to separate the condensate into two effectively. It should be noted that, as V_0 increases, Λ also increases, since E_J decreases and E_C increases. However, because $\omega = E_J \sqrt{\Lambda} + 1$, the decreasing E_J term outside the square root has a larger effect on ω than the increasing Λ inside the root. The non-linearity of the graph arises from the increasing competition between E_C and E_J ; however, it is the decrease in tunnelling energy that dictates the behaviour of ω , and we can see that as we approach $V_0 \approx 2.7$, ω decreases ever more rapidly towards zero; the oscillations become faster. At this point, we are entering the critical region, in which E_C and E_J are of similar magnitude, causing the unusual-looking oscillations displayed in Figure 2.1 (c). Unfortunately, my numerics were not precise enough to reproduce this solution; however, by increasing the height of the barrier to $V_0 = 2.75$, I was able to observe macroscopoic quantum self-trapping, which we shall discuss in the next section.



Figure 4.8: Time evolution of z(t) for different values of V_0 ; $V_0 = 0.5$ (green dashed); $V_0 = 1.5$ (red solid); $V_0 = 2.5$ (blue dash-dot)

Figure 4.8 shows how the population imbalance changes in three specific cases: $V_0 = 0.5$ (green), $V_0 = 1.5$ (red), and $V_0 = 2.5$ (blue). All three fall

within the Josephson oscillations regime, as we can see from z(t) oscillating about zero. However, as well as a small change in amplitude of oscillations, we see that the period of oscillation nearly doubles between potentials of $V_0 = 0.5$ and $V_0 = 2.5$.

4.3 Macroscopic Quantum Self Trapping

So far we have considered only the Josephson oscillations effect, in which the population difference and phase difference both oscillate about zero. However, if we increase the potential barrier further, to values of $V_0 \ge 2.75$, we see instead macroscopic quantum self trapping. This is what we would expect, as by increasing V_0 , we are raising the potential through which the atoms have to tunnel. This decreases the Josephson coupling energy, E_J , and increases the atomic self-interaction energy, E_C , and so the value of Λ increases. Figures 4.9 and 4.10 shows the behaviour of population and phase differences under such a regime.



Figure 4.9: Time-evolution of population difference for $V_0 = 2.75$, within the self-trapping regime.

Although the oscillations for z(t) are imperfect, they display the characteristic behaviour of self-trapping, notably that the changes in population difference no longer oscillate between the two condensates, but instead the condensate with the higher initial population retains more of the atoms. We can also observe the "running" phase; for the purposes of this graph it is bounded by $[-\pi,\pi]$, but in reality the phase increases continually, rather than resetting each 2π -phase jump.



Figure 4.10: Time-evolution of phase difference for $V_0 = 2.75$, within the self-trapping regime.



Figure 4.11: Plot of z vs ϕ : upper trajectory shows solution for z(0) > 0, lower trajectory shows solution for z(0) < 0.

As before, we can plot z vs ϕ , which is shown in Figure 4.11. Unlike in the case of Josephson oscillations, we instead see two distinct open trajectories, which correspond to the non-oscillatory running phase. The upper trajectory shows the solution for initial population imbalance z(0) > 0 (using initial potential imbalance $\gamma = 0.5$), the lower trajectory the solution for negative population imbalance, z(0) < 0 ($\gamma = -0.5$). The trajectories remain approximately the same after each phase jump, which reflects the the oscillations in population difference, but, as expected for MQST, neither trajectory crosses the z-axis.

Chapter 5

Summary and Future Work

5.1 Summary

We have seen that the results produced from my simulations match both numerical and experimental results produced by others produced by others, in both the Josephson oscillations and macroscopic quantum self-trapping schemes. This can be summarised neatly by Figure 5.1, which shows the plots of z vs. ϕ , for my simulated results (left), and for the Albiez experimental data (right).



Figure 5.1: Plots of population difference vs. phase difference for simulated results (left) and experimental data (right). Left: Josephson oscillations (red solid line), MQST (blue dashed line); Right: Josephson oscillations (black points), MQST (white points) [20].

We have see that my results have good agreement in trend with Josephson effects observed experimentally, despite the different parameters used. We have a closed (almost) elliptical solution in the case of the JO case, reflecting its oscillatory phase and population differences, whereas in the MQST case, we have an open trajectory, which reflects its characteristic running phase. Note that in MQST, the z trajectory remains approximately the same for each phase loop, corresponding to the oscillatory nature of the population difference; however, it never crosses the z = 0 axis, again characteristic of the MQST oscillations.

The key difference between my results and those of the experiment is the amplitudes for the two different effects; consider the value of z_{max} . My results show z_{max} to be approximately equal for both Josephson oscillations and MQST, whereas the experimental data puts z_{max} much higher for MQST. This is caused by the different methods used to initiate the separate effects; the experimental data was attained by increasing the initial population difference z(0) past a critical value, whereas I increased the potential barrier between the condensates to prohibit tunnelling, which causes only a very minor alteration to z(0).

In general though, my results display strong qualitative similarities to both analytical predictions, and experimental data.

5.2 Future Work

Initially, any future work in this topic would include improving my nuemrical methods; although the issues experienced with energy drift did not appear to have a noticeable effect on the Josephson effects at $|z| \ll 1$, this was no longer the case for larger values of |z|. This would potentially involve implementing the Crank-Nicholson method for my timestep, which is not restricted by the stability condition as the Runge-Kutta 4th Order method is. I would also investigate higher order schemes for approximating $\partial^2 \psi / \partial x^2$.

Once the numerics were running more smoothly, I would like to investigate the critical value of Λ in more detail, and ideally to produce plots analogous to those produced in Figure 2.1 (c, d), for $\Lambda \to \Lambda_C^-$, $\Lambda = \Lambda_C$ respectively. I would also like to alter my parameters, chosen for computational convenience, to those used in the Albiez experiment, in order to see if I could replicate their results quantitatively. One study which particularly interested me was that of J. Thywissen et al [21], which was concerned with the crossover region from Josephson effects to hydrodynamics, when different potential barriers are used, specifically a decaying frequency signal observed with higher barriers. Although this decaying signal is not the same as the damping observed in my results, it was this which first drew my attention to this paper, and I would like to study it in more detail, in order to improve my understanding of Josephson effects within Bose-Einstein condensates.

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