From Disordered Bosons to Dipolar Fermions - Theoretical Studies in Ultracold Atoms

Joseph Towers

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Abstract

We use numerical simulation to study ultracold, quantum degenerate, atomic gases. In the first part of the thesis we study the effects of disorder, introduced via a bichromatic optical lattice, in one and two dimensional systems. We employ the Aubry-André model and use time-dependent numerical simulations to investigate the disorder dependent transition to strong localisation present in the model. Weak s-wave interactions are added to the model and we observe the interaction between localisation and interaction induced self-trapping. We then add a tilted lattice potential to the model. In the homogeneous model this induces Bloch oscillations. While one might expect that a strong enough force will break the strong localisation or self-trapping, within the bounds of the single-band model, the trapping effect of the Bloch oscillations reinforces both of the other effects leading to increased confinement, albeit lacking the clear single frequency oscillation signature of pure Bloch oscillations.

Along with the two dimensional bichromatic optical lattice we add a term to the Hamiltonian equivalent to that of a uniform external magnetic field on charged particles. Since the experimental realisation of this model would employ neutral atoms, the magnetic field is synthetic, the equivalent effect being produced by an appropriate set of lasers and magnetic fields. We show that in the ballistic regime (weak bichromatic disorder) the system displays positive magnetoresistance. Conversely in the strong localisation regime the system exhibits negative magnetoresistance.

In the latter part of the thesis we use density functional theory to calculate the ground-state density of a harmonically trapped dipolar Fermi gas. We then use these to calculate the lowest energy collective mode oscillation frequencies under the hydrodynamic approximation. We find that increasing the strength of the dipoles has the effect of increasing the mode frequencies. The increase saturates for large dipole strengths. We verify this analytically and show that such is due to the local nature of the two dimensional energy functional and not dependent on the specific equation of state.

We employ an average density approximation to construct an energy functional for the inhomogeneous, 2D degenerate Fermi gas. The ground-state densities for a cylindrically symmetric harmonic trap are compared to the
Kohn-Sham results, showing extremely good agreement in the tail region and good agreement with the exact ground-state energy. We then do the same for higher order polynomial traps and obtain improved agreement for higher degree.
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Chapter 1

Introduction and Outline of the Thesis

The advent of laser cooling [1] has lead to a rapid expansion in studies and applications of ultra-cold atomic physics. The notion of using the momentum change from elastic collisions with photons from an incident laser, to slow and cool a gas of particles, allowed physicists to access unparalleled low temperatures in the sub-micro Kelvin range.

At such low temperatures, the cloud of atoms is able to be trapped in the intensity peak of an off-resonant laser beam. Slowly reducing the dipolar trap or selectively exciting the higher energy particles out of the trap, reduces the average energy of the particles in the cloud, and hence, further reduces the temperature. This evaporative cooling enables a gas to be cooled to the nano Kelvin range.

In 1995 these methods allowed two groups [2, 3] to reduce the temperature of a gas of bosons to the point of condensation, a sudden macroscopic occupation of the lowest energy state. This state of matter is known as a Bose-Einstein condensate, a concept predicted by Einstein in 1924.

The attainment of the first Bose-Einstein condensate has allowed unprecedented access to the quantum regime. The same and similar techniques can be used to reduce a cloud of fermions to degeneracy. Such precision control of the position and momentum of a gas, allows the production of systems with both simple and complex Hamiltonians. Careful manipulation of the system allows one to manufacture Hamiltonians found in other fields of Physics that are difficult or impossible to explore directly. This type of emulation of quantum systems was labelled a “quantum simulator” by Feynman in 1981 [4].

In this way we can simulate the behaviour of the electrons in a metal, but still have full control of the particle interactions and lattice spacing, control which is impossible
in solid-state physics.

Similarly, we can explore the physics of the electronic structure of molecules by studying the behaviour of fermions in simple potentials. Density functional theory allows us to numerically calculate the ground-state properties of these systems with much less computational cost. Most functionals have been developed for the Coulomb interaction. Dipolar gases have different long-range interactions and so alternate energy functionals must be developed, particularly in 2D configurations.

1.1 Thesis Outline

The first part of this thesis explores the effects of disorder on some one and two dimensional ultra-cold Bose gases. We first explore, via numerical integration, the dynamic behaviour of a non-interacting, and interacting, Bose gas in a 1D bichromatic optical lattice potential, and compare to experimental observations. We also explore the incarnation of Bloch oscillations in the bichromatic optical lattice.

We then numerically simulate the dynamics of an ultra-cold Bose gas in a 2D bichromatic optical lattice potential, in the presence of an effective external magnetic field. We explore the interplay of magneto-resistance and disorder induced localisation in the Bose gas.

The second part of the thesis is dedicated to using density functional theory to explore the structure of electron clouds. We first use the Thomas-Fermi-von Weiszäcker method to calculate the frequencies of the collective mode oscillations of a 2D spin-polarised, dipolar Fermi gas in a harmonic potential. The collective mode frequencies are readily measured in experiment, so are of immediate use to future experimental studies.

In the last chapter we develop and implement an average density approximation approach to find the ground-state density of a 2D spin-degenerate Fermi gas. We make use of a discrete Hankel transform to efficiently calculate the ground-state, providing an algorithm that is less numerically difficult than the current methods while maintaining sufficient accuracy.

1.2 Publication History

Over the course of my ph.D. study I have contributed to the publishing of four academic papers.
The first paper, I wrote all the code for the simulations, performed all the simulations with the aid of S. Cormack, and wrote the paper text under the supervisorship of D. A. W. Hutchinson. This paper contributes to the content of Chapter 3 and builds from the results from the earlier chapters.

The second paper, is a joint collaboration with B. P. van Zyl et al. I was called upon to develop and implement a numerical solver for the proposed Average Density Approximation method. I was then involved in the writing and editing of the results section. This paper contributes to the theory and the first set of numerical results in Chapter 5.

For the third paper I was only involved in the late editing stage, preparing the paper for resubmission. The bulk of the work was performed by the other authors, however, the content is similar to that presented in the first two chapters of this thesis.

The final paper was again a collaboration with B. P. van Zyl et al., this time I was involved throughout. I contributed to the theory, particularly the analytical results, developed and executed all the numerical calculations, and was involved in the writing and editing. This paper contributes to the content of Chapter 4.


Part I

Disordered Media
Chapter 2

Introduction

Disorder is unavoidable in any realistic system, whether it be lattice misalignment or impurities in solid-state materials, or background noise in general. The effects of varying degrees of disorder can be hard to predict even when seemingly negligible. In contrast to the rest of solid-state physics, where disorder is an inconvenience and all attempts are made to negate its effects, a large interest has arisen in the phenomena where disorder is useful.

Disorder in bulk materials can be difficult to study due to the large number of other phenomena occurring at the same time, and the extremely small scale of the atomic separation. Fortunately, we can turn to other systems that have the same or similar Hamiltonian as the system of interest, as suggested by Feynman [4]. The test system may be easier to manipulate and its behaviour will be the same or similar to the original system, after suitable matching of the problem parameters.

In 1995 the production of the first Bose-Einstein condensate (BEC) [2, 3] opened up a whole new field in the study of disordered media. The dipole potential of a laser standing wave provides a very suitable lattice structure so that the BEC can simulate the behaviour of electrons in the crystalline lattice of bulk metals. The site separation of the simulator is on the order of the micron and tunable by the light’s wavelength, the strength of the lattice is tunable by varying the light intensity, and even the particle interactions may be tuned by applying an external magnetic field near a Feshbach resonance [5]. This superior degree of control has sparked many theoretical and experimental studies into various types of disorder and lattice arrangements.
2.1 The Quantum Limit

A classical particle in a disordered potential will traverse space, changing speed depending on the topology of the potential, until it encounters a peak in the potential with greater energy than its own. It is forbidden to pass the barrier and so it will be perfectly reflected.

![Wavefunction of a particle in the region of a finite square barrier.](image)

Figure 2.1: Wavefunction of a particle in the region of a finite square barrier. If the size of the barrier is much larger than the particle’s wavelength then it is reflected. If it is smaller, there is a finite probability of transmission through the barrier.

In a quantum system, the density probability of the particle extends through the barrier (see Fig. 2.1), and hence, there is a finite probability that the particle will be transmitted past, even though its energy is less than the peak. This so-called "quantum tunnelling" is the basis of many modern technologies including the tunnelling electron microscope.

The flip-side of the quantum treatment is that the particle has a finite probability of reflecting off any peak in the potential, even if the energy of the peak is far smaller than the particle’s energy.

The system enters the quantum regime when the free-energy of the particles - given by $\epsilon = \hbar^2 k^2 / 2m$, where $k = 2\pi / \lambda$, with $\lambda$ as the particle’s de Broglie wavelength, and $m$ is their mass - is smaller than the correlation energy of the potential [6] - defined as $E_c = \hbar^2 / 2m R_c^2$, which corresponds to the recoil energy of a particle trapped in a well of size $R_c$, where $R_c$ is the correlation length. This is equivalent to $\epsilon / E_c = (kR_c)^2 \ll 1$, i.e.
the correlation length of the disorder is much shorter than the de Broglie wavelength of the particles. This is a similar, but stronger, condition than the Ioffe-Regel criterion

\[ l < \lambda, \quad (2.1) \]

where, \( l \), is the mean free path, the average distance a particle will travel before scattering off the disordered potential. The mean free path is a measure of the size and density of the potential peaks, and the de Broglie wavelength effects the decay rate of the probability density through a barrier. Colder particles, with lower momentum, will have a larger wavelength. Hence, an experimentalist will cool down a system to enter the quantum regime.

### 2.2 Weak Localisation

A particle in a disordered region does not simply travel from point A to B in a straight line, it will scatter off the features of the disorder field as it moves, similar to the classical picture of electronic resistance in a metal wire. The motion is diffusive, as opposed to the ballistic motion of free space.

In the path integral formulation of quantum mechanics, all possible classical paths contribute to the transmission probability, and the amplitudes of all the paths must be summed. Some paths are more important than others, for instance, the paths that cross themselves, the so-called "looped paths" have greater weight. Consider the looped trajectory I in Fig. 2.2 from point A, through point B and back to A. Trajectory II

Figure 2.2: If two waves follow the same path from A to B, one going clockwise and the other anti-clockwise, they interfere constructively on returning to A. **Figure credit to [7].**

A particle in a disordered region does not simply travel from point A to B in a straight line, it will scatter off the features of the disorder field as it moves, similar to the classical picture of electronic resistance in a metal wire. The motion is diffusive, as opposed to the ballistic motion of free space.
follows the same path except in the opposite direction. The phase accumulated is the same for either, and hence, they constructively interfere. The tendency to promote looped paths reduces the transmission probability, and hence, the conductance of the material [8, 9]. This effect is known as "Weak localisation".

2.3 Anderson Localisation

Given an ultra-cold gas of non-interacting particles in a disordered potential such that the system is firmly in the quantum regime, we expect that, as the probability of transmission through any barrier is finite, the gas will eventually expand to fill the entire system.

However, in 1958 Anderson [10] predicted that electrons in a crystal lattice structure would demonstrate an “absence of diffusion” in the presence of a uniformly random disordered potential. Such a random potential could be the effect of a frustrated lattice or impurities in the crystalline material. The standard and intuitive, perturbative approach fails to predict this behaviour.

Anderson presented a model for a gas of particles occupying the sites of a 3D lattice with energy $E_j$, and the energy associated with "hopping" between pairs of sites is $V_{jk}$. The evolution of the probability amplitude of the site occupation is then governed by the equation

$$i \dot{a}_j = E_j a_j + \sum_{k \neq j} V_{jk} a_k.$$  \hspace{1cm} (2.2)

The onsite energies, $E_j$, are uniformly distributed on the interval $-W/2 < E_j < W/2$, and the site-to-site hopping energies, $V_{jk}$, decay with distance faster than the potential

$$V(r) = \frac{1}{r^3},$$  \hspace{1cm} (2.3)

i.e. the theory is not supported for dipolar interactions.

Anderson used the Laplace transform to show that the probability of transmission, after infinite time, to a site distant from the initially seeded site, decays exponentially with distance. i.e. that the probability distribution at infinite time is

$$|\psi(r)|^2 \sim e^{-|r-r_0|/L_{loc}},$$  \hspace{1cm} (2.4)

where, $L_{loc}$, is the localisation length. Other than this “virtual” transmission, all other transmission processes (i.e. ballistic or diffusive expansion) are suspended.

Anderson attributed the localisation to “the failure of the energies of neighbouring sites to match sufficiently well for $V_{jk}$ to cause real transport. [...] More distant sites
are not important because the probability of finding one with the right energy increases much more slowly with distance than the interaction decreases”.

### 2.4 The Mobility Edge

The main signature of Anderson localisation is the exponentially decaying profile of the single-particle eigen-states of the Hamiltonian. However, as was pointed out by Mott in 1967 [11], if the strength of the disorder potential is less than a certain critical value, then there exists an energy, $E_c$, known as the “mobility edge”, above which, the eigen-states need not be localised.

Mott further conjectures that a localised state and an extended state cannot exist in the same energy region. If they were close enough together, a small perturbation would cause them to form a pair of hybrid states, both of which are extended. Therefore, all states with energy above the mobility edge must be extended. The material would then be a metal if the Fermi energy, $E_F$, is greater than $E_c$, as transmission is possible via the extended states, or an insulator, if $E_F < E_c$.

Fig. 2.3 gives a sketch of the density of states of the Anderson band of the system. The states are localised in the low-density tails of the band (shaded regions), i.e. the states with energy below $E_c$ or above $E_c'$. As the strength of the disorder potential, $W$, is raised, the two critical energies come together until there are no extended states.

![Density of states in an Anderson band. $E_c$ and $E_c'$ mark the two mobility edges. Figure credit to [12].](image)

Figure 2.3: Density of states in an Anderson band. $E_c$ and $E_c'$ mark the two mobility edges. **Figure credit to** [12].
2.5 Scaling Theory

The original Anderson model, and Mott’s considerations of the mobility edge, were for a 3D disordered material, however, the dimensionality (\(d\)) of the system proves critical in determining the existence of a mobility edge.

In 1979 Abrahams et al. [13] published a scaling theory extending the Anderson model to other dimensions. They presented arguments for the behaviour of a scaling function \(\beta(g)\) for various dimensionless, local conductances \(g\). If this scaling function is positive, then the conductance of the system increases with \(L\) (the system size), i.e. the system is not localised. Alternatively if the scaling function is negative then the conductance of the system decreases with \(L\). A sketch of the scaling function is plotted in Fig. 2.4 for various dimensionalities.

![Figure 2.4: Plot of \(\beta(g)\) vs \(\ln g\) for dimensionality \(d > 2\), \(d = 2\), and \(d < 2\). \(g(L)\) is the normalised “local conductance”. For \(d > 2\), the point \(g = g_c\) where \(\beta = 0\) indicates a transition from localised to extended states. For \(d \leq 2\), this point does not exist, hence, all states are always localised. Figure credit to [13].](\)

In a \(d > 2\) system, there exists a critical local conductance, \(g_c\), at which the scaling function crosses from negative to positive. This indicates a transition from localised states to extended states, i.e. a mobility edge [14, 15].

For systems with \(d \leq 2\), the cross-over does not exist, and hence, no mobility edge is present. These systems are always localised for any finite disorder.
2.6 Experimental Realisations of Anderson Localisation

While Anderson’s original model was for free electrons in a crystalline lattice, Anderson localisation is not restricted to quantum particles. It is a wave effect, and so it can also be observed with light waves or any medium governed by a wave equation with an appropriate disorder potential. However, it is not so easy to find an optical material with a sufficiently small mean-free path that Anderson localisation can be observed in light waves, especially while competing with optical absorption in the disordered medium. Wiersma et al. [16] reported the experimental observation of the Anderson localisation of light waves in a powder of GaAs semiconductor. The near infra-red light lies in a low absorption band-gap of the semiconductor and the extremely small mean-free path provided by the many scattering surfaces of the powdered solid provides ideal conditions for the observation. There are further experimental reports of Anderson localisation of light waves [17–20].

Anderson localisation has also been experimentally observed in microwaves [21, 22] and sound waves [23, 24].

It wasn’t until the late 2000s that Anderson localisation was directly observed for matter waves. The small scale and large inter-particle interactions made such an observation impossible in a solid-state system. However, with the attainment of the first BEC, experimentalists finally had the tools to explore a whole range of systems that were previously only theoretical. Inter-particle interactions can be made negligible in a BEC or ultra-cold system by using a sufficiently diffuse gas or via an external magnetic field near a Feshbach resonance. The dipolar potential provided by a laser-light field can then be used to produce a multitude of different Hamiltonians. In particular, such a laser could be passed through a diffuser plate to produce a speckle potential [25, 26], a random set of intensity peaks. Billy et al. [27] experimentally observed Anderson localisation in a 1D speckle potential in 2006. Their set-up is detailed in Fig. 2.5, a laser dipole potential provides strong confinement in the transverse directions of the 3D Bose gas, decoupling the transverse degrees-of-freedom and making the system pseudo-1D. A magneto-optical trap (MOT) weakly confines the gas in the longitudinal direction. The ultra-cold Bose gas is then free to expand (or not) in the hybrid potential. Anderson localisation has since been observed for a 3D speckle potential [28, 29].

This thesis explores the effect of bichromatic disorder on a Bose gas. This system was experimentally investigated by Roati et al. [30] in the same year. We will compare
Figure 2.5: a) A small BEC \((1.7 \times 10^4\) atoms\) is formed in a hybrid trap that is the combination of a horizontal optical waveguide, ensuring a strong transverse confinement, and a loose magnetic longitudinal trap. A weak disordered optical potential, transversely invariant over the atomic cloud, is superimposed (disorder amplitude \(V_R\) low in comparison with the chemical potential \(\mu_{in}\) of the initial BEC). b) When the longitudinal trap is switched off, the BEC starts expanding and then localises, as observed by direct imaging of the fluorescence of the atoms irradiated by a resonant probe. In a and b, false-colour images and sketched profiles are for illustration purposes; they are not exactly to scale. **Figure credit to [27].**

our numerical results to this experiment.
In this chapter we explore the effects of disorder in a 1D lattice. We choose to introduce the disorder using interference with a second lattice of a different wavelength. This is termed “bichromatic” disorder, or “pseudo-disorder”. There has been much debate and discussion as to whether the localisation caused by this type of disorder can truly be called “Anderson” localisation. We will return to the topic later, however, in the mean-time we will refrain from using the word “Anderson” in the context of bichromatic disorder.

We explore the effects of weak inter-particle interactions on the dynamics of the system and also the incarnation of Bloch oscillations in the bichromatic potential.

3.1 The model

3.1.1 Dipolar Laser Potential and the Optical Lattice

The electrons and protons of a neutral atom in the beam of an off-resonant laser will experience the Coulomb force due to the electric field of the laser-light in opposite directions. This induces a temporary separation of the charges and an overall electric dipole, thus shifting the atom’s energy levels. The effect of light with an angular frequency $\omega$ on an atomic energy level with resonance frequency $\omega_{\text{res}}$ is to induce the AC Stark shift:

$$\Delta \epsilon = \alpha(\omega)|\langle E(r, t) \rangle^2|,$$  \hspace{1cm} (3.1)
where $\alpha(\omega_{\text{res}} + \Delta)$ is the dynamic polarisability of the atomic level and $\Delta$ is the detuning from the resonance. If $\Delta < 0$ then the field is red-detuned and the atom will experience a time averaged force in the direction of increasing light intensity. If $\Delta > 0$ then it is blue-detuned and the force will be in the direction of decreasing intensity. This provides an effective and convenient method of manipulating cold gasses of atoms. It has wide application in the field of cold-atom physics and was instrumental in the achievement of the long-sought BEC.

In our application, a gas of ultra-cold bosons placed in the red-detuned light field of a pair of counter-propagating lasers. The bosons experience a force towards the anti-nodes of the resulting laser standing wave. If the laser is strong enough and the bosons cold enough, the bosons will be confined to the ground state of the wells centred at each anti-node. The bosons may tunnel between adjacent wells and interact with other bosons within the same well.

In the transverse directions, the bosons are confined by the width of the laser standing wave. The cloud is optimally positioned at the waist or narrowest point of the transverse laser profile. If the waist is sufficiently narrow and the thermal energy of the cloud sufficiently small, then excitation of the transverse oscillator modes will be effectively “frozen” out and the system will be pseudo-1D. It is important to note that the mean scattering length of the atoms is still much smaller than the transverse oscillator length, and so the inter-particle interactions remain 3D. This proves useful in manipulating the interaction properties.

If a stronger transverse trapping is desired, an alternative method is to take a fully 3D optical lattice formed using 3 pairs of counter-propagating lasers. Two of the pairs are set to a much stronger intensity such that tunnelling between the sites in the transverse directions is negligible. The result is a set of pseudo-1D optical lattices.

### 3.1.2 The Many-Body Hamiltonian

In an ultra-cold system, and in particular the idealised case of zero temperature, the energy of the inter-particle collisions is low enough that only s-wave scattering need be included. The system is then well described by the many-body Hamiltonian:

$$\hat{H} = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{U_0}{2} \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}),$$

(3.2)

where $U_0 = 4\pi a_s \hbar^2 / m$, $a_s$ is the s-wave scattering length, and $\hat{\psi}(\mathbf{r})$ is the field annihilation operator defined by the operation $\hat{\psi}(\mathbf{r}) |\psi(\mathbf{r})\rangle = |0\rangle$ and its adjoint, the field
creation operator, \( \hat{\psi}(r)|0\rangle = |\psi(r)\rangle \). These operators obey the Boson commutation relations

\[
[\hat{\psi}(r), \hat{\psi}(r')] = 0, \quad (3.3)
\]
\[
[\hat{\psi}^\dagger(r), \hat{\psi}^\dagger(r')] = 0, \quad (3.4)
\]
\[
[\hat{\psi}(r), \hat{\psi}^\dagger(r')] = \delta(r - r'). \quad (3.5)
\]

### 3.1.3 The Wannier States

The external potential for a 1D optical lattice with wavelength \( \lambda_1 = 2\pi/k_1 \) is

\[
V_{\text{ext}}(x) = s_1 E_R \sin^2(k_1 x), \quad (3.6)
\]

where \( E_R = \frac{\hbar^2 k_1^2}{2m} \) is the recoil energy, the natural energy scale of the Schrödinger equation. The eigen-states of the resulting single-particle Hamiltonian are the Bloch states that have the form

\[
\phi_{n,q}(x) = e^{iqx} u_{n,q}(x), \quad (3.7)
\]

where \( n \) is the band index, \( q \) is the quasi-momentum, and the function \( u_{n,q}(x) \) has the same periodicity as the optical lattice. Inserting this into the Schrödinger equation and solving for energy results in the band structure shown in Fig. 3.1.

![Figure 3.1](image.png)

Figure 3.1: The lowest energy bands w.r.t. pseudo-momentum of a (a) weak and (b) strong optical lattice.

In the tight-binding limit [31], \( s_1 \gg 1 \), the energy gap between the lowest band and the first excited band is large and if the system is cold enough, then only the lowest band need be considered. It is then more convenient to describe the system using
the localised Wannier functions [32], which are given as superpositions of the Bloch
functions by

\[ W(R_j, x) = \frac{2}{\lambda_1} \int dq e^{iR_j \cdot q} \phi_{n,q}(x). \]  

(3.8)

These are a set of localised basis states, centred at each lattice well (site). Each Wannier
function has a gaussian-like profile close to the centre, but decays slower in the tails.

![Figure 3.2: The Wannier function centred at \( x = 0 \) in a strong optical lattice where \( a_1 = \lambda_1 / 2 \) is the site separation length and \( \lambda_1 \) is the lattice wavelength.](image)

3.1.4 The Bose-Hubbard Hamiltonian

The system is tightly confined in the transverse directions, either by a harmonic po-
tential or a set of much stronger optical lattices. We therefore write the field operator as

\[ \hat{\psi}(\mathbf{r}, t) = \sum_j \hat{a}_j(t) \psi_j(\mathbf{r}), \]  

(3.9)

where \( \psi_j(\mathbf{r}) \) is the product of the Wannier state centred at site \( j \) and the lowest
eigen-state of the transverse directions. \( \hat{a}_j(t) \) is the time-dependent Bose annihilation
operator that removes a particle in the \( j^{th} \) well at time \( t \). The Hermitian conjugate
to this is \( a_j^\dagger \), the Bose creation operator that creates a particle in the \( j^{th} \) well. The
annihilation/creation operators have the commutation relations

\[ [\hat{a}_j, \hat{a}_k] = 0, \quad (3.10) \]
\[ [\hat{a}_j^\dagger, \hat{a}_k^\dagger] = 0, \quad (3.11) \]
\[ [\hat{a}_j, \hat{a}_k^\dagger] = \delta_{j,k}. \quad (3.12) \]

Inserting the ansatz (3.9) into the many-body Hamiltonian (3.2), and applying a few assumptions (see below), we may simplify it into the Bose-Hubbard Hamiltonian defined as

\[ \hat{H} = -\sum_{j\neq k} J_{j,k} \hat{a}_j^\dagger \hat{a}_k + \sum_j \epsilon_j \hat{n}_j + \frac{U}{2} \sum_j \hat{n}_j(\hat{n}_j - 1), \quad (3.13) \]

where \( \hat{n}_j = \hat{a}_j^\dagger \hat{a}_j \) is the particle number operator for the \( j \)th site, \( J_{j,k} \) is the energy associated with tunnelling from \( j \) to \( k \), \( \epsilon_j \) is the on-site energy and \( U \) is the energy associated with s-wave particle-particle interactions.

These parameters can be calculated from physical parameters via [33]

\[ J_{j,k} = -\int dr \psi_j^*(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) \right] \psi_k(r), \quad (3.14) \]
\[ \epsilon_j = -J_{j,j}, \quad (3.15) \]
\[ U = U_0 \int dr |\psi_j(r)|^4. \quad (3.16) \]

In getting to the Bose-Hubbard Hamiltonian we have assumed that only the lowest Bloch band is able to be occupied. This assumption is justified if the interactions are kept small enough that there is virtually no possibility of exciting a particle up to the next band. In the deep well limit, \( s_1 \gg 1 \), the main lattice potential is approximately harmonic

\[ V_{\text{ext}}(x) \approx s_1 E_{R_1} k^2 x^2 = \frac{1}{2} m \omega^2 \parallel x^2, \quad (3.17) \]

and so the energy gap between the lowest and first excited bands is approximately [34]

\[ \Delta E \approx \hbar \omega \parallel = 2 s_1 E_{R_1}, \quad (3.18) \]

so the condition for the single-band approximation is

\[ U \langle \hat{n}_j \rangle \ll 2 s_1 E_{R_1}, \quad (3.19) \]

for the most populated site.

We have also required that only the lowest eigen-state of the transverse trapping potential is occupied. The condition for avoiding transverse mode excitations is

\[ U \langle \hat{n}_j \rangle \ll \hbar \omega \perp, \quad (3.20) \]
where $\omega_{\perp}$ is the characteristic harmonic oscillator frequency of the transverse trap.

The terms for interactions between particles in different sites was discarded in the Bose-Hubbard Hamiltonian. These terms are much smaller than the onsite particle interaction terms, and so if the onsite interaction terms are small or comparable to the onsite potential energy and hopping terms, then they may be safely discarded.

$J_{j,k}$ decays exponentially with $|j - k|$ so we neglect tunnelling beyond the nearest neighbours [35–38].

The interaction parameter $U$ inherits proportionality with the atomic scattering length ($a_s$) from its ancestor in the many-body Hamiltonian. Therefore the interaction parameter is tunable, in experiment, independent of the tunnelling and on-site parameters, via an external magnetic field near one of the atoms Feshbach resonances. With care, the interaction parameter may even be tuned to zero so that we have a non-interacting system with a single-particle Hamiltonian.

We proceed by inserting (3.13) into the Heisenberg equation-of-motion

\[ i\hbar \frac{d\hat{a}_j(t)}{dt} = [\hat{a}_j(t), \hat{H}] \tag{3.21} \]

The annihilation operators may be expanded in the Bogoliubov treatment [39] into a complex scalar part, equal to its mean or expectation value, and a fluctuating part, i.e.

\[ \hat{a}_j = \sqrt{N}z_j(t) + \delta \hat{a}_j(t), \tag{3.22} \]

where $z_j = \langle \hat{a}_j \rangle / N$ and $N$ is the total number of particles in the system. The modulus squared of the expectation value, $n_{c,j} = N|z_j|^2$, is termed the condensate density. We will assume that the number of particles in the system is large, on the order of $10^5$ to $10^6$, so that the fluctuating term is negligible in comparison, and so we employ the mean-field approximation, i.e. $\hat{a}_j \approx \sqrt{N}z_j$.

The equations of motion (EOM) of the system take the form of a discrete Gross-Pitaevskii (GP) system of equations given as

\[ i\dot{z}_j = -\sum_{(j,k)} \tilde{J}_{j,k} z_k + \bar{\epsilon}_j z_j + \bar{U}|z_j|^2 z_j \tag{3.23} \]

where the derivative is taken with respect to scaled time $\tilde{t} = Jt/\hbar$. $(j,k)$ indicates the nearest neighbours of site $j$ and we have defined $\tilde{J}_{j,k} = J_{j,k}/J$, $\bar{\epsilon}_j = \epsilon_j/J$ and $\bar{U} = UN/J$, where $J$ is the mean value of the site-to-site tunnelling energies $J_{j,k}$.

The tunnelling energy for the homogeneous lattice in the deep-well limit is given analytically by [40]

\[ J = \frac{4}{\sqrt{\pi}} s_1^{3/4} \exp(-2\sqrt{s_1}) E_{R_1} \]. \tag{3.24}
Combining this with (3.19), the limit on \( \bar{U} \) imposed by the single-band model is

\[
\bar{U} \bar{n}_j \ll \frac{8}{\sqrt{\pi}} s_1^{1/4} \exp(2\sqrt{s_1}),
\]

(3.25)

where \( \bar{n}_j = n_j/N \) is the fraction of particles in site \( j \). For a lattice with depth \( s_1 = 10 \), this gives \( \bar{U} \bar{n}_j \ll 278.14 \).

From here on we will drop the bars and, unless otherwise stated, use \( a_1 = \lambda_1/2 \) for spatial units, \( \hbar/J \) for time units and \( J \) for energy units.

In most of our simulations we examine the size of a wave-packet of bosons. As a measure of the size of a bunched wave-packet, we define the rms. half-width, given by

\[
w = \sqrt{\sum_j |z_j|^2 x_j^2 - \left( \sum_j |z_j|^2 x_j \right)^2}
\]

(3.26)

in our adopted dimension-less units, which is the standard deviation of position and equals the 1/e-half-width of the best-fit Gaussian curve.

### 3.1.5 Two Colour Lattice

A bichromatic lattice is created by superimposing a much weaker lattice with a different lattice wavenumber, \( k_2 = 2\pi/\lambda_2 \), onto the primary lattice. The external potential is then given by

\[
V_{\text{ext}}(x) = s_1 E_{R_1} \sin^2(k_1 x) + s_2 E_{R_2} \sin^2(k_2 x),
\]

(3.27)

where \( E_{R_2} = \hbar^2 k_2^2 / 2m \) is the secondary lattice’s recoil energy.

The effect of the second lattice is weak enough that the Wannier states remain unchanged, but the depth of each potential well is shifted by a small pseudo-random amount. The external potential is accounted for in the Bose-Hubbard Hamiltonian through the on-site energy

\[
\epsilon_j = \Delta \cos(2\pi \alpha j + \phi),
\]

(3.28)

where \( \alpha = \lambda_1/\lambda_2 \) is the ratio of the wavelengths of the lattices and \( \phi \) displaces the secondary lattice relative to the primary in order to break the associated spatial symmetry. The external potential also imparts a cosine variation in the site-to-site tunnelling energies \( J_{j,k} \), however, the variation is orders of magnitude smaller than the onsite energy variations due to the exponential decay of the site-to-site tunnelling, hence, the variations are discarded and it is assumed that \( J_{j,k} = J \).
The set of on-site energies produced by the secondary lattice has a pseudo-period ($\lambda_b$) produced by the beating between the two lattice frequencies defined as:

$$\lambda_b = \frac{1}{|\alpha - 1|},$$

(3.29)

that is $\sim 5$ lattice sites for the typical wavelengths we employ. However, the pattern only exactly repeats every $m$ sites, where $m$ is the denominator of the reduced fraction $\alpha = \frac{n}{m}$, and does not ever repeat when $\alpha$ is irrational.

### 3.1.6 The Aubry-André Model

The model of a single particle in a bichromatic lattice was presented by S. Aubry and S. André in their 1980 paper[41]. They analytically show that for irrational $\alpha$, the system will have localised eigenstates for $\Delta > 2$; extended states for $\Delta < 2$ and $\Delta = 2$ is the marginal case.

The time-independent discrete Shrödinger equation for the Aubry-André (AA) model is

$$-z_{j-1} - z_{j+1} + \Delta \cos(2\pi \alpha j + \phi)z_j = Ez_j.$$  

(3.30)

The periodic nature of the potential suggests that we search for solutions of the form

$$z_j = e^{-ikj} \sum_m f_m e^{-im(2\pi \alpha j + \phi)}.$$  

(3.31)
This gives us the dual equation

\[-f_{m-1} - f_{m+1} + \frac{4}{\Delta} \cos(2\pi \alpha m + k) f_m = -\frac{2E}{\Delta} f_m, \quad (3.32)\]

which has the same form as the GP equation (3.30). This implies that the number of states with energy less than \(-\frac{2E}{\Delta}\) for the dual model, is the same as the number of states with energy less than \(E\) for the GP model, i.e.

\[N_{\frac{1}{2}} \left( -\frac{2E}{\Delta} \right) = N_\Delta(E). \quad (3.33)\]

Thouless, in his 1972 paper[42], presents an argument that for an equation of the form (3.30), the characteristic exponent, \(\lambda_\beta\), which has the definition

\[\lambda_\beta = \lim_{N \to \infty} \left\{ (N - 1)^{-1} \sum_{\alpha \neq \beta} \ln |E_\beta - E_\alpha| \right\}, \quad (3.34)\]

will tend to zero for non-localised states, and have a finite positive value for localised states, that is equal to the fall-off distance of the eigen-state, i.e. the localisation length.

For a long and statistically homogeneous chain of sites, the sum can be replaced by an integral so that

\[\lambda(E) = \int dx \rho(x) \ln |E - x|, \quad (3.35)\]

where \(\rho(x)\) is the density-of-states.

The density-of-states is defined such that

\[N(E) = \int_{-\infty}^{E} \rho(x) dx, \quad (3.36)\]

so the density-of-states of the two models are related by

\[\rho_\Delta(E) = -\frac{2}{\Delta} \rho_{\frac{1}{2}} \left( -\frac{2E}{\Delta} \right). \quad (3.37)\]

Therefore, the characteristic exponents of the two models are related by

\[\lambda_\Delta(E) = \lambda_{\frac{1}{2}} \left( -\frac{2E}{\Delta} \right) + \ln \frac{\Delta}{2}. \quad (3.38)\]

By definition, the characteristic exponents are positive. Therefore, when \(\Delta > 2\),

\[\lambda_\Delta(E) \geq \ln \frac{\Delta}{2} > 0, \quad (3.39)\]

and hence, the eigen-states of (3.30) are all localised.
In the case where $\Delta < 2$, Eq. 3.38 gives us that
\[ \lambda_\pm \left( -\frac{2E}{\Delta} \right) > 0, \tag{3.40} \]
i.e. the eigen-states of the dual model, (3.32), are localised. From the dual transform, (3.31), it is obvious that if the dual model eigen-states are localised then the AA model’s eigen-states must be extended.

The characteristic equation relation (3.38) gives us no indication of the behaviour at $\Delta = 2$.

### 3.1.7 Bichromatic Disorder: Anderson Localisation or Not?

It has long been known that bichromatic disorder did not fit with the other types of disorder that lead to Anderson localisation. The existence of the localisation transition clearly violates the scaling theory of Abrahams et al. For a 1D disordered potential, all eigen-states should be localised for any disorder strength.

In 2010, Albert and Leboeuf [43] argued that the localisation exhibited in the AA model arises from purely classical trapping in the potential barriers and not due to destructive interference processes.

Albert and Leboeuf show that a simple transformation of the Hamiltonian allows one to calculate and display the phase-space trajectories of the associated pseudo-particles. These trajectories are localised in the pseudo-momentum direction for $\Delta < 2$ and localised in the position direction for $\Delta > 2$, leading to the same observations as the AA analysis.

Albert and Leboeuf conclude that the existence of these trajectories proves that the confinement is due to the classical trapping. However, the AA equation is a wave equation and the potential at the edge of the system is not infinite, or even very much larger than at the centre, so we would expect that without the interference processes, the particles would eventually escape by tunnelling through any finite barriers.

Moratti and Modugno discuss the necessity of the interference processes in the quasi-periodic model in their 2012 paper [44].

### 3.2 Numerical Integration Methods

The equations of motion are evolved in time via the 4th order Runge-Kutta method (RK4) combined with double step error checking. This method is particularly useful
when a portion of the EOM is able to be factorised and treated exactly as all samples of the gradient are taken at regular time intervals.

3.2.1 Runge-Kutta Methods

The simplest explicit method for numerically solving an ordinary differential equation (ODE) is known as Euler’s method. The method evaluates the derivative of the system at a point and then treats that derivative as constant to extrapolate to the next point. i.e. Given the ODE

$$\frac{dx}{dt} = f[t, x(t)],$$  \hspace{1cm} (3.41)

and the point \( x_n \) at \( t = t_n \), then next point is found from

$$x_{n+1} = x_n + hf[t_n, x_n],$$  \hspace{1cm} (3.42)

at \( t_{n+1} = t_n + h \).

The Euler method may be improved upon by recognising that the slope is only sampled at the beginning of the interval. A more balanced approach is to also sample it at the end and then average the two. This method is known as the midpoint method.

The Euler method and the Midpoint method described above are one and two step examples of a more general class of numerical integration methods known as Runge-Kutta methods. Named after the work of C. Runge and M. W. Kutta around 1900. The explicit q-step Runge-Kutta integration method to solve (3.41) is found using

$$x_{n+1} = x_n + h \sum_{i=1}^{q} \omega_i k_i,$$  \hspace{1cm} (3.43)

and

$$k_i = f \left[ t + h\alpha_i, x_n + h \sum_{j=1}^{i-1} \beta_{ij} k_j \right],$$  \hspace{1cm} (3.44)

with \( \alpha_1 = 0 \). The coefficients \( \alpha_i, \omega_i \) and \( \beta_{ij} \) are computed by matching the terms of (3.43) to the truncated Taylor expansion of (3.41), and solving the resulting system of equations. The order of the method is the greatest power of \( h \) before truncation, hence the Euler method is 1\(^{st}\) order and the Midpoint method is 2\(^{nd}\) order. The order determines the local truncation error, or step error, which extrapolates to the global error, or accumulated error after many steps.

For a given number of steps, the above equations admit a variety of methods of different orders, however, it is the unproven rule that the minimum number of steps to get a \( p \)^{th} order truncation is at least \( p \). For \( p \leq 4 \) it has been proven that \( q_{\text{min}} = p \).
but for \( p > 4 \) the few solutions found require greater than \( p \) steps. Of course the more steps required, the more computer time required, however, a lower truncation order will require smaller integration steps in order to maintain accuracy, and hence, a larger global computer time.

The optimum is generally held to be the 4th order methods with 4 steps. One such method which is known as the 4th order Runge-Kutta (RK4) method proceeds as follows:

Given the ODE, \( \frac{dx}{dt} = f(t, x(t)) \),

\[
\begin{align*}
    k_1 &= f(t, x(t))h \\
    k_2 &= f\left(t + \frac{1}{2}h, x(t) + \frac{1}{2}k_1\right)h \\
    k_3 &= f\left(t + \frac{1}{2}h, x(t) + \frac{1}{2}k_2\right)h \\
    k_4 &= f\left(t + h, x(t) + k_3\right)h \\
    x(t+h) &= x(t) + \frac{1}{6}(k_1 + 2(k_2 + k_3) + k_4).
\end{align*}
\]

In general, the global error cannot be known unless an exact calculation is performed. This is possible in limited cases, but if it was easy, there would be no point to the approximate methods. Instead we can form estimates of the step error and extrapolate to the global error, assuming that nothing drastic is occurring.

The common approach to estimate the step error in the RK4 method is to also use the standard RK5 method. The difference in the two methods is then proportional to \( h^5 \). The combined method is known as RK45, it has the advantage that some of the derivative evaluations for the two branches are the same and hence it only requires 11 steps total.

In contrast, we prefer a double step method. In this version the RK4 step is performed in one full step \( (h) \), and concurrently in two half steps \( (h/2) \). The difference is also 5th order, but it requires 12 steps. The advantage comes from the even spacing of the steps which allows the partial factorisation of the derivative as described in the next section.

### 3.2.2 RK4DS

The EOM have the form \( \dot{z} = -i\hat{a}z - i\hat{b}z - i\hat{G}z \). An improvement on the basic RK4 algorithm is to factorize by the exponentials of \( \hat{a} \) and \( \hat{b} \) via the transformation

\[
y = e^{i\hat{a}(\tau - \tau_0)}e^{i\hat{b}(\tau - \tau_0)}z. \tag{3.45}
\]
The algorithm proceeds as follows:

At \( \tau = \tau_n \) choose \( \tau_0 = \tau_n - h/2 \) and define \( \hat{A} = e^{-i\hat{a}h/2} \) and \( \hat{B} = e^{-i\hat{b}h/2} \).

\[
y \leftarrow \hat{A} \hat{B} z_n
\]

\[
k_1 \leftarrow -ih\hat{A}(\hat{a}, \hat{B}) \hat{B} z_n
\]

\[
k_2 \leftarrow -ih\hat{G}(y + \frac{1}{2}k_1)
\]

\[
k_3 \leftarrow -ih\hat{G}(y + \frac{1}{2}k_2)
\]

\[
k_4 \leftarrow ih(\hat{a}, \hat{B}) + \hat{G} \hat{B}) \hat{A}(y + k_3)
\]

\[
z_{n+1} \leftarrow \hat{A} \left( y + \frac{1}{6}(k_1 + 2(k_2 + k_3)) \right) - \frac{1}{6}k_4.
\]

\( k_4 \) has been altered from the basic RK4 to save two extra operations and the operators \( \hat{A} \) and \( \hat{B} \) can be precomputed for a given step size.

The accuracy of each step is measured by evolving the system one full step, \( h \), and concurrently via two half steps. If the maximum difference of any element via the two paths exceeds a fixed target \( (10^{-10}) \) then the step size is reduced. The difference of the two methods is accurate to 5th order in \( h \) so if a step of size \( h_1 \) measures \( \Delta_1 \) then the target error \( \Delta_0 \) can be achieved by redoing the step with size \( h_0 = h_1(\Delta_0/\Delta_1)^{1/5} \).

Changes in the step size are relatively expensive so the step size is only readjusted if the error exceeds 1.7 of the target. In order to optimise the simulation time, the step size is increased if the error drops below 0.5 of the target.

In addition, the particle number is monitored and if it drifts by more than 1 part in \( 10^6 \) over the duration of the simulation then the simulation is restarted with a smaller target step accuracy.

The elements of the Hamiltonian can be put into the operators \( \hat{a}, \hat{b} \) and \( \hat{G} \) in different combinations which will affect the efficiency and memory requirements of the algorithm, but collectively we will call this method "4th order Runge-Kutta with Double Step error correction" (RK4DS). The particular variants are:

**Method 1** - The fastest and most accurate algorithm is achieved by putting the local elements into \( \hat{a} \) and the non-local elements into \( \hat{G} \) leaving \( \hat{b} = 0 \). This method is exact (aside from rounding errors) in a purely linear system, however, it requires the evaluation of a matrix exponential which quickly becomes memory limited.

**Method 2** - The second option is to put the local, linear elements into \( \hat{G} \). We can
then take advantage of the fact that
\[
-z_{j-1} - z_{j+1} = -\frac{2}{M} \sum_{p=0}^{M-1} \tilde{z}_p \cos \left( \frac{2\pi p}{M} \right) e^{\frac{2\pi i}{M}j} = \tilde{F}^{-1} \hat{\omega} \hat{F} \tilde{z}_j.
\] (3.46)

Then
\[
\hat{A} = e^{-i\hat{a} \frac{\hat{h}}{2}} = e^{-i\hat{F}^{-1} \hat{\omega} \frac{\hat{h}}{2}} = \hat{F}^{-1} e^{-i\hat{\omega} \frac{\hat{h}}{2}} \hat{F} = \hat{F}^{-1} \hat{\Omega} \hat{F},
\] (3.47)

where
\[
[\hat{\Omega} \tilde{z}]_p = e^{i h \cos \left( \frac{2\pi p}{M} \right)} \tilde{z}_p.
\] (3.48)

is a diagonal matrix and the Fourier transforms are evaluated using the Fast Fourier Transform (FFT) algorithms in the fftw library.

**Method 3** - When the local, linear elements become large, the algorithm can be further improved by inserting these elements into \( \hat{b} \), the accuracy then depends on the convolution between the local and non-local, linear elements.

### 3.2.3 Efficiency Analysis

The computer time required to complete a simulation depends on the desired accuracy of the result. We expect to have simulations of a few million steps so we set the target accuracy at \(10^{-10}\) for each step.

As expected, the error of both of the approximate methods is clearly 5th order in \( h \), as seen in Fig. 3.4. This trend is very convenient as doubling the number of steps will increase the accuracy by 32 times.

As can be observed in Fig. 3.5, factorising the local and non-local linear elements separately (method 3) is less accurate when \( \Delta < 1 \), but quickly becomes more accurate when \( \Delta > 1 \). This reflects the fact that evolving the larger energy term exactly, where possible, will bring greater accuracy to the algorithm.

Neither method proves better than the other when the interaction term is finite. For low interaction strength, Fig. 3.6 shows that the efficiency is determined by the disorder term. As the interaction term is increased, smaller step-size is required until the accuracy required by the disorder term is automatically satisfied by the higher level required by the interaction term. At this point both method 2 and 3 give the same accuracy. Therefore, the method should be chosen to best suit the secondary lattice parameter.

Multi-threading may be employed to significantly speed up the algorithm, however, it is not as simple as tasking more and more CPUs. Most of the algorithm is serial
Figure 3.4: Double step accuracy $\max[\Delta z]$ vs. step size ($h$), with fits, for secondary lattice strength $\Delta = 3$. $M = 256$.

Figure 3.5: Step size ($h$) required to achieve double step accuracy $\max[\Delta z] \leq 10^{-10}$ vs. secondary lattice strength ($\Delta$). $M = 256$. 
Figure 3.6: Step size ($h$) required to achieve double step accuracy $\max[\Delta z] \leq 10^{-10}$ vs. particle interaction strength ($U$) at secondary lattice strength $\Delta = 10^{-2}$. $M = 256$.

in nature so that each step must be performed in its place, and even the parts that branch, and so may run in parallel, join up again before the next step, thus requiring synchronisation of the threads. This always creates delays as one thread pauses to wait on another to finish and then is restarted, and if one is not careful these delays may be longer than the benefit of the parallelisation.

We employ parallelisation along two natural lines in the algorithm. The first is to calculate the full and half step branches on separate threads. In practice, this split into two threads reduces the computer time to $\sim 60\%$ of the original. Additionally, in the non-interacting system, $k_2$ and $k_3$ are zero and $k_1$ and $k_4$ may be calculated on separate threads. Employing this, in addition to the previous split, uses four threads and reduces the computer time to $\sim 40\%$ of the original. In the 1D simulations, where the computer time is on the order of minutes to an hour, these gains are irrelevant, however, later in this thesis we explore a 2D model where the typical simulation time is 24-300 hours. Thus the gains become significant. It is obvious that further parallelisation will provide diminishing returns as the overhead becomes larger than the gain, it is far more efficient to use the spare cpus to run other simulations in the parameter space of interest.
3.3 Results

At $t = 0$, a cloud of ultra-cold bosons is prepared in the ground state of a tight harmonic trap and the primary lattice. i.e. the ground state is found for a system with the external potential

$$
\epsilon_j = v_t j^2, \quad (3.49)
$$

where $v_t$, the trap strength, is set to $10^{-2}$. The trap is then instantaneously turned off and the secondary lattice is simultaneously turned on.

For the homogeneous system ($\Delta = 0$), the cloud expands ballistically, analogous with a gas in free space with an increased effective mass. This occurs because the initial wave-packet mainly occupies the bottom of the cosine dispersion relation which is approximately quadratic as in free space, albeit with an increased second derivative (effective mass) [45]. This is clearly seen in Fig. 3.7 where the initial, tight Gaussian ($w(t = 0) = 2.22$), wave-packet expands at a constant rate, maintaining its Gaussian profile.

3.3.1 Commensurate Lattice

The behaviour in a weak, commensurate secondary lattice ($\Delta = 1$ and $\alpha = 6/5$ in Fig. 3.8 and Fig. 3.10) appears as a two component gas, one component with an increased group velocity and the larger component with a reduced group velocity. The faster component is due to the momentum “kick” imparted when the secondary lattice is switched on.

In a strong, commensurate lattice ($\Delta = 3$ in Fig. 3.9), the faster component has
disappeared, returning the gas to a single component, ballistically expanding with an increased effective mass inversely dependent on the strength of the secondary lattice. The pseudo-period, which in the commensurate case is the true period, of the external potential is readily apparent as every $\sim 5^{th}$ site is heavily populated and the betwixt sites are sparsely populated. The density appears to tunnel between the pseudo period wells as it expands.

Figure 3.8: Spatial density (logarithmic) for a weak, commensurate secondary lattice ($\Delta = 1$, $\alpha = 6/5$). Initial trap $v_t = 10^{-2}$.

Figure 3.9: Spatial density (logarithmic) for a strong, commensurate secondary lattice ($\Delta = 3$, $\alpha = 6/5$). Initial trap $v_t = 10^{-2}$.

### 3.3.2 Incommensurate Lattice

The weak, incommensurate system ($\Delta = 1$ and $\alpha = 1025/863$ in Fig. 3.11) is qualitatively identical to the commensurate lattice. However, in the strong, incommensurate
lattice ($\Delta = 3$ in Fig. 3.12) we observe a completely different behaviour, the wave-packet has expanded slightly and relaxed into the pseudo-lattice but compared to the commensurate case it is clear that the wave-packet is strongly localised. The spatial density plot in Fig. 3.12 clearly shows that this localisation is persistent and shows no sign of dissipating over the duration of our simulation.

3.3.3 What is Commensurability?

Aubry and André show that if $\alpha$ is irrational and $\Delta > 2$, then all eigenstates will be of the form $z_{i,j} \sim e^{-\lambda_i |c_i - j|}$ as $|c_i - j| \to \infty$ where $c_i$ is the centre of the $i^{th}$ eigenstate which is exponentially localised with fall-off distance $\lambda_i^{-1}$. Although the condition that $\alpha$ is
Figure 3.12: Spatial density (logarithmic) for a strong, incommensurate secondary lattice ($\Delta = 3, \alpha = 1025/863$). Initial trap $v_t = 10^{-2}$.

Figure 3.13: Size ($w$) vs. lattice ratio ($\alpha$) of a cloud of bosons $10^6 t_0$ after release from a trap ($v_t = 10^{-2}$) in a bichromatic optical lattice with secondary lattice strength $\Delta = 3$.

irrational is required for their proof, our numerical results show that it is not, in fact, required to have localisation; nor is the localisation length ($\lambda_{\text{loc}} = \max \{\lambda_i^{-1}\}$) related to the irrationality of $\alpha$. The localisation length tends to smoothly approach infinity at discrete values of $\alpha = n/m$ that are the ratio of small positive integers with unity greatest common divisor. As the denominator, $m$, exceeds $\sim 30$ the potential becomes indistinguishable from one with an infinite denominator (irrational $\alpha$) and we observe localisation for $\Delta > 2$. The smallest localisation lengths are then achieved with those $\alpha$, rational or irrational, furthest away from one of these commensurate values.

A common approach of groups in the literature is to approximate an irrational
value (usually the inverse golden mean) as one of the rational convergents from its
continued fraction representation. As better convergents are used, the $\alpha$ becomes more
irrational, however, if the target irrational value is near a commensurate ratio then the
localisation length of the system increases; this approach provides limited insight into
the transition from periodic lattices to pseudo-disorder.

3.3.4 Disorder Averaging

We are interested in those properties of the system that are independent of the initial state of the wave-packet and the particular realisation of the external potential, however, we explore these properties by measuring the width of the wave-packet after simulating time propagation, which most certainly does depend on this.

The common approach in a system with speckle disorder is to average over an independent set of randomly generated external potentials, all with the same disorder properties. An equivalent in the bichromatic system is to displace the secondary lattice from the primary by a random length and average over several such realisations. However, the pseudo-period is a strong feature in the on-site energies and this results in wildly differing initial momenta when the secondary lattice is switched on at $t = 0$.

Our approach is to select a set of lattice ratios $\{\alpha_k\}$ in the region of $\alpha = 6/5$ that are sufficiently far from a commensurate ratio and have a similar localisation length for a given secondary lattice strength. The width calculated from the simulations performed at each ratio is then averaged. Unless otherwise stated, the width shall be calculated in this manner from here on. The plot in Fig. 3.14 shows the set of lattice ratios that we selected as red vertical lines, superimposed on the previous $\alpha$ vs. $\Delta$ plot. The only criteria we have used to select this set is that they not be near any peaked feature on the plot, otherwise we have simply taken a uniform sample across the spectrum.

3.3.5 The Localisation Transition

If $\alpha$ is chosen as one of the many incommensurate values then for $\Delta > 2$, all eigenstates will be exponentially localised and bulk transport in the system will be forbidden. The wave-packet still exchanges density via virtual transport over an exponentially decreasing range with characteristic length $\lambda_{loc}$, the localisation length. Therefore, a wave-packet released from a tight harmonic trap will increase rapidly to the localisation length, but no further.

This can be observed in Fig. 3.16 where we have plotted the width of a wave-packet.
Figure 3.14: The set of lattice ratios (α) used for disorder averaging (red vertical lines), superimposed on the previously shown lattice ratio vs. disorder strength plot.

in time in an incommensurate lattice for a selection of disorder strengths. The traces for Δ < 2 expand ballistically after a short settling period, this is indicated by the gradient of the traces on the log-log plot which is approximately 1 for t > 100. The Δ > 2 traces expand a small amount in this settling period, but have a zero gradient afterward. In Fig. 3.15, the blue curve shows the width at t = 1000 in the disorder-averaged incommensurate system. There is a strong feature precisely at the predicted Δ = 2.

In contrast, the width of the commensurate system (green curve in Fig. 3.15) reduces gradually with increasing disorder strength as the collisions with the disorder potential increase, analogous with increasing resistance in a classical system. Transport is not completely forbidden as in the incommensurate case, however, even with strong disorder.

In Fig. 3.17 we present for comparison the experimental results published by Roati et al. [30] in 2008. Roati et al. claim to have eliminated the inter-particle interactions to a negligible degree and so have exactly the model presented above. However, when comparing the shape of the rms. half-width curve near the localisation transition, we can’t help but find more qualitative agreement with the commensurate curve (α = 6/5) than with the incommensurate one in Fig. 3.15. There is no clear transition to localisation, instead there is the gradual suppression of transport due to the squashing of the band’s width as the secondary lattice’s strength increases. This effect is almost
Figure 3.15: Width of the wave-packet vs. secondary lattice strength in: (solid circles) the disorder-averaged incommensurate lattice and (empty circles) a commensurate lattice ($\alpha = 6/5$), at $t = 1000$. $v_t = 10^{-2}$, $M = 8192$.

Figure 3.16: Disorder averaged rms. half-width of the particle cloud vs. time during evolution in an incommensurate lattice with strength: (circle) $\Delta = 0$, (triangle) $\Delta = 1$, (square) $\Delta = 1.8$, (cross) $\Delta = 2.2$, (diamond) $\Delta = 5$. $v_t = 10^{-2}$ and $M = 8192$. 

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Figure 3.17: a) *In situ* absorption images of the BEC diffusing along the quasi-periodic lattice for different values of $\Delta$ and $J/h = 153$ Hz (where $h$ denotes Planck’s constant). For $\Delta/J > 7$ the size of the condensate remains at its original value, reflecting the onset of localisation. b) rms. size of the condensate for three different values of $J$, at a fixed evolution time of 750 ms, versus the rescaled disorder strength $\Delta/J$. The dashed line indicates the initial size of the condensate. The onset of localisation appears in the same range of values of $\Delta/J$ in all three cases. Vertical error bars, 95% confidence level (±2 s.e.m.); horizontal error bars, 10% uncertainty due to the nonlinearity of the modulators’ response. *Excerpt from [30]. The $\Delta/J$ displayed here corresponds to $\Delta$ in this thesis and time is not scaled here.*
completely set-in at $\Delta = 7$, which is the value that Roati et al. empirically identify as the critical disorder. Further experiments are required to resolve the ambiguity.
3.3.6 Inter-particle Interactions

The dependency of the interaction term in (3.26) on the scattering length \( a_s \) of the atoms provides an excellent method, in experiment, of manipulating the inter-particle interactions, independent of the other parameters. Even so, these interactions must not exceed the excitation energy of the lattice wells as our model only takes into account the first Bloch band.

The dispersion relation of the homogeneous lattice is a cosine with the maximum energy at the edge of the first Brillouin zone. The maximum amount of energy that can be converted from interaction energy to kinetic energy is to take the lowest energy quasi-momentum state and promote it to the highest. If the initial interaction energy exceeds this limit then the excess cannot be dissipated and the wave-packet cannot spread to infinity. A portion of the wave-packet will hold onto the interaction energy in the form of a soliton or in the case of our initially trapped wave-packet, remain localised. This is referred to as "self-trapping" and is independent of disorder induced localisation and classical trapping.

The total saturation of the upper energy states only provides an extreme upper limit to the self-trapping regime. In practice the effect will kick-in a lot sooner when the interaction energy dissipated by the spread of the wave-packet exceeds the ability of the dispersion relation to contain it in its current configuration.

What results is a very dynamic form of trapping with some of the wave-packet escaping before the kinetic energy saturates, some escaping as solitons and the rest remaining localised. This remaining population attains a messy top-hat profile with the wave-packet trapped between two steep-sloped sides. This was observed in experiment and compared with theory by Oberthaler et al. [46]. We have included two figures from their paper (Fig. 3.18 and Fig. 3.19) that clearly show the top-hat signature and compares this effect to the self-trapping found in the well-known double-well system which itself maps onto a classical non-rigid pendulum [47].

In this section we only explore in detail interactions in the commensurate bichromatic lattice, however, Larcher et al. [48] explore the effect of interactions on the incommensurate system. They find that interactions break the localisation when the interaction strength is below the self-trapping limit. Albeit they must employ very large simulation time and lattice sizes to see it. They find that the size of the wave-packet has a \( t^{1/3} \) behaviour in the long-time limit, which is in accordance with the results from purely disordered systems.

Due to the dependence of the self-tapping on the initial interaction energy and
Figure 3.18: Excerpt from Oberthaler et al. [46]: Comparison between theory and experiment for $s = 10, 7.6(5)$ $\mu$m initial rms width and $5000 \pm 600$ atoms. The upper graphs show the measured density distribution for different propagation times. During the initial expansion in the self-trapping regime the wave packet develops steep edges which act as stationary boundaries for the subsequent internal dynamics. The results of the numerical integration (depicted in the lower graphs) are in very good agreement. For $t = 50$ ms a 1.5 mrad deviation of the waveguides horizontal orientation (consistent with the experimental uncertainty) is taken into account and reproduces the experimentally observed asymmetry (gray line).

hence the size of the initial wave-packet, we start from a Gaussian wave-packet of fixed width ($w_0 = 6$) for these simulations. This is equivalent to preparing the cloud in the ground-state of a fairly tight harmonic trap in the optical lattice, and then releasing the cloud into the disordered medium at $t = 0$ by simultaneously switching off the trapping potential and switching on the disorder potential.

In Fig. 3.20 we show the evolution of the wavepacket when the interactions are small in a bichromatic lattice with commensurate wavelengths, $\alpha = 6/5$ and strong secondary lattice $\Delta = 3$. If compared to Fig. 3.9, one can already see that the central peak is maintaining more of the population, however, given enough time this central peak will dissipate.

In Fig. 3.21 we show the evolution with a much stronger interaction ($U = 10$). Most of the cloud remains in the central peak, with only a very small fraction escaping. The central peak is stable and persistent and the fragments that escape tend to do so in clumps that hold together. These are solitons.

We next show the width of the cloud, $t = 1000$ after release, vs. interaction strength (see Fig. 3.22). The initial trend of increasing the interaction strength is to increase
Figure 3.19: Excerpt from Oberthaler et al.[46]: A numerical investigation of the site-to-site tunnelling dynamics. (a) The atomic distribution $N_j$ of the wave packet for $t = 0$ and 50 ms. (b) The relative population difference $\Delta N_j$ time averaged over the expansion time indicates two regions with different dynamics. (c) The dynamics of $\Delta N_j$ and the phase difference $\phi_j$ for the marked site oscillate around zero known as the zero-phase mode of the boson Josephson junction. (d) The dynamics in the edge region is characterised by long time periods where $|\Delta N_j|$ is close to 1 while at the same time $\Delta \phi_j$ winds up very quickly (phase is plotted modulo $\pi$) known as "running phase self-trapping mode" in boson Josephson junctions. Thus the expansion of the wave packet is stopped due to the inhibited site-to-site tunnelling at the edge of the wave packet.

The spread rate of the cloud as more energy is transformed into kinetic energy. A critical point is then reached and increasing the interaction strength further will instead decrease the spread rate as the momentum states become saturated and the cloud starts experiencing self-trapping.

If we fix the interaction strength at a weak value ($U = 0.1$) and vary the secondary lattice strength (see Fig. 3.23), there is no qualitative difference from the non-interacting case (Fig. 3.15). When the interactions are much stronger ($U = 10$), the spread rate is larger in the weak secondary lattice region, as the larger interaction energy is converted to kinetic energy. Increasing the secondary lattice strength reduces
Figure 3.20: Site occupation (logarithmic) of an interacting ($U = 10^{-3}$) Bose gas in a commensurate bichromatic lattice ($\alpha = 6/5$, $\Delta = 3$), at $t = 1000$ after release from a $w_0 = 6$ sized initial state.

Figure 3.21: Site occupation (logarithmic) of an interacting ($U = 10$) Bose gas in a commensurate bichromatic lattice ($\alpha = 6/5$, $\Delta = 3$), at $t = 1000$ after release from a $w_0 = 6$ sized initial state.
Figure 3.22: Rms. half-width vs. interaction strength of an interacting Bose gas in a commensurate bichromatic lattice ($\alpha = 6/5$, $\Delta = 3$), at $t = 1000$ after release from a $w_0 = 6$ sized initial state.

Figure 3.23: Rms. half-width vs. secondary lattice strength of an interacting Bose gas in a commensurate bichromatic lattice ($\alpha = 6/5$), at $t = 200$ after release from a $w_0 = 6$ sized initial state. The blue curve is for $U = 0.1$ and the green curve is for $U = 10$. 
the spread rate of the cloud as the bandwidth of the modified Bloch band reduces, and self-trapping sets in. The result is to suppress the transmission of the cloud much faster than for the non-interacting case.
3.3.7 Tilted Optical Lattice

Bloch oscillations are a well known quantum effect in condensed matter physics, where the periodic nature of the reciprocal of the optical lattice causes an accelerating particle to Bragg scatter off the Brillouin zone edge, setting up a harmonic oscillation in position space when only single particle dynamics are relevant. Inter-particle interactions destroy the effect as collisions tend to reset the momentum of the particle before it reaches the Brillouin zone edge. For this reason Bloch oscillations escaped observation in experiment for a long time, however, modern techniques and control of the interaction strength allow observation of this interesting and purely quantum effect \[49, 50\]. In this section we examine its incarnation in the presence of pseudo-disorder and interaction induced self-trapping.

An appropriate constant force could be implemented in experiment by tilting the optical lattice from the horizontal in a gravitational field. In our model this is accounted for by including

\[
\epsilon_j^F = -F_j
\]

in the onsite energy \((\epsilon_j)\) of (3.23). In the otherwise homogeneous, non-interacting system we obtain the analytic solution

\[
z_j(\tau) = \frac{1}{M} \sum_p \tilde{z}_p \exp i \left[ \frac{2\pi}{F} \left( \sin [k_p(0)] - \sin [k_p(\tau)] \right) - k_p(\tau)j \right],
\]

where

\[
k_p(\tau) = \frac{2\pi}{M}p - F\tau
\]

\[
\tilde{z}_p = \sum_j z_j(0) \exp i \left[ \frac{2\pi}{M}pj \right],
\]

which is periodic in time with period \(T = 2\pi/F\). After every period, \(T\), the cloud is back in its initial state. This is obvious in the density vs. time plot in Fig. 3.24, but is most clearly seen in the “center-of-mass” \((\mu)\) and “size” \((w)\) traces plotted in Fig. 3.25, as the cloud has both a dipolar (center-of-mass) and a breathing (size) oscillation with the same period.

When we include a secondary lattice, the dynamics becomes much more complex. In the commensurate case, where the lattice’s wavelength ratio is \(\alpha = n/m\), the Brillouin zone of the homogeneous lattice is split into \(m\) bands. The reduced Brillouin zone is \(1/m\) of the homogeneous one. The main oscillation period of the centre-of-mass is therefore given by

\[
T_c = \frac{2\pi}{Fm}.
\]
Figure 3.24: Site occupation of the homogeneous lattice ($\Delta = 0$) in the presence of a uniform force. Bloch parameter is $F = 2 \times 10^{-2}$ giving a Bloch oscillation period of $T = 314.16$. $v_t = 10^{-2}$.

Figure 3.25: Mean position (blue) and rms. half-width (green) of the homogeneous lattice ($\Delta = 0$) in the presence of a uniform force. Bloch parameter is $F = 2 \times 10^{-2}$ giving a Bloch oscillation period of $T = 314.16$. $v_t = 10^{-2}$ and $M = 1024$. 
Note that this means we must use a Bloch parameter, $F$, 5 times smaller, when $\alpha = 6/5$, to get a period similar to the homogeneous case. This period is clearly visible in Fig. 3.26, where $T_c \approx 419$. The increased effective mass reduces the position fluctuation (seen in the reduced axes scales for $\mu$ and $w$ in Fig. 3.27), even as the reduced period increases the oscillation frequency. Hence, the oscillation is most obvious as a breathing oscillation, i.e. the expansion and contraction of the clouds width, rather than the centre-of-mass. The plot is presented on a log scale in order to more easily see the oscillation, however, it should be noted that in experiment, an oscillation this small will be difficult to see by the usual absorption imaging.

In the incommensurate case (Fig. 3.28), multiple oscillation frequencies seem to be present. The localisation is not broken by tilting the lattice, however, the cloud is still able to oscillate in the virtual transition zone, i.e. within a localisation length of the start position. The multiple frequencies leads to a decay of the periodicity, which can already be seen on the time scale presented in Fig. 3.29, and will eventually destroy the periodicity completely. The oscillations in this simulation are even smaller than for the commensurate lattice, and while it is of theoretical interest, may be impossible to observe in experiment.

If we include interactions in the commensurate lattice, we would expect that the collisions will tend to reset the particles as they traverse the Brillouin zone, and hence, prevent some of the particles from Bragg scattering off the zone edge, allowing transmission. However, the mean field treatment that we apply cannot support this behaviour. In the absence of quantum fluctuations and confined to the single-band model, the Bloch oscillations remain unbroken. Added to this is the confining effect of the interaction induced self-trapping. The combined effect is impossible to distinguish from the localised case above when the interactions are strong enough.

Due to the extremely similar behaviour between a disorder localised cloud and a self-trapped cloud in a tilted optical lattice, we conclude that any external potential will be of limited use in distinguishing the two effects from experimental data. We would expect that applying an external potential to a self-trapped gas will shift the centre-of-mass of the gas, however, any potential that varies by more than the bandwidth of the bichromatic lattice will induce Bloch oscillations. Increasing the slope will only make the oscillation frequency larger and the displacement smaller.
Figure 3.26: Site occupation (logarithmic) in the presence of a uniform force and a strong commensurate secondary lattice ($\alpha = 6/5$ and $\Delta = 3$). Bloch parameter is $F = 5 \times 10^{-3}$ and $v_t = 10^{-2}$.

Figure 3.27: Mean position (blue) and rms. half-width (green) in the presence of a uniform force and a commensurate secondary lattice ($\alpha = 6/5$ and $\Delta = 3$). Bloch parameter is $F = 3 \times 10^{-3}$ giving a Bloch oscillation period of $T = 418.88$. $v_t = 10^{-2}$ and $M = 256$. 
Figure 3.28: Site occupation (logarithmic) in the presence of a uniform force and an incommensurate secondary lattice ($\alpha = 1025/863$ and $\Delta = 3$). Bloch parameter is $F = 3 \times 10^{-3}$ and $v_t = 10^{-2}$.

Figure 3.29: Mean position (blue) and rms. half-width (green) in the presence of a uniform force and an incommensurate secondary lattice ($\alpha = 1025/863$ and $\Delta = 3$). Bloch parameter is $F = 3 \times 10^{-3}$, $v_t = 10^{-2}$, and $M = 256$. 
Figure 3.30: Site occupation (logarithmic) of an interacting Bose gas \((U = 1)\) in the presence of a uniform force and a commensurate secondary lattice \((\alpha = 6/5 \text{ and } \Delta = 3)\). Bloch parameter is \(F = 3 \times 10^{-3}\) and \(v_t = 10^{-2}\).

Figure 3.31: Mean position (blue) and rms. half-width (green) of an interacting Bose gas \((U = 1)\) in the presence of a uniform force and a commensurate secondary lattice \((\alpha = 6/5 \text{ and } \Delta = 3)\). Bloch parameter is \(F = 3 \times 10^{-3}\), \(v_t = 10^{-2}\), and \(M = 256\).
3.4 Conclusions

In this chapter we have simulated the behaviour of a non-interacting and interacting Bose gas in a disordered optical lattice, where the disorder is introduced via interference with a second optical lattice. The simulations are consistent with the findings of Aubry and André [41], i.e. for an incommensurate bichromatic lattice, there exists a critical disorder strength ($\Delta_c = 2$), beyond which there is an absence of diffusion.

We have demonstrated the effect of inter-particle interactions in the single band model, in particular the self-trapping that confines the particle cloud as interactions increase. The self-trapping effect is enhanced by a secondary lattice due to the decreased bandwidth.

Finally we have included a linear force in the simulations, which causes Bloch oscillations in the gas. The Bloch oscillations are enhanced by a secondary lattice and do not break the strong localisation of an incommensurate lattice. Surprisingly, the force term does not significantly break the self-trapping if the interactions are strong enough.
Chapter 4

Synthetic Magnetic Fields in the 2D Lattice Model

In this chapter we explore the effect of an external magnetic field on charged particles in a 2D disordered lattice.

The classical effect of an external magnetic field is to cause the particles to take looped paths which should lead to a decrease in the conductance of material as magnetic field increases. Despite this, there are materials that exhibit a negative magneto-resistance, an increase in the conductance in response to an increasing magnetic field. The mechanism behind this phenomenon was a thirty year puzzle until it was finally explained in the context of Anderson localisation [51, 52] in 1980.

Both negative magneto-resistance and localisation are interference effects, so it is of interest how the two effects interact.

The disorder is introduced via a secondary lattice, as in the 1D bichromatic model presented earlier, however, we compare the results to a truly random disorder potential (as in the Anderson model) in the final section.

4.1 The Model

4.1.1 Magneto-resistance

If a source of charged particles is placed at S and a detector at D and $A_i$ is the amplitude of the $i^{th}$ classical trajectory from S to D then the probability of detecting a particle from the source at the detector is

$$W = \left| \sum_i A_i \right|^2 = \sum_i |A_i|^2 + \sum_{i \neq j} A_i^* A_j.$$  \hfill (4.1)
The first term is the sum of the probabilities of the classical trajectories, while the second is the quantum interference of those paths. The second term is usually neglected as the trajectory length is much larger than the wavelength of the particle and hence the paths effectively arrive with random phase and sum to zero. However, in the case where the source and the detector are at the same position then the trajectories form closed loops, the time-reversed trajectory, which is the same path traversed in the opposite direction, has the same amplitude. If a particle follows a trajectory with amplitude \( A_1 \), which is also the amplitude of time-reversed trajectory, then the sum of their contribution to the probability is \( w_1 = 4|A_1|^2 \), instead of the \( w_1 = 2|A_1|^2 \) that results if we neglect the second term. The difference in the contributions is large but comes from only a small number of paths. The overall result is to reduce the conduction of the particles from the classically expected result. This effect is known as "Weak localisation" and can be observed in even well conducting materials.

In the presence of a uniform magnetic field, the time-reversal symmetry is broken and a phase difference is imposed between the amplitude of the looped trajectory \( A_1 \) and its time-reversed amplitude \( A_2 \), proportional to the magnetic flux enclosed by the loop. This is the result of the Aharonov-Bohm effect. Their combined probability is then reduced from the magnetic field-free case, and the conduction of the particles is increased.

A full quantum treatment will show that the conduction of the particles is composed of a classical Drude conduction and a negative quantum correction. The Drude conduction decreases with increasing magnetic field, but for weak magnetic field the magnitude of the quantum term decreases faster. This saturates for larger magnetic field, but for weak field the net trend is negative. The material then has an increasing conduction with increasing magnetic field, and hence, a negative magneto-resistance.
4.1.2 Synthetic Magnetic Fields in Continuous Space

The ultra-cold model used in the previous chapter proves to be a powerful tool for examining the properties of crystalline materials without the complexities of working with the materials themselves. However, using charged particles in those systems is prohibitive due to the large Coulomb force, and hence, we would like to use a neutral bosonic system that has the same Hamiltonian as that of charged particles in a magnetic field.

To this end we examine the Hamiltonian for such a system

\[ \hat{H}_A = \frac{1}{2m} (p + qA)^2 + V(r), \]  

(4.2)

where \( q \) is the charge of the particle and \( A \) is the gauge-invariant vector potential such that \( B = \nabla \times A \) for a given magnetic field \( B \). Essentially, the momentum is shifted from its free-space value by \( qA \).

We can simulate this effect in a gas of neutral bosons by synthesising a Hamiltonian of the same form. For example, the force on a particle in a rotating frame is given by the Coriolis force \( F_c = 2mv \times \Omega \), resulting in the Hamiltonian [53]

\[ \hat{H}_c = \frac{1}{2m} (p - m\Omega \times r)^2 + V(r) - \frac{1}{2}m(\Omega \times r)^2. \]  

(4.3)

Care must be taken to cancel the resulting harmonic potential terms to keep the system stable, and the issues arising from having a rapidly spinning experimental apparatus are prohibitive.

An alternative scheme proposed by Spielman et al. [54] uses Raman laser fields to couple the \( F = 1 \) spin-states of \(^{87}\text{Rb} \) atoms that have been split by an external magnetic field via the Zeeman effect. Thus, they are able to produce a \( y \)-dependent shift in the \( x \)-component of momentum (Fig. 4.2d), that is tunable by the external magnetic field. The advantage of this method is that light fields are faster to switch on and off than a real magnetic field, the apparatus is stationary and it is possible to produce synthetic magnetic fields much stronger than real ones as conventional electromagnets are restricted by resistance and inductance in the electrical wires. Furthermore it is relatively simple to add a periodic lattice to simulate crystalline materials.

4.1.3 Magnetic Field in a Tight-Binding Optical Lattice

In a lattice system we include the effect of a magnetic field by first assuming that we still have an orthogonal set of basis states, centred at each lattice site, similar to
Figure 4.2: Experiment summary for synthesising magnetic fields employed by [54].

a, The BEC is in a crossed dipole trap in a magnetic field $B = (B_0 - b'y)\hat{y}$. Two Raman beams propagating along $\hat{y} \pm \hat{x}$ (linearly polarised along $\hat{y} \pm \hat{x}$) have frequencies $\omega_L$ and $\omega_L + \Delta \omega_L$. b, Raman coupling scheme within the $F = 1$ manifold: $\omega_Z$ and $\epsilon$ are the linear and quadratic Zeeman shifts, and $\delta$ is the Raman detuning. c, Energy-momentum dispersion relations. The grey curves represent the states without Raman coupling; the three coloured curves represent $E_j(k_x)$ of the dressed states. The arrow indicates the minimum at $k_{\text{min}}$. d, Vector potential $q^* A_z^* = \hbar k_{\text{min}}$ versus Raman detuning $\delta$. The insets show the dispersion $E_1(k_x)$ for $\hbar \delta = 0$ (top inset) and $-2E_L$ (bottom inset).
the Wannier basis. The requirement that the system is gauge invariant [55–57] then motivates the modification to the hopping terms

\[ J_{n,m} \rightarrow J'_{n,m} = J_{n,m} e^{iq \int_{x_n}^{x_m} A \cdot dl} \] (4.4)

where the integral is taken over the shortest path from site \( n \) to \( m \).

Eq. 4.4 provides us with a new set of tools to synthesise magnetic fields in the tight-binding model as we do not need to alter the momentum of the particles, only manufacture a phase shift on the site-to-site hopping.

One such experimental set-up proposed by Zoller et al. [58], summarised in Fig. 4.3, takes advantage of two optical lattices, one for each of two different internal states of the atoms. The light assisted transition from one species to the other provides the required phase shift on hopping in the \( x \)-direction, while the particles hop in the normal manner in the \( y \)-direction. By spatially varying the Raman laser beams in the \( y \)-direction, the phase shift is made site dependent and traversing a lattice plaquette accumulates a overall phase consistent with an excited particle in an external magnetic field in the tight-binding model. The adjacent lattice plaquette has the opposite flux, however, forming a chequered pattern instead of the desired uniform magnetic field. For this reason we favour the method of Speilman et al.

Alternative schemes have been proposed by [59–62].
Figure 4.3: **Optical lattice set-up employed by [58].** Open (closed) circles denote atoms in state $|g⟩$ ($|e⟩$). (a) Hopping in the y-direction is due to kinetic energy and described by the hopping matrix element $J^y$ being the same for particles in states $|e⟩$ and $|g⟩$. Along the x-direction hopping amplitudes are due to the additional lasers. (b) Trapping potential in the x-direction. Adjacent sites are offset by an energy $Δ$ because of the acceleration or a static inhomogeneous electric field. The laser $Ω_1$ is resonant for transitions $|g⟩ ↔ |e⟩$ while $Ω_2$ is resonant for transitions $|e⟩ ↔ |g⟩$ due to the offset of the lattice sites. Because of the spatial dependence of $Ω_{1,2}$ atoms hopping around one plaquette get phase shifts of $2πα = -φ_m + 0 + φ_{m+1} + 0$ where $φ_m = m q λ / 4 π$ as indicated in (a).
4.1.4 Equations of Motion

We are free to choose the most convenient gauge in (4.4). This turns out to be the Landau gauge \( \mathbf{A} = -B y \mathbf{x} \) for a uniform magnetic field as it eliminates the imposed phase shifts from the non-local terms in one dimension. The EOM are then given by

\[
i \dot{z}_{j,k} = -z_{j-1,k} - z_{j+1,k} - e^{-i \varphi j} z_{j,k-1} - e^{i \varphi j} z_{j,k+1} + \epsilon_{j,k} z_{j,k}
\]

(4.5)

for \(-\pi \leq \varphi < \pi\). The phase accumulated traversing the closed loop that is the perimeter of one lattice plaquette is \(0 + \varphi(j + 1) + 0 - \varphi j = \varphi\). This is directly proportional to the effective magnetic flux through that plaquette due to the synthetic magnetic field.

Any external potentials enter the EOM through the onsite potential energy, \(\epsilon_{j,k}\). In the case of the 2D bichromatic lattice, this takes the form

\[
\epsilon_{j,k} = \Delta \left( \cos(2\pi \alpha j + \phi_y) + \cos(2\pi \alpha k + \phi_x) \right).
\]

(4.6)

Note that this potential is separable into two independent 1D potentials. In the last section of this chapter, the onsite potential is replaced by a uniformly random potential to simulate true disorder. This potential is not separable.

In the pure lattice model, where \(\epsilon_{j,k} = 0\), transforming to Fourier space in the \(x\)-direction, i.e.

\[
z_{j,k} = \sum_q \tilde{z}_{j,q} e^{i q k},
\]

(4.7)

changes the time-independent equation into a set of 1D equations,

\[
-\tilde{z}_{j-1,q} - \tilde{z}_{j+1,q} - 2 \cos(\varphi j - q) \tilde{z}_{j,q} = E \tilde{z}_{j,q}
\]

(4.8)

This has the same form as the 1D Aubry-André equation (3.30) at the critical value of \(\Delta = 2\). This approach is analogous to the continuous version in [63].

The following simulations are started from the ground state of the primary lattice and a harmonic trap \((v_t = 10^{-2})\). The secondary lattice and synthetic magnetic field are then instantaneously switched on and the simulation proceeds. However, the switching on of the synthetic magnetic field effectively gives the wave-packet a momentum kick. In the symmetric gauge the \(x\) and \(y\) terms cancel leaving the initial wave-packet the same, but in the Landau gauge we must apply the transform

\[
z_{j,k}^L = e^{i \varphi j k/2} z_{j,k}^S
\]

(4.9)

to get the initial state. This effect is the same as that measured experimentally by Spielman et al. [64] as it is essentially the result of a time-varying synthetic field or
equivalently a synthetic electric field in the instant that the synthetic magnetic field ramps up.

4.2 Numerics

We again use the RK4DS method to time evolve the system. The particular variant depends on the strength of the magnetic and disorder terms. Method 1 is not practical for a 2D system as the matrix to contain the linear part of (4.5) is $M^2 \times M^2$. A desktop PC could only handle systems up to $M \sim 70$, and more powerful computers will not do significantly better. We desire to simulate a lattice with $M \sim 1000$ or larger.

We can again take advantage of Fourier transforms to reduce the memory requirements of the algorithm. One configuration is to arrange the terms so that

$$\hat{a}_z j,k = -z_{j-1,k} - z_{j+1,k} = [\hat{F}_Y^{-1}\hat{\omega}_Y \hat{F}_Y z]_{j,k}, \quad (4.10)$$

$$\hat{b}_z j,k = -e^{-i\varphi j} z_{j,k-1} - e^{i\varphi j} z_{j,k+1} = [\hat{F}_X^{-1}\hat{\omega}_X \hat{F}_X z]_{j,k}, \quad (4.11)$$

where $\hat{F}_Y (\hat{F}_X)$ is the 1D Fourier transform in the y-direction (x-direction) and

$$[\hat{\omega}_Y x]_{p,k} = -2 \cos \left( \frac{2\pi p}{M} \right) x_{p,k}, \quad (4.12)$$

$$[\hat{\omega}_X x]_{j,q} = -2 \cos \left( \frac{2\pi q + \varphi j}{M} \right) x_{j,q}. \quad (4.13)$$

This is the 2D, magnetic version of method 2.

If the onsite energy is separable such that $\epsilon_{j,k} = \epsilon^Y_j + \epsilon^X_k$, then we can instead use

$$\hat{a}_z j,k = -z_{j-1,k} - z_{j+1,k} + \epsilon^X_k = [\hat{F}_Y^{-1}\hat{\omega}_Y \hat{F}_Y z]_{j,k}, \quad (4.14)$$

$$\hat{b}_z j,k = -e^{-i\varphi j} z_{j,k-1} - e^{i\varphi j} z_{j,k+1} + \epsilon^Y_j = [\hat{F}_X^{-1}\hat{\omega}_X \hat{F}_X z]_{j,k}, \quad (4.15)$$

where

$$[\hat{\omega}_Y x]_{p,k} = \left[ \epsilon^X_k - 2 \cos \left( \frac{2\pi p}{M} \right) \right] x_{p,k}, \quad (4.16)$$

$$[\hat{\omega}_X x]_{j,q} = \left[ \epsilon^Y_j - 2 \cos \left( \frac{2\pi q + \varphi j}{M} \right) \right] x_{j,q}. \quad (4.17)$$

This is the 2D, magnetic version of method 3.

Fig. 4.4 and Fig. 4.5 show the step size required to get a step accuracy of $10^{-10}$. Method 3 is again more efficient than method 2 when the disorder strength is large, as was the case in the 1D algorithm. For low magnetic field, the efficiency is dominated by the disorder term. When the magnetic flux becomes large enough, the step size for the disorder term is not small enough. After this point neither method is better than the other. Therefore, the method should be chosen for the disorder strength.
Figure 4.4: Step size ($h$) required to achieve double step accuracy $\max[\Delta z] \leq 10^{-10}$ vs. synthetic magnetic field flux ($\varphi$) when secondary lattice strength $\Delta = 1$.

Figure 4.5: Step size ($h$) required to achieve double step accuracy $\max[\Delta z] \leq 10^{-10}$ vs. synthetic magnetic field flux ($\varphi$) when secondary lattice strength $\Delta = 3$. 
4.3 Results

4.3.1 Symmetries and the Brillouin Zone

In the limit of vanishing synthetic magnetic field, the dispersion relation of the primary lattice is a pure cosine. The low momentum dispersion is approximately equivalent to a quadratic, hence the appearance of ballistic transport in the homogeneous system. The secondary lattice in the case of weak localisation ($\Delta < 2$) does not significantly alter the shape of the dispersion relation and so the wave-packet released from a harmonic trap evolves from the initial circular shape (Fig. 4.6a) into a square symmetry of the 2D square reciprocal lattice (Fig. 4.6b). Classically this is evident from the position-velocity relation: $x(t, p) = x(0, p) + v(p)t$, so as $t$ increases the shape of the momentum distribution comes to dominate over the bias of the initial position. This square symmetry was observed experimentally in a non-interacting Fermi gas by Schneider et al. [65].

When the synthetic magnetic field is stronger, time-reversal symmetry is broken and hence the $\sigma_x$ and $\sigma_y$ symmetries (reflection in the $x=0$ and $y=0$ planes respectively) are also broken [66]. The $C_2 = \sigma_x \sigma_y$ symmetry (rotation by $\pi$) is preserved, however, so the solid points in Fig. 4.7 are each self-similar and the Bravais lattice and hence the reciprocal lattice is now rotated by $\pi/2$. This results in the diamond symmetry of Fig. 4.8a, a signature that would be clearly observable in time-of-flight
Figure 4.7: Diagram of the primary lattice depicting the phase accumulated around a lattice plaquette in the synthetic gauge field and the symmetries, $\sigma_x$ and $\sigma_y$, which are broken. Filled and unfilled dots indicate the loss of self-similarity between these sets of sites due to symmetry breaking.

type experiments. Furthermore, the lattice parameter is increased by a factor of $\sqrt{2}$ and hence the “volume” of the Brillouin zone is reduced by half causing some of the particles that were in the low-momentum region to now not be. Therefore, in a very strong gauge field (Fig. 4.8b), the wave-packet maintains some of the radial symmetry, losing the diamond-like structure.

Figure 4.8: Spatial density $t = 1000$ after release in the presence of a synthetic magnetic field with (a) $\varphi = 0.1$ and (b) $\varphi = 1$ in a homogeneous optical lattice ($\Delta = 0$). $v_t = 10^{-2}$. 
4.3.2 Weak Secondary Lattice

At long times, increasing the magnetic field has the effect of decreasing the cloud’s rate of expansion (Fig. 4.9). The classical analogy is that the particles are completing more of their tighter circular orbits, and hence traversing less linear distance, before being scattered off the pseudo-random secondary lattice. This is therefore analogous with normal, positive magneto-resistance.

The durations of the simulations shown in Fig. 4.9 are limited by the system size, the simulation is terminated when the effect of the periodic boundary conditions becomes noticeable.

Figure 4.9: Disorder averaged rms. half-width of the particle cloud vs. time during evolution in a weak incommensurate lattice with strength $\Delta = 1$ and synthetic gauge field: (triangle) $\varphi = 0.001$; (square) $\varphi = 0.01$; (cross) $\varphi = 0.1$; (circle) $\varphi = 1$. $v_t = 10^{-2}$ and $M = 1024$.

Figure 4.10: Long-time scaling ($w \propto t^\gamma$) of the width of the cloud. Data points are retrieved from a temporal average of the gradient of the log($w$) vs. log($t$) plot at long time. The error bars are the standard deviations of the samples.

In Fig. 4.10 we plot $\gamma = \frac{\text{d}\log_{10}(w)}{\text{d}\log_{10}(t)}$ at long times for a selection of gauge field strengths. The data points are obtained using a temporal average about each point. The error bars reflect the variance in the data. The long time behaviour of the size of the cloud approaches $t^{1/2}$ with very strong magnetic field, which is characteristic of diffusive expansion.
To summarise, for weak disorder, the effect of the magnetic field is therefore to change the transport from ballistic to diffusive expansion. Furthermore, with increasing field strength, the diffusion coefficient is reduced, consistent with positive magneto-resistance.

4.3.3 Strong Secondary Lattice

![Figure 4.11: Disorder averaged Rms. half-width of the particle cloud vs. time during evolution in a strong incommensurate lattice with strength $\Delta = 3$ and synthetic gauge field: (cross) $\varphi = 0.001$; (circle) $\varphi = 0.01$; (square) $\varphi = 0.1$; (diamond) $\varphi = 0.5$; (triangle) $\varphi = 1$. $v_t = 10^{-2}$ and $M = 1024$.](image)

In the strongly localised regime, $\Delta > 2$, we observe the confinement of the wave-packet consistent with the Aubry-André model for a sufficiently weak gauge field [Fig. 4.11 - cross]. This localisation is the result of the total destructive interference of multiply scattered matter-waves for any sites beyond the localisation length.

Considering any path that loops back to its origin, the same path traversed in the opposite (time-reversed) direction is of the same length and hence will return the same phase. Any closed path and its time-reversed partner will therefore interfere constructively. In the presence of a gauge field, however, the phase is displaced proportional to the flux enclosed which has opposite sign for each direction (the Aharonov-Bohm effect). The two paths will then interfere with an essentially random phase. When averaged over many paths, the backscattering of the matter-waves is now dramatically reduced, resulting in the destruction of the localisation and a positive expansion of the wave-packet.

For a sufficiently strong gauge field we clearly observe the destruction of the strong localisation [Fig. 4.11]. Furthermore, increasing the magnetic field increases the rate of expansion of the cloud, characteristic of negative magneto-resistance. The transition occurs continuously suggesting that the localisation is broken for any magnetic field strength, although it may be undetectable for the system run times that we can simulate.
Figure 4.12: Total particles vs. time when $\Delta = 3$, $\varphi = 1$ and using a 25 site absorbing boundary layer in a $256 \times 256$ site system (thus attenuating extended states). (dashed line) Full system, (solid line) $31 \times 31$ sites at centre of the system.

It is interesting to note that localisation is not completely broken for all states. Some of the eigen-states remain localised. In Fig. 4.12 we demonstrate the presence of localised eigen-states. For this plot we have included a large negative-imaginary term in the local part of the Hamiltonian for sites within 25 sites of the system edge (in a $256 \times 256$ site system). When released from the harmonic trap, the outward bound population enters the absorbing layer and is quickly attenuated before it can reflect off the system edge. In practice there is still a finite reflection off the boundary between the system and the absorbing layer but this can be minimised by ramping the absorption strength quadratically in the outward direction. In a continuous model there are methods such as phase matching [67] that would completely cancel any outbound waves, however, this does not work for discrete systems and is only ever approximate for numerical simulations of continuous systems.

In the plot we observe that the decay of the total population saturates as all the extended states are attenuated when they reach the edge of the simulation grid, leaving behind the surviving localised states. This is most pronounced for the $31 \times 31$ sites at the centre of the system. Such behaviour could be observed experimentally by taking in situ absorption images and observing the change in particle number with time.

4.3.4 True Disorder

Up to this point we have considered disorder introduced through a quasi-periodic potential as in the experiments of Roati et al. [30] and Schulte et al. [68].

We now compare these results to those obtained using a true disorder potential defined by replacing the previous $\epsilon_{j,k}$ with

$$\epsilon_{j,k} = W\text{Rand}(j,k),$$

(4.18)
where $W$ is the strength of the disorder and $\text{Rand}()$ is MATLAB’s random number generator producing pseudo-random numbers on the interval [0,1] for each lattice site. This model, while strictly unachievable in current experiments, is an approximation to those using 2D laser speckle patterns [27]. However, the disorder potential produced through laser speckle contains correlations due to the grain size which are not included here. This model could, of course, be extended to include these correlations, but is very parameter-specific and so neglected here in this more general treatment.

Figure 4.13: Disorder averaged rms. width of the particle cloud vs. time during evolution in a uniformly random on-site potential with energies in the range [0, 6]. Synthetic gauge field switched on at $t = 0$ with strength: (circle) $\varphi = 0$, (square) $\varphi = 0.001$, (cross) $\varphi = 0.01$, (diamond) $\varphi = 0.1$, (triangle) $\varphi = 0.5$ and (asterisk) $\varphi = 1$. $\nu_t = 10^{-2}$ and $M = 1024$.

Figure 4.14: Disorder averaged rms. width of the particle cloud vs. time during evolution in a uniformly random on-site potential with energies in the range [0, 9]. Synthetic gauge field switched on at $t = 0$ with strength: (circle) $\varphi = 0$, (square) $\varphi = 0.001$, (cross) $\varphi = 0.01$, (diamond) $\varphi = 0.1$, (triangle) $\varphi = 0.5$ and (asterisk) $\varphi = 1$. $\nu_t = 10^{-2}$ and $M = 1024$.

With true disorder in the 2D system, in principle, all states are localised for any finite strength of the disorder [69]. However, the localisation length for vanishingly weak disorder can be larger than the size of our system. We therefore present calculations performed with $W = 6$ (Fig. 4.13), $W = 9$ (Fig. 4.14), and $W = 12$ (Fig. 4.15) as this results in localisation lengths small enough to contain in our numerical simulations. We ran each simulation ten times with different realisations of the disorder potential.
Figure 4.15: Disorder averaged rms. width of the particle cloud vs. time during evolution in a uniformly random on-site potential with energies in the range $[0, 12]$. Synthetic gauge field switched on at $t = 0$ with strength: (circle) $\varphi = 0$, (square) $\varphi = 0.001$, (cross) $\varphi = 0.01$, (diamond) $\varphi = 0.1$, (triangle) $\varphi = 0.5$ and (asterisk) $\varphi = 1$. $v_t = 10^{-2}$ and $M = 1024$.

and present the average of the wave-packet size vs. time. In this model, the wave-packet remains localised for any phase ($\varphi$) of the gauge potential as one expects from the scaling theory. However, the localisation length is increased with increasing field strength, consistent with the appearance of negative magneto-resistance in a truly disordered system.

### 4.4 Conclusions

In conclusion, we have used numerical simulations to demonstrate the interplay between synthetic gauge fields and strong localisation in the Aubrey-André model. We observe firstly positive magneto-resistance in the extended regime and then negative magneto-resistance in the strong localisation regime. We have demonstrated distinctive behaviours for each regime that should be experimentally observable through straightforward absorption imaging techniques. Especially, the observation of negative magneto-resistance can only be explained in the context of an interference phenomenon. This would therefore be an unambiguous signature that localisation, destroyed or reduced by the imposition of a magnetic field, had such interference as its origin, distinguishing it from classical trapping or interaction-induced self-trapping. This is especially important in 2D where ambiguity in the origin of localisation in experiments still resides. Whilst our study has concentrated on the use of quasi-periodic lattices for the experimental introduction of the disorder potential, we have demonstrated qualitative agreement for our conclusions using a true disorder potential. We therefore believe our results will carry over to experiments using laser speckle.
Part II

Density Functional Theory
Chapter 5

Introduction

The study of the electronic structure of molecules and bulk materials is a difficult but important problem in quantum theory. Continued research of the topic could allow quantum chemists and physicists to understand current natural phenomena, and predict new ones that may prove useful in science and technology.

A common method for solving quantum many-body problems is the Hartree-Fock (HF) method [70]. The HF method assumes that the many-body wavefunction be expressed as a Slater determinant, in the case of fermionic particles, or as a single permanent of $N$ single-particle orbitals, for bosons, where $N$ is the number of particles. Although this is an approximation, it proves very accurate for a wide range of applications. However, as an example, the rigid nature of the single Slater determinant does not allow the model to account for the correlation effects caused by Coulomb repulsion. To do this one must turn to the many post-HF methods, the best of which, scales as $\sim N^5$, i.e. fifth order with particle number, so are very computationally expensive.

For a system of $N$ fermions, the basic HF theory requires self-consistently solving a system of $N$ equations with 3 spatial coordinates. However, the Hohenberg-Kohn theorems [71] show that to measure the expectation value of any observable on the ground-state, all that is needed is the ground-state density, $\rho_0(r)$, which is a function of only 3 spatial coordinates.

The essence of density functional theory (DFT) is to construct the energy functional, $E[\rho]$, dependent on density, of a non-interacting system that has the same ground-state as the full interacting system. One then uses conventional optimisation techniques to find the ground-state of this new system, and hence, of the original many-body system, which can then be used to calculate any desired observables on the ground-state.

The energy functional of a suitable non-interacting system may not, \textit{a priori}, be
known. In fact, it may not even be possible to write down the energy functional in a concise or practical form. In this case we choose an approximate energy functional that shares desirable qualities with the system we are studying. In some cases one might also choose to do this when the energy functional is computationally too time-consuming to calculate.

The HF theory will always remain the method of choice for many-body systems with a small number of particles (at most 10-15), however, the DFT is a much more attractive method in the case of large particle numbers, due to the much improved scaling. The goal of DFT studies is then to find better functionals that more accurately predict the desired properties of the systems under consideration.

There is a vast publication base for DFT. It has a long history in both quantum chemistry and cold-atom physics. Although some of the concepts of DFT have been around since the start of quantum theory, the theory was not put on a solid theoretical foundation until the aforementioned work of Hohenberg and Kohn in 1964. Even after this, the theory was not of much practical use until Kohn and Sham presented their DFT scheme a year later [72]. Since then DFT has seen much mainstream use. In the next few sections we will review some of the concepts of DFT, but for a more complete review see [73]. Most attention to date has been paid to 1D and 3D systems, this thesis aims to fill in some gaps by extending these methods to their 2D equivalents.

The first and most basic form of DFT is the local density approximation (LDA). The LDA assumes that the total energy functional is only formed from powers of the local particle density. When the kinetic energy is considered in the LDA, this results in the Thomas-Fermi functional. Thomas and Fermi developed this model separately in 1927 by considering the statistical distribution of Fermi particles; it is considered to be the precursor to true DFT. This model is very limited and it fails to predict many properties. However, its simplicity is very attractive and much effort has been expended to expand the model without losing this simplicity.

This thesis employs the Thomas-Fermi-von Weizsäcker (TFvW) method, where a local gradient term with a fitted parameter is employed. The TFvW method enjoys great success over the basic TF model, however, it still fails to predict the expected oscillating density structure of a trapped Fermi gas. We apply the TFvW method to a harmonically trapped, dipolar Fermi gas, where the dipolar interactions are considered in the LDA. We extend the prior work of Zaremba and van Zyl [74] to calculate the low energy collective oscillation frequencies, a property which is often readily measurable in experiment. The TFvW method is quite suited to the calculation of the collective
frequencies as they are less sensitive to the local details of the ground-state density [75–78].

After that we present a method, inspired by the TFvW method, where the kinetic energy functional is an integral over an “average” density function. The weight function of the density average is then determined by a desired physical property, the exact static linear response. This method automatically employs the local gradient of the density, as in the TFvW, however, it does not require any parameter to be fitted.

In order to simplify constants, we will use atomic units ($\hbar = m = 1$) for this part of the thesis, unless otherwise stated. For convenience, we also introduce the wavefunction defined by $\psi(r) = \sqrt{\rho(r)}$, and note that as $\psi(r) \geq 0$, minimising w.r.t. $\psi(r)$ is equivalent to minimising w.r.t. $\rho(r)$.

### 5.0.1 Many-Body Fermionic System

The particles in the first part of this thesis were Bosons, particles with integer intrinsic spin and symmetric many-body wavefunctions, i.e. the particles are indistinguishable and any two particles may be switched simply by switching their position coordinates in the wavefunction. The particles under consideration in this part of the thesis are Fermionic. They have half-integer spin and the many body wavefunctions are antisymmetric, exchanging the position of any two particles in the many-body system will result in a $\pi$ phase shift in the many body wavefunction, i.e.

$$\Psi(r_1, ..., r_i, ..., r_j, ..., r_N) = -\Psi(r_1, ..., r_j, ..., r_i, ..., r_N) \tag{5.1}$$

This is the cause of the famous Pauli exclusion principle, two fermions may not occupy the same quantum state at the same position.

The Hamiltonian for a standard many-body fermionic system is constructed as

$$\hat{H} = \hat{T} + \hat{V}_{\text{ext}} + \hat{W}, \tag{5.2}$$

where $\hat{T}$ is the kinetic energy operator, $\hat{V}_{\text{ext}}$ is the external potential energy, and $\hat{W}$ is the inter-particle interaction energy.

### 5.1 Hohenberg-Kohn Theorem

If we consider a system with external potential, $v_{\text{ext}}(r)$, we can obtain the many-body stationary states by solving the Schrödinger equation

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle. \tag{5.3}$$
In particular we may find the ground-state, $|\Psi_0\rangle$, for the given external potential. Hence, we may consider the Schrödinger equation to be a map from the external potentials to their ground-states. The first Hohenberg-Kohn (HK) theorem [71] tells us that if the ground state is non-degenerate, then the ground-state is unique for any external potential plus an arbitrary constant, i.e. $v_{\text{ext}}(\mathbf{r})$ and $v_{\text{ext}}'(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + C$ ($C$ is an arbitrary scalar constant) will lead to the same ground state, however, another external potential that does not fit this form will not. The map is therefore one-to-one.

If we introduce the ground-state density,

$$\rho_0(\mathbf{r}) = \langle \Psi_0|\hat{\rho}(\mathbf{r})|\Psi_0 \rangle,$$

the second HK theorem tells us that the density function obtained is unique to that ground-state. Hence, there is a one-to-one map from ground-states to ground-state density functions.

The combination of the two maps insures that the ground-state density functional is uniquely determined for a given external potential plus a constant, and hence, that any operator, measured on the ground-state, can be calculated from the ground-state density function. Therefore, the observable is a functional (function of a function) of the density function. In particular, the total energy

$$E[\rho] = \langle \Psi|\hat{H}|\Psi \rangle,$$

is a functional of $\rho$, and when combined with the Ritz variational principal, gives us that

$$E[\rho_0] = \min_{\rho \in \mathcal{N}} E[\rho],$$

where $\mathcal{N}$ is the set of normalised density functions, i.e. the minimisation of the total energy functional, under the normalisation constraint, gives the ground-state density functional.

The original formulation of the HK theorems relied crucially on non-degenerate ground-states. However, one can show that the degenerate ground-states of a particular external potential are unique to that external potential plus a constant. Furthermore, though the ground-state density functions may be identical or different for the degenerate ground-states of a particular external potential, the degenerate ground-states for a different external potential will not share any ground-state density functions with the former. Thus, the above results are valid for degenerate systems.

This then is the essence of density functional theory, to find the correct total energy functional and minimise it to find the ground-state density. The density is a function
of \(d\) spatial coordinates, in a \(d\)-dimensional system, this is much less than the \(dN\)-dimensional space of the HF method, where \(N\) is the number of particles.

Note, however, that the HK theorems give no help whatsoever in finding the correct total energy functional, indeed there is no guarantee that one even exists in explicit form, or that it may be easily calculated. There have been many attempts to find suitable approximate functionals in the absence of the true form.

### 5.2 The Kohn-Sham Scheme

The birth of DFT may have been in the 1920’s with the TF model, however, it was not until Kohn and Sham released their paper in 1965 [72] that the kinetic energy functionals proved accurate enough in solving realistic problems.

The idea of the Kohn-Sham (KS) scheme is to separate, from the total energy functional, the effective single-particle kinetic energy, \(T[\rho]\), and let the rest form an effective potential energy functional, i.e.

\[
E[\rho] = T[\rho] + \int d\mathbf{r} \ v_{\text{eff}}(\mathbf{r}) \rho(\mathbf{r}),
\]

where

\[
v_{\text{eff}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(\mathbf{r})},
\]

and \(E_{\text{int}}[\rho]\), the interaction energy functional, contains the usual Hartree and exchange-correlation functionals as well as any additional particle interaction functionals.

The effective single-particle kinetic energy functional is defined by

\[
T[\rho] = \sum_{i=0}^{N-1} \int d\mathbf{r} \ \phi_i^*(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \phi_i(\mathbf{r}).
\]

The \(\phi_i(\mathbf{r})\), the single-particle orbitals, are the first \(N\) lowest-energy eigenstates of the Schrödinger equation

\[
-\frac{\hbar^2}{2m} \nabla^2 \phi_i(\mathbf{r}) + v_{\text{eff}}(\mathbf{r}) \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r}).
\]

The density is then recovered from

\[
\rho(\mathbf{r}) = \sum_{i=0}^{N-1} \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}),
\]

subject to the normalisation constraint

\[
N = \int d\mathbf{r} \ \rho(\mathbf{r}).
\]
The single-particle orbitals depend on the ground-state density and \textit{vice versa}, therefore the equations must be solved self-consistently.

The exact form for the interaction energy functional, $E_{\text{int}}[\rho]$, is most often unknown, some approximation must be made of its true form. The effective single-particle kinetic energy functional in the KS functional tends to be much more important than the exchange-correlation energy, hence the KS scheme remains fairly accurate, even with rough estimates for the exchange-correlation energy functional. However, the calculation of the single-particle orbitals for a large number of particles or for highly non-linear interaction energy functionals, may be prohibitive.

For a 2D, non-interacting, spin-polarised, degenerate Fermi gas in a harmonic external potential with circular symmetry, the KS calculation can be solved exactly by employing the Laplace transform method, and results in the density \cite{79, 80}

$$\rho(r) = \frac{1}{\pi} \sum_{n=0}^{M} (-1)^n (M - n + 1) L_n(2r^2)e^{-r^2}, \quad (5.13)$$

where $L_n(x)$ is the $n^{th}$ Laguerre polynomial. $M + 1$ is the number of filled oscillator shells and is related to the particle number via

$$N(M) = \frac{1}{2} (M + 1)(M + 2). \quad (5.14)$$

The total energy is then given by

$$E_{\text{ex}} = \frac{\hbar \omega_0}{3} N \sqrt{1 + 8N}. \quad (5.15)$$
Chapter 6

Numerical Minimisation

6.1 Functionals and the Functional Derivative

A scalar or a function that can be written as a function of functions is called a functional. A basic example of the former is the external potential energy functional, which is a function of the external potential and the particle density, which are both functions of position, i.e.

$$V_{\text{ext}}[\rho, v_{\text{ext}}] = \int d\mathbf{r} v_{\text{ext}}(\mathbf{r})\rho(\mathbf{r}).$$

(6.1)

The “free” functions are put in square brackets. An example of the latter type is the Fourier transform

$$F[f](\mathbf{k}) = \tilde{f}(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k} \cdot \mathbf{r}} f(\mathbf{r}),$$

(6.2)

where the round brackets contain the free variables of the resulting function.

Any function can be written as a functional of the second type simply by making use of the Dirac delta function, i.e.

$$\rho[\rho](\mathbf{r}) = \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r}).$$

(6.3)

It is of interest in this work to know the reaction of a functional to an infinitesimal change in the dependent function. This infinitesimal change can be written as

$$\delta \rho(\mathbf{r}) = \epsilon \varphi(\mathbf{r}),$$

(6.4)

where $\varphi(\mathbf{r})$ is normalised to unity, and $\epsilon$ is an infinitesimal scalar. To proceed we perform a standard Taylor expansion in terms of $\epsilon$ about $\rho$,

$$E[\rho + \epsilon \varphi] = E[\rho] + \left. \frac{dE[\rho + \epsilon \varphi]}{d\epsilon} \right|_{\epsilon=0} \epsilon + \left. \frac{d^2E[\rho + \epsilon \varphi]}{d\epsilon^2} \right|_{\epsilon=0} \epsilon^2 + O(\epsilon^3).$$

(6.5)
The linear term in $\varepsilon$ gives us the definition of the first functional derivative
\[
\int d\mathbf{r} \frac{\delta E[\rho]}{\delta \rho(\mathbf{r})} \varphi(\mathbf{r}) = \frac{dE[\rho + \varepsilon \varphi]}{d\varepsilon} \bigg|_{\varepsilon=0}.
\] (6.6)

The function $\varphi(\mathbf{r})$ is a test function. It can be any function that $\rho(\mathbf{r})$ itself can attain. The functional derivative, $\frac{\delta E[\rho]}{\delta \rho(\mathbf{r})}$, does not depend on the test function, it is a property of the functional.

The functional derivative is the continuous analogue of the total derivative of a function of many variables, i.e.
\[
df = \sum_i \frac{\partial f}{\partial x_i} dx_i.
\] (6.7)

### 6.2 Constrained Minimisation

The ground-state of a system is found by minimising the energy functional, $E[\rho]$, w.r.t. density, under the normalisation constraint:
\[
N[\rho] = \int d\mathbf{r} \rho(\mathbf{r}) = N.
\] (6.8)

Any numerical method will require a finite spatial grid at which to sample the density, and perhaps an analogue of the integral operation, in order to form a discretised approximation of the energy functional. The optimum choice of the set of spatial grid points, $\{\mathbf{r}_k\}$, is determined by the particular method employed. The wavefunction samples then form the set $\{\psi_k = \psi(\mathbf{r}_k)\}$.

Most numerical minimisation algorithms are only suitable for unconstrained minimisation. Fortunately, there are many methods to convert a constrained problem to an unconstrained problem, however, at some cost in difficulty to implement and compute. The usual approach is to employ a Lagrangian multiplier, $\mu$, and minimise the functional
\[
G[\rho] = E[\rho] - \mu N[\rho].
\] (6.9)

This is minimised when
\[
\frac{\delta E[\rho]}{\delta \rho} - \mu = 0,
\] (6.10)

which can be multiplied by $\psi$, and rearranged to the Schrödinger-like form required by the Imaginary-Time Propagation method,
\[
\frac{\delta E[\rho]}{\delta \rho} \psi = \mu \psi,
\] (6.11)
if the LHS gives a Laplacian term and an effective potential term.

Employing more advanced methods, like Steepest-Descent and the Conjugate-Gradient method is problematic, in this approach, as the optima of $E[\rho]$ are saddle-points of (6.9). A "downhill" method will skip over these points, except in the extremely unlikely event that a step lands close enough to suit the exit condition. This can be overcome by, instead, seeking the minima of the square magnitude of the gradient of $G[\rho]$ in (6.10), i.e.

$$H[\rho] = |\nabla_\rho G[\rho]|^2 + \left(\frac{\partial G[\rho]}{\partial \mu}\right)^2.$$  \hspace{1cm} (6.12)

However, this makes all the optima of $E[\rho]$ into minima of $H[\rho]$, including the maxima. The start state, which is at best a guess, of the minimiser then plays an extremely important role in the result.

We find that a much better scheme, similar to that employed by [81, 82], is to instead choose to minimise the functional

$$G[\psi] = E\left[\frac{N_0 \rho}{N[\rho]}\right] + \frac{1}{4}(N[\rho] - N_0)^2.$$  \hspace{1cm} (6.13)

The first term evaluates the energy of the normalised density, and the second term is minimised when the density is properly normalised. This method avoids some of the drawbacks of using a Lagrangian multiplier scheme as the constrained maxima of $E[\rho]$ are the same as the maxima of $G[\psi]$. Thus ensuring that proceeding "downhill" in this unconstrained system will always bring the system to a local energy minimum. The $\frac{1}{4}$ prefactor is included purely to simplify constants in a later chapter.

### 6.3 Imaginary-Time Propagation Method

Imaginary-Time Propagation (ITP) is a fairly simple and intuitive method for finding the minimum (or maximum) energy state of an eigen-system. Given the Shrödinger equation

$$\hat{H}\psi(r) = E\psi(r),$$  \hspace{1cm} (6.14)

then the time-propagation of a general wavefunction can be expressed as

$$\psi(r, t) = e^{-i\hat{H}t}\psi(r) = \sum_n c_n e^{-iE nt}\psi_n(r),$$  \hspace{1cm} (6.15)

where $E_n$ is the $n^{th}$ smallest eigen-energy of (6.14) with corresponding state $\psi_n$. 

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By making the substitution $t \rightarrow -it$, we transform the system such that forward in $t$, is backward in imaginary time, (6.15) then becomes

$$\psi(r, t) = \sum_n c_n e^{-E_n t} \psi_n(r).$$

(6.16)

The coefficients are growing (or decaying) exponentially in $t$, therefore, in the $t \rightarrow \infty$ limit, the wavefunction reduces to

$$\psi(r, t) \approx c_0 e^{-E_0 t} \psi_0(r),$$

(6.17)

as the lowest eigen-energy state grows the fastest (if it is negative), or decays the slowest (if it is positive). The method is best employed iteratively, normalising after each step to avoid infinities. The step size of the imaginary-time propagations is restricted by the numerical accuracy of the propagator.

Performing the iterations also allows us to solve non-linear eigen-systems. At each step, the non-linear potential is linearised, and the linear propagation completed. As the ground-state is approached, the inaccuracy introduced by the linearisation becomes more important, and so smaller and smaller steps must be taken to improve accuracy. For severe non-linearities, this is an issue as the number of steps required may be prohibitive. The non-linear method will not necessarily find the global ground-state, but will find a local energy minimum. However, this is true for all non-linear methods.

### 6.4 Steepest-Descent Method

The Steepest-Descent (SD) method is one of the more intuitive non-linear minimising methods. Its main advantage is that one can easily visualise what is occurring. Our set of $n$ sample points $\{\psi_k\}$, we treat as spatial coordinates $x$, in an $n$-dimensional space, and the energy functional for each configuration is visualised as the elevation of a surface in that space, $f(x)$. Given a starting position, $x_0$, we first find the SD direction at this point

$$g_0 = -\nabla f(x_0).$$

(6.18)

Then, searching along a line in the SD direction, through the start position,

$$x_1 = x_0 + \epsilon_0 g_0,$$

(6.19)

we find the first minimum. We repeat this process until the updated position is within a tolerable distance from the last. Intuitively we can see that always proceeding "down-hill" in this manner, we must arrive at the local minimum.
The SD method runs into some trouble when navigating along a long narrow valley, one might hope that, from a start point on the lip of the valley, the first step will find a point on the bottom of the valley, and the next will find the local minimum along the valley. However, the minimum along the SD direction from the start point is the point where this line meets the iso-contours of $f(x)$ at a tangent. The next SD direction will be perpendicular to the last, as it is also perpendicular to the contours. And so on. The result is that the algorithm will be forced to take many small steps as it zig-zags down towards the minimum.

6.5 The Conjugate-Gradient Method

The Conjugate-Gradient (CG) method is most efficient when the function to minimise is approximately a quadratic form,

$$f(x) \approx c - b^T x + \frac{1}{2} x^T A x,$$

(6.20)

where $A$ is a positive definite matrix. The vectors $u$ and $v$ are considered to be conjugate with respect to $A$ if they satisfy

$$u^T A v = 0.$$  

(6.21)

Conjugacy is the analogue of orthogonality with an inner product based on $A$ instead of the identity matrix.

Minimising $f(x)$ is equivalent to solving $\nabla f(x) = A x - b = 0$. The idea of the CG method is to expand $x$ in a basis constructed from mutually conjugate vectors, $\{p_k\}$, i.e.

$$x = \sum_j \alpha_j p_j.$$  

(6.22)

Therefore

$$p_k^T b = \sum_j \alpha_j p_k^T A p_j = \alpha_k p_k^T A p_k,$$

(6.23)

and so

$$\alpha_k = \frac{p_k^T b}{p_k^T A p_k}.$$  

(6.24)

As an iterative method, we can build up the solution successively as $x_{k+1} = x_k + \alpha_k p_k$. The basis vectors are generated in a Gram-Schmidt orthogonalisation-like process that may be performed in a number of equivalent ways. The resulting recursion relation has the form

$$p_{k+1} = g_{k+1} + \beta_k p_k,$$

(6.25)
and in the Fletcher-Reeves derivation, the $\beta$ are given by

$$ \beta_{k}^{\text{FR}} = \frac{g_{k+1}^T g_{k+1}}{g_{k}^T g_{k}}. $$

(6.26)

The generating vectors are chosen to be $g_{k} = -\nabla f(x_{k})$, the SD direction. If $f(x)$ is the exact equation, the CG method will find the solution in $n$ steps, where $n$ is the number of elements in $x$.

In the case where $f(x)$ is not exact, as in the non-linear functions we are interested in, we do not have direct knowledge of $A$ and $b$. We modify the method to handle this by using the conjugate basis vectors as search directions as in the SD method, and the coefficients, $\alpha_{k}$, are found by minimising $f(x)$ along the line through $x_{k}$ in the direction of $p_{k}$. We also alter the $\beta$ to that of the Polak-Ribiére revision, and set $\beta_{k} = \max[0, \beta_{k}^{\text{PR}}]$, where

$$ \beta_{k}^{\text{PR}} = \frac{g_{k+1}^T (g_{k+1} - g_{k})}{g_{k}^T g_{k}}. $$

(6.27)

This has the advantage of resetting the CG algorithm when numerical error grows to the point where it hinders the conjugation process.

The full non-linear conjugate-gradient method we employ is summarised as:

Given an initial guess $x_{0}$, set $p_{0} = g_{0} = -\nabla f(x_{0})$.

From $k = 0$, iterate over:

- Find $\alpha_{k}$ that minimises $f(x_{k} + \alpha_{k} p_{k})$.
- Calculate $\beta_{k}$.
- Update $x_{k+1} = x_{k} + \alpha_{k} p_{k}$, $g_{k+1} = -\nabla f(x_{k+1})$, and $p_{k+1} = g_{k+1} + \beta_{k} p_{k}$.
- Break if $|g_{k+1}|^2 < \text{tol}$.

Each iteration only requires one evaluation of the functions derivative, and one line minimisation. Its cost is only slightly more than the SD method, however, the number of steps required is vastly reduced.

Whereas the ITP method slowed down as it approached the ground-state and more accuracy is required, the function $f(x)$ becomes more quadratic as it approaches a minimum, and hence, the CG method accelerates to the solution. However, it requires the calculation of the second derivative, or at least an approximation of it, in order to perform the line minimisations. This makes it a lot more difficult to implement than the ITP method.

For a more complete review of the CG method, and explicit example algorithms, see [83].
6.6 The Discrete Hankel Transform

The problems we will work on all involve a 2D geometry with cylindrically symmetric trapping potentials. We expect to apply the Laplacian operator as well as performing Fourier transforms on the functions, and we must have some efficient discretisation scheme. In cylindrical coordinates, the 2D Fourier transform of a circularly symmetric function

$$F(k) = \int_0^\infty f(r)J_0(kr)rdr,$$  \hspace{1cm} (6.28)

is simply the 0th-order Hankel transform. The $\nu$th-order Hankel transform is defined as

$$\tilde{f}_\nu(k) = \mathcal{H}_\nu\{f(r)\}(k) = \int_0^\infty f(r)J_\nu(kr)rdr,$$  \hspace{1cm} (6.29)

where $J_\nu(z)$ is the $\nu$th-order Bessel function of the first kind. Simply switching $k$ and $r$ in (6.29) gives the inverse transform.

If the function $f(r)$ is effectively zero for $r \geq R$ and its Hankel transform, $\tilde{f}_\nu(k)$, is effectively zero for $k \geq K$, then we can sample the integrals at the quadrature points

$$r_n = j_{\nu n}/K, \quad n = 0, 1, 2, \ldots$$  \hspace{1cm} (6.30)

$$k_m = j_{\nu m}/R, \quad m = 0, 1, 2, \ldots$$  \hspace{1cm} (6.31)

where the $j_{\nu n}$ are the solutions of $J_\nu(j_{\nu n}) = 0$. Then (6.29) is very well approximated [81, 84] by

$$\tilde{f}_\nu(k_m) \simeq \frac{2}{K^2} \sum_{n=0}^{M-1} \frac{f(r_n)}{J_{\nu+1}(j_{\nu n})^2} J_\nu \left( j_{\nu n} j_{\nu m} \frac{R}{K} \right).$$  \hspace{1cm} (6.32)

This approximation can be derived by expanding $f(r)$ in a truncated Fourier-Bessel series, inserting this into (6.29) and evaluating at the quadrature points. Imposing the boundary conditions $f(R) = \tilde{f}(K) = 0$ requires that $RK = j_{\nu M}$. The inverse transform is, again, found simply by switching the roles of $r$ and $k$.

A well known identity,

$$-\nabla^2 f(r) = \mathcal{H}_0\{k^2 \tilde{f}_0(k)\}(r),$$  \hspace{1cm} (6.33)

gives us a convenient method to apply the Laplacian operator, allowing us to write an $M$ point discretised approximation to the Laplacian operation on a circularly symmetric function,

$$[-\nabla^2 f(r)]_n = \sum_{l=0}^{M-1} D_{nl} f(r_l)$$  \hspace{1cm} (6.34)

$$D_{nl} = \frac{4}{R^2} \sum_{m=0}^{M-1} k_m^2 \frac{J_0(j_m j_l/j_M)J_0(j_m j_l/j_M)}{J_1(j_m)^2J_1(j_l)^2}.$$  \hspace{1cm} (6.35)
The extension to non-symmetric functions is trivial, however, it requires interpolating between different order grids, and so is avoided in this work.

The discretisation scheme also provides a convenient quadrature scheme found by evaluating (6.32) at $k = 0$ [81, 85]. It can immediately be seen that (6.29) evaluated with $\nu = 0$ at $k = 0$ recovers the spatial integral in cylindrical coordinates. Thus we have

$$\int_0^R f(r)rdr \simeq \frac{2R^2}{j_M^2} \sum_{n=0}^{M-1} \frac{f(r_n)}{J_1(j_n)^2}. \quad (6.36)$$
Chapter 7

Thomas-Fermi-von-Weizsacker Theory

7.1 The Local Density Approximation

In the general case, the KS scheme requires solving (5.10), a set of $N$ self-consistent equations. This can be very computationally expensive. To reduce this one can attempt to construct an explicit definition for the kinetic energy functional in terms of density alone, this orbital-free DFT is more in keeping with the true spirit of DFT. As the explicit definition of the kinetic energy functional is not known, approximations of its true form must be made.

The most basic approximation for the construction of an explicit kinetic energy functional is the so-called local-density approximation (LDA). In this approximation, the local kinetic energy for an inhomogeneous system is assumed to be the same as that of a uniform system. This assumption is most accurate in systems where the external potential is only slowly varying.

The LDA for a degenerate 2D fermi gas results in the Thomas-Fermi (TF) energy functional

$$T_{\text{TF}}[\rho] = C_2 \int d\mathbf{r} \rho^2(\mathbf{r}),$$

where $C_2 = \frac{\pi}{2}$ for a spin-degenerate Fermi gas, or $C_2 = \pi$ for a spin-polarised Fermi gas (in atomic units).

The variational minimisation of the total energy functional in the LDA, under the normalisation constraint (Eq. 5.12), results in

$$\rho_{\text{TF}}(\mathbf{r}) = \begin{cases} \frac{1}{2C_2} (\mu_{TF} - v_{\text{ext}}(\mathbf{r})) & , v_{\text{ext}}(\mathbf{r}) < \mu_{TF} \\ 0 & , v_{\text{ext}}(\mathbf{r}) \geq \mu_{TF} \end{cases}$$

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where $\mu_{TF}$ is a Lagrange multiplier, determined by the normalisation condition. This results in an unphysical cusp in the density on the boundary defined by $v_{\text{ext}}(r) = \mu_{TF}$.

In particular, we look at a spin-polarised Fermi gas in a 2D harmonic potential

$$v_{\text{ext}}(r) = \frac{1}{2} r^2,$$  

(7.3)

in cylindrical coordinates and harmonic length units ($l_{\text{osc}} = \sqrt{\hbar/m\omega}$). The Thomas-Fermi ground-state is then given by

$$\rho_{TF}(r) = \begin{cases} \frac{(R^2-r^2)}{4\pi}, & r < R \\ 0, & r \geq R \end{cases},$$  

(7.4)

where $R = (8N)^{\frac{1}{4}}$.

### 7.2 The Thomas-Fermi-von Weizsäcker Scheme

We can improve on the LDA by introducing local gradient corrections to smooth the cusp. The simplest gradient correction takes the form of the von-Weizsäcker (vW) energy functional [86]

$$T_{\text{vW}}[\rho] = \frac{1}{8} \int dr \frac{|\nabla \rho(r)|^2}{\rho(r)}.$$  

(7.5)

Higher order gradient terms may be added but are not guaranteed to improve the result, and may even harm it [87].

The total energy functional for the Thomas-Fermi-von Weizsäcker (TFvW) scheme is given as

$$E[\rho] = \int dr \left[ C_2 \rho(r)^2 + \lambda_{\text{vW}} \frac{1}{8} \frac{|\nabla \rho(r)|^2}{\rho(r)} + v_{\text{ext}}(r)\rho(r) \right] + E_{\text{int}}[\rho],$$  

(7.6)

where $\lambda_{\text{vW}}$ is the vW parameter, which may be tuned to get the best agreement with the KS orbital calculation.

We are interested in employing the TFvW scheme for a 2D harmonically trapped, spin-polarised Fermi gas. To do this we employ the CG method to find the ground state for each trial $\lambda_{\text{vW}}$; the equations for the line minimisations involved in the CG method are explicitly stated in Appendix A. A simple ‘golden ratio’ line minimiser will find the ground-state energy closest to the exact energy from (5.15), by varying $\lambda_{\text{vW}}$. This results in the points plotted in Fig. 7.1, where we have also fitted it to the equation $\lambda_{\text{vW}} = \lambda_{\text{vW}}^\infty + a/N^b$. This implies that there is a non-zero limiting value as $N \to \infty$. 

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In Fig. 7.2 we show the ground-state calculated via the TFvW method for a few $N$ values, and in Fig. 7.3 we directly compare the exact density and the TF density for $N = 10^3$. The TF solution is very close to the exact result for $r \ll R$, however, the sharp cusp at $r = R$ is very different to the qualitative behaviour of the exact density. The TFvW density, in contrast, has the same exponentially decaying tail that the exact result does, however, neither result captures the density oscillations at low $r$. Both results get closer to the exact result as $N \to \infty$, as the density oscillations become relatively weaker and the density decays to zero much more sharply after $r = R$.

![Graph showing the von Weizsäcker parameter $\lambda_{vW}$ (Dots) vs. the logarithm of the number of particles $N$. Best fit (line) to the equation $\lambda_{vW} = \lambda_{\infty}^{vW} + a/N^b$ with $\lambda_{\infty}^{vW} = 0.0181, a = 0.0594, b = 0.1594$. (This is a reproduction of a figure from [74]).](image)

7.3 TFvW Method for a Spin-Polarised Dipolar Fermi Gas

So far in this thesis we have restricted our study to short range interactions. For dilute bosons in the low energy regime this eliminated all interactions except for the s-wave scattering, which took the form of a delta function pseudopotential in the interaction potential. Fermions, which must obey the Pauli exchange principle, are forbidden to
Figure 7.2: Ground-state density vs. radial distance for a 2D spin-polarised fermi gas calculated using the TFvW method.

Figure 7.3: The exact ground-state density (green), the TFvW ground-state (blue), and the TF ground-state (red) vs. radial coordinate for a spin-polarised fermi gas with $N = 1000$ particles, where $R \approx 9.4574$. 
interact on the s-wave scattering channel. The lowest allowed channel is the d-wave, which is frozen out at low enough collision energy.

For a typical gas of neutral atoms, the dominant interaction is due to van der Waals forces. Reducing the density and temperature of the gas will eliminate such long-range interactions and bring it into the short-range interaction regime [88]. However, this is not always the case. Some atoms exhibit strong magnetic dipoles that remain significant even in the low energy regime. Chromium has a particularly large magnetic dipole moment of $6\mu_b$, where $\mu_b$ is the Bohr magneton.

Molecular gases can also exhibit electric dipoles that are much stronger than their magnetic analogues [89]. With typical electric dipole strengths on the order of a Debye, molecular dipoles can provide the equivalent of a magnetic dipole strength on the order of $100\mu_b$. Observing the effects of interest in the dipolar gas requires a BEC or degenerate Fermi gas. However, the usual method of laser cooling is significantly harder due to the much more complex spectral properties of the molecules [90–92], and the obtained temperatures are still orders of magnitude above degeneracy [93]. A promising alternative involves cooling the component elements first and then using laser assisted collisions to chemically bond them into molecules [94–96], the difficulty then is to avoid dumping the released chemical bond energy into the thermal cloud.

We will write the formalism for magnetic dipoles, as the electric dipole formalism is directly equivalent. If all the dipoles in the gas are aligned to the $z$-axis by an external field, then the potential field felt by a dipole at the origin due to a dipole at $r$ (see Fig. 7.4) is given by

$$V_{dd}(r) = \frac{\mu_0 \mu^2}{4\pi r^3} \left( 1 - \frac{3\cos^2 \theta}{r^3} \right),$$

where $\theta$ is the angle between $r$ and the $z$-axis, and $\mu$ is the magnitude of the dipole moment of each particle. In the pseudo-2D system, where the $z$-direction is frozen out by a strong harmonic trap, the angle is effectively always $\theta = \pi/2$ and the dipole potential is given by

$$V_{dd}(r) = \frac{\mu_0 \mu^2}{4\pi r^3}.$$  

(7.8)

The dipole interaction energy functional is formed from the sum of the pairwise interaction energies given as

$$E_{dd} = \frac{1}{2} \sum_{kk'} \rho_k \rho_{k'} \left( \langle kk' | V_{dd} | kk' \rangle - \langle kk' | V_{dd} | k' k \rangle \right).$$

(7.9)

The first term is the direct interaction, and the second term is the exchange interaction. In contrast to the 3D system, where both these terms are finite, in the pseudo-2D system they are separately infinite, however, the sum of the two terms remains finite.
Fang and Englert [98] use the LDA assumptions to derive the result

\[ E_{dd} = E_{dd}^{(1)} + E_{dd}^{(2)}, \]  

(7.10)

where

\[ E_{dd}^{(1)} = \frac{\mu_0 \mu^2}{4\pi} \frac{256}{45} \sqrt{\pi} \int dr \rho(r)^{5/2}, \]  

(7.11)

\[ E_{dd}^{(2)} = -\frac{\mu_0 \mu^2}{4\pi} \pi \int dr \rho(r)\sqrt{-\nabla^2 \rho(r)}. \]  

(7.12)

These terms do not correspond to the direct and exchange contributions. The second term scales with particle number, \( N \), as \( N^{-1/2} \), so may be discarded under the assumption that \( N \gg 1 \).

Alternative derivations of (7.10) have been published by Bruun and Taylor [99] and van Zyl and Zaremba [74], of which, this work is an extension.

In particular van Zyl and Zaremba suggest that the interaction energy functional in the LDA can be defined as

\[ E^{\text{LDA}}_{dd}[\rho] = \frac{2}{5} C_{dd} \int dr \rho(r)^{5/2}, \]  

(7.13)

where \( C_{dd} = 32\mu_0 \mu^2/9\sqrt{\pi} \).

Our approximation of the total energy functional for a spin-polarised, dipolar, 2D Fermi gas in a cylindrically symmetric potential, is given by

\[ E[\rho] = \int dr \left[ \pi \rho(r)^2 + \lambda_{\text{W}} \frac{1}{8} \frac{|\nabla \rho(r)|^2}{\rho(r)} + \frac{1}{2} r^2 \rho(r) + \frac{2}{5} C_{dd} \rho(r)^{5/2} \right], \]  

(7.14)
which leads to the equilibrium condition

\[-\lambda vW \nabla^2 \psi + \frac{1}{2} \mu^2 \psi + 2\pi \psi^3 + C_{dd} \psi^4 = \mu \psi.\]  

(7.15)

We employ the CG method as before except that the equation to be solved for the line minimisations is a radical function and more care must be taken. The details are in Appendix A. In addition, the wavefunction tends to drift to negative values if care is not taken to keep it strictly positive. This is achieved simply by changing one of the factors of \( \psi \) in the dipole interaction term in to \( |\psi| \).

In Fig. 7.5, we have plotted a selection of the ground-state densities, calculated via the TFvW method, for a gas with \( N = 1000 \) particles. The effect of the dipole interaction, is to stretch the profile of the density in the radial direction. In the full 3D view, the pancake shape of the gas would appear to get flatter and wider. In the \( C_{dd} \rightarrow 0 \) limit, the point after which the density rapidly decays to zero is the TF radius, \( R = (8N)^{\frac{3}{4}} \). In the opposite (\( C_{dd} \rightarrow \infty \)) limit, this point is instead

\[ R = \left( \frac{5N}{3\pi} \right)^{\frac{3}{10}} (2C_{dd})^{\frac{1}{5}}, \]  

(7.16)

which we will prove in a later section.

7.3.1 Benchmark of Numerical Methods

In the ‘Numerical Minimisation’ section we described three methods for finding the ground-state of a non-linear eigen-system. We have implemented all three methods for solving the TFvW eigen-equation for the 2D spin-polarised dipolar Fermi gas.

The ITP method is a variation of the RKDS method from Part I of this thesis. The step size is set by trial-and-error for each configuration to be the largest multiple of 10 that reaches convergence. This depends on the size of the non-linearity, i.e. \( N \) and \( C_{dd} \), but is insensitive to grid size \( M \). Each iteration of the ITP method is roughly equivalent to 12 function evaluations of the CG method. The CG method requires 1 function evaluation to obtain the search direction and the equivalent of 6 in the polynomial line minimiser. Therefore, the cost of each iteration is roughly the same for both.

The SD method uses the same code as the CG method, but with the SD direction used instead of the CG direction at each iteration.

In Table 7.1 we have displayed the number of iterations and the computation time (excluding the precalculation of the DHT coefficients etc...) when performed on a
Figure 7.5: The ground-state density vs. radius in a 2D spin-polarised dipolar Fermi gas with \( N = 1000 \) particles, calculated via the TFvW method. The parameter \( C_{dd} \) indicates the dipole interaction strength.

3.2GHz Intel processor. The grid size for this data is small \( M = 100 \), and so all of the methods can easily complete the calculation in a reasonable time. Even so, the CG method is 2 orders of magnitude quicker than the other methods.

The cost of each method is shown most clearly by the number of iterations required to achieve convergence. The ITP method performs well for low particle numbers, where the non-linear TF and dipole terms are small, however at large particle numbers it quickly grows to an unacceptably high cost. The SD method has a comparable cost at low particle numbers, but is a marked improvement at the highest particle number. The CG method, on the other hand, always out-performs the other two methods. The cost of the CG method grows by less than 600% over 4 orders of magnitude.

If the ITP method has any advantage over the SD and CG methods, it is that it is insensitive to the grid size, as seen in Table 7.2. The cost of each iteration grows with grid size, however, the number of iterations remains the same. The ITP method is effectively minimising the total energy by varying the coefficients of the linear part’s eigen-basis. The number of occupied basis-states does not depend on the grid and so the number of iterations remains constant as the grid size is increased.

The SD method minimises by varying the \( M \) elements and so is expected to search
Table 7.1: Numerical performance, at different particle numbers $N$, of the implemented Thomas-Fermi-von Weizsäcker ground-state finder using an imaginary-time propagation (ITP), steepest-descent (SD), and conjugate-gradient (CG) non-linear minimiser. Dipole interaction strength $C_{dd} = 10$, von Weizsäcker parameter $\lambda_{vW} = 0.05$, grid size $M = 100$, and convergence condition $||\nabla \psi||^2 \leq 10^{-10}N$. The ‘time’ is for the iterative part of the algorithm, excluding any precalculations, performed on a 3.2GHz Intel processor.

<table>
<thead>
<tr>
<th>$N$</th>
<th>ITP iter. time</th>
<th>SD iter. time</th>
<th>CG iter. time</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^1$</td>
<td>680 0.29</td>
<td>413 0.069</td>
<td>65 0.012</td>
</tr>
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<td>$10^2$</td>
<td>2420 1.0</td>
<td>444 0.069</td>
<td>71 0.012</td>
</tr>
<tr>
<td>$10^3$</td>
<td>7720 3.3</td>
<td>1089 0.16</td>
<td>110 0.019</td>
</tr>
<tr>
<td>$10^4$</td>
<td>19780 8.4</td>
<td>4185 0.62</td>
<td>219 0.035</td>
</tr>
<tr>
<td>$10^5$</td>
<td>67300 29</td>
<td>16611 2.6</td>
<td>387 0.063</td>
</tr>
</tbody>
</table>

Table 7.2: Numerical performance, at different grid sizes $M$, of the implemented Thomas-Fermi-von Weizsäcker ground-state finder using an imaginary-time propagation (ITP), steepest-descent (SD), and conjugate-gradient (CG) non-linear minimiser. Dipole interaction strength $C_{dd} = 10$, particle number $N = 10^3$, von Weizsäcker parameter $\lambda_{vW} = 0.05$, and convergence condition $||\nabla \psi||^2 \leq 10^{-10}N$. The ‘time’ is for the iterative part of the algorithm, excluding any precalculations, performed on a 3.2GHz Intel processor.

<table>
<thead>
<tr>
<th>$M$</th>
<th>ITP iter. time</th>
<th>SD iter. time</th>
<th>CG iter. time</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>7720 3.3</td>
<td>1089 0.16</td>
<td>110 0.019</td>
</tr>
<tr>
<td>200</td>
<td>7740 13</td>
<td>1255 0.30</td>
<td>118 0.030</td>
</tr>
<tr>
<td>300</td>
<td>7740 30</td>
<td>1537 0.57</td>
<td>158 0.062</td>
</tr>
<tr>
<td>500</td>
<td>7740 90</td>
<td>2449 2.0</td>
<td>189 0.16</td>
</tr>
<tr>
<td>1000</td>
<td>7740 380</td>
<td>6357 19</td>
<td>271 0.81</td>
</tr>
</tbody>
</table>

at least $M$ directions. Therefore, the number of iterations increases with the number of grid points, but even for the larger grid it outperforms the ITP method.

The CG method, with its smarter choice of search directions, drastically reduces the number of iterations required. The number required is still dependent on the grid
size, but to a much lesser degree.

The true benefit of the CG method is seen when you extrapolate these benchmarks to the maximum particle numbers, dipole strengths, and grid sizes required in the next few sections. The maximum we calculate uses $N = 10^5$, $C_{dd} = 100$, and $M = 2000$. The CG method performs these in a few minutes, whereas we expect that the ITP method would require hours.

In addition to this, we need to find the optimum vW parameter, which we do via a golden mean minimiser requiring $\sim 5$ separate minimisations. The algorithm will then be run over hundreds of different particle number and dipole strength settings.

### 7.3.2 Hydrodynamic Collective Mode Oscillations

An important property of any system or material is its reaction to external stimuli. In particular the reaction of a system in its ground-state to small perturbations in the external potential exciting collective mode oscillations. The lowest lying collective modes, such as the dipole mode (also known as the Kohn mode [100]), that is the collective oscillation of the gases centre-of-mass, and the breathing mode, the cylindrically symmetric bunching and spreading oscillation of the gas, are readily measurable in cold-atom systems, and so provide a powerful and convenient tool for directly comparing theory to empirical results.

In our highly degenerate Fermi system, Pauli exclusion suppresses the elastic collisions and hence this regime is known as the collisionless regime. The collective oscillations remain undamped in this regime. As the temperature is raised, the collisions may no longer be ignored and the collective modes become damped. However, if the collisions occur much more often than the typical timescale of the collective oscillations (dependent on the trap frequency), then the gas will remain, locally, in equilibrium and the system enters the hydrodynamic (HD) regime. The collective modes are again dissipationless in the HD regime. Babadi and Demler [101] suggest that if the system obeys the condition

$$N \left( \frac{a_{dd}}{a_{ho}} \right)^2 \gg 1, \quad (7.17)$$

then it is in the HD regime. In the above equation we have introduced, $a_{dd} = \mu_0 D^2 M / (4\pi\hbar^2)$, the dipole interaction length, and $a_{ho}$, the harmonic oscillator length. As an example, if we take the value $\omega_0 = 2\pi \times 1500$ Hz which gives $(a_{dd}/a_{ho})^2 \approx 10^{-2}$ for $^{161}$Dy, then we are in the HD regime for $N \gtrsim 10^3$.

The dynamics in the HD regime are determined by the HD equations of differential
mass, energy, and momentum conservation. The HD equations (in atomic units) are

\[ \dot{\rho} + \nabla \cdot (\rho \mathbf{v}) = 0 \] (7.18)
\[ \dot{\mathbf{v}} + \mathbf{v} \cdot \nabla \mathbf{v} = \mathbf{F} \] (7.19)

where the dot indicates the derivative w.r.t. time and the gradient is w.r.t. \( \mathbf{r} \).

From the equilibrium equation (7.15), we define the force as

\[ \mathbf{F} = -\nabla \left[ -\frac{\lambda_{vW}}{2} \frac{\nabla^2 \psi}{\psi} + \frac{1}{2} r^2 + 2\pi \psi^2 + C_{dd} \psi^3 \right]. \] (7.20)

We are only interested in small displacements from the equilibrium state, so we expand the equations in a Taylor expansion in \( \delta \rho \) about \( \rho_0 \), and discard the terms beyond first order, noting that as \( \rho_0 \) is an equilibrium state, \( \dot{\rho}_0 = 0 \). The linearised HD equations are then

\[ \dot{\delta \rho} + \nabla \cdot (\rho_0 \mathbf{v}) = 0, \] (7.21)
\[ \dot{\mathbf{v}} = \delta \mathbf{F} = -\nabla f, \] (7.22)

where

\[ f = \left( 4\pi \psi_0 + 3C_{dd} \psi_0^2 + \frac{1}{\psi_0} \hat{h} \right) \delta \psi, \] (7.23)

with

\[ \hat{h} = -\frac{\lambda_{vW}}{2} \nabla^2 + \frac{1}{2} r^2 + 2\pi \psi_0^2 + C_{dd} \psi_0^3 - \mu. \] (7.24)

Taking the time derivative of (7.21) and combining with (7.22) leads to the eigen-equation

\[ \omega^2 \delta \psi + \frac{1}{2\psi_0} \nabla \cdot (\psi_0^2 \nabla f) = 0, \] (7.25)

where the eigen-frequency, \( \omega \), is scaled by the harmonic oscillator frequency, \( \omega_0 \).

Using the orthogonal basis formed from the solutions of

\[ \hat{h} \phi_j = \epsilon_j \phi_j, \] (7.26)

where \( \int d\mathbf{r} \phi_j^* \phi_l = \delta_{jl} \), we expand the mode wave-functions via

\[ \delta \psi = \sum_j c_j \phi_j, \] (7.27)

and the eigenvalue problem (7.25) reduces to

\[ \omega^2 c_j = \frac{\epsilon_j}{\lambda_{vW}} \sum_j M_{jl} c_j, \] (7.28)
where
\[ M_{jl} = \int d^3r \phi_j^* (4\pi \psi_0^4 + 3C_{dd} \psi_0^4 + \epsilon_j) \phi_l. \] (7.29)

From the circular symmetry of our problem we have \( \phi_j(r) \to \phi_j(r)e^{im\theta} \), and the Laplace operator evaluates as
\[ -\nabla^2 (\phi_j(r)e^{im\theta}) = \left( -\nabla^2 \phi_j(r) + m^2 r^2 \phi_j(r) \right)e^{im\theta}, \] (7.30)
allowing (7.26) to be discretised using (6.34) and solved using MATLAB’s eigenvalue packages. \( M_{jl} \) is then block diagonal for each \( m \).

The linear basis is infinite, however, if we truncate the basis at \( k_{\text{max}} \) and solve (7.28) via MATLAB, then we observe that the frequencies converge for large enough \( k_{\text{max}} \). This is because the basis state occupancies \( \{|c_j|^2\} \) decay exponentially with state number as observed in Fig. 7.6 and hence the contribution from states beyond the cut-off is negligible. The decay rate is smaller for systems with more particles or larger interaction energy, and hence, more basis states are required for these, however, the most difficult system that we calculate requires only \( k_{\text{max}} \approx 2000 \). MATLAB can easily solve eigen-problems of this size so we use this truncation for all the calculations.

In Fig. 7.7, Fig. 7.8, and Fig. 7.9, we have plotted the first 3 angular modes \((m)\) for the first 3 radial modes \((n)\). Note that the \((m, n) = (0, 0)\) mode is the ground-state, \( \rho_0 \), and so, is excluded.

All modes have a sharp peak near \( r = R \), this is the place where the ground-state is quickly decaying to zero. Succeeding angular states get sharper and sharper peaks at \( r = R \), as \( m \) increases.

The \( m = 0 \) modes have \( n \) nodes, plus one at infinity, and have an anti-node at \( r = 0 \). The \( m > 0 \) modes have a node at \( r = 0 \), and therefore have \( n + 1 \) nodes, plus one at infinity.

Increasing the dipole strength, \( C_{dd} \), stretches out the modes radially, as it did the ground-state density, however, it also increases the sharpness of the peak, which we expect will increase the frequency of the mode. Increasing the number of particles, \( N \), will have a similar effect.

The frequencies of the \( n = 0 \) modes, Fig. 7.10, are all fairly constant w.r.t. \( C_{dd} \), and seem to follow the rule \( \omega_{(m,0)} = \sqrt{m} \). However, on closer inspection this is only the case for the dipole mode \((m = 1)\). We will prove this analytically in the next section. The higher states start at a slightly higher frequency and rapidly decay to their asymptotic values as dipole strength increases. The quadrupole mode \((m = 2)\) is hard to see as the dispersion is on the order of the numerical error, however, in Fig. 7.11 we show a
zoom in on the $m = 6$, $n = 0$ mode where it can clearly be seen. This effect is more pronounced for low particle number, $N$, where the vW term has more importance.

All the higher order modes, Fig. 7.12 and Fig. 7.13, have a frequency that increases to their asymptote as dipole strength increases.

Figure 7.6: The basis state occupancy (logarithmic) vs. basis state number for the Kohn mode of the (blue) $N = 10^3$, $C_{dd} = 0$ and (green) $N = 10^5$, $C_{dd} = 100$ systems.
Figure 7.7: The first 3, $n = 0$ collective mode densities for a spin-polarised, fermi gas ($C_{dd} = 0$) with $N = 1000$ particles. The naming convention in the legend is $(m, n)$.

Figure 7.8: The first 3, $n = 1$ collective mode densities for a spin-polarised, fermi gas ($C_{dd} = 0$) with $N = 1000$ particles. The naming convention in the legend is $(m, n)$. 
Figure 7.9: The first 3, $n = 2$ collective mode densities for a spin-polarised, fermi gas ($C_{dd} = 0$) with $N = 1000$ particles. The naming convention in the legend is $(m,n)$.

Figure 7.10: The $n = 0$ collective mode angular frequencies for a spin-polarised, dipole, fermi gas with $N = 1000$ particles vs. dipole interaction strength. The naming convention in the labels is $(m,n)$.
Figure 7.11: The $m = 6$, $n = 0$ collective mode angular frequencies for a spin-polarised, dipole, fermi gas with $N = 1000$ particles vs. dipole interaction strength.

Figure 7.12: The $n = 1$ collective mode angular frequencies for a spin-polarised, dipole, fermi gas with $N = 1000$ particles vs. dipole interaction strength. The naming convention in the labels is $(m,n)$. 
Figure 7.13: The $n = 2$ collective mode angular frequencies for a spin-polarised, dipole, fermi gas with $N = 1000$ particles vs. dipole interaction strength. The naming convention in the labels is $(m, n)$. 
7.3.3 The Dipole Mode

The first excited mode \((n = 0, m = 1)\), is the dipole mode, also known as the Kohn mode [100]. It is of particular interest as it can be proven to be independent of the particle interactions in a harmonic trap. The dipole mode is characterised by a sloshing motion, where the centre-of-mass of the gas oscillates in the trap, while the profile of the gas remains constant relative to it. The constant profile is what makes the interaction energy constant, and hence, the dipole state is purely an oscillation between the translational kinetic energy of the centre of mass and the potential energy of the trap.

We are looking for a solution of the form

\[
\rho(r, t) = \rho_0(r'(t)),
\]

where \(r'(t) = r - \eta(t)\) and \(\eta(t)\) is the centre-of-mass vector. The force on the gas is then

\[
F(r, t) = -\nabla \left[ -\frac{\lambda_{W}}{2} \frac{\nabla^2 \psi(r, t)}{\psi(r, t)} + \frac{1}{2} r^2 + 2\pi \psi(r, t)^2 + C_{dd} \psi(r, t)^3 \right]
\]

\[
= F_0(r') + \nabla \left[ \frac{1}{2} (r')^2 - \frac{1}{2} r^2 \right],
\]

\[
= -\eta(t) = \dot{v},
\]

since, by definition, the force on the equilibrium state is zero, i.e. \(F_0(r') = 0\).

From the continuity equation we get

\[
\dot{\rho}(v, t) + \nabla \cdot (\rho(r, t)v) = \nabla \cdot \rho_0(r') \cdot \dot{r}' + \nabla \rho_0(r') \cdot v
\]

\[
= \nabla \rho_0(r') \cdot (v - \dot{\eta})
\]

\[
= 0,
\]

since \(v\) must be independent of position. This is true for all \(r\), hence, \(v = \dot{\eta}\). Combining this with (7.32) we get the ODE

\[
\ddot{\eta} = \dot{v} = -\eta,
\]

which has the real solution \(\eta(t) = \cos(t)\eta_0\). Hence, the angular frequency of the dipole mode is \(\omega = 1\), which can clearly be observed in the numerical results in Fig. 7.10. Furthermore, if we expand \(\rho(r, t)\) in a Taylor series in \(\eta\) about \(r\), we get

\[
\rho(r, t) = \rho_0(r) - \nabla \rho_0(r) \cdot \eta + \ldots
\]

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and therefore,
\[ \delta \rho(r, t) = \rho(r, t) - \rho_0 = - \cos(t) \rho_0 \mathbf{r} \cdot \eta_0. \] (7.36)

The dipole mode density is proportional to the first derivative of the ground-state. This is a tidy and convenient check for the accuracy of the numerical results, as we indeed see in Fig. 7.14. The ratio of the attained dipole mode to the first derivative of the ground-state is a constant. The large error for \( r > 10 \) is due to the numerical noise introduced by the numerical derivative and dividing two numbers that are extremely small.

![Figure 7.14](image)

Figure 7.14: The dipole mode density \((m = 1, n = 0)\) divided by the first derivative of the ground-state for a spin-polarised, dipolar, fermi gas with \( N = 1000 \) particles.

Checking the dipole mode is also a common technique in experiments, as it is applicable in a large range of systems and can be used to establish or verify the time or frequency scale of the experiment.

### 7.3.4 Large Dipole Interaction and HD Limits

As stated in (7.17), the HD limit is achieved when the particle number or the dipole interaction strength tends to infinity. In this case the derivative terms in the energy functional become negligible. In our TFvW formulation this can be achieved by simply
setting the vW parameter to zero, and therefore the equilibrium equation is

$$\frac{1}{2}r^2\psi + 2\pi\psi^2 + C_{dd}\psi^3 = \mu\psi. \quad (7.37)$$

In the limiting case of large dipole interactions, where $C_{dd} \gg 2\pi$, the TF term is negligible compared to the dipole term except at the very edge of the cloud in the low density region. The equilibrium equation in the bulk of the cloud is then

$$\frac{1}{2}r^2\psi + C_{dd}\psi^3 = \mu\psi. \quad (7.38)$$

The opposite limiting case is when the dipole interactions are reduced to zero. The particle number must be increased simultaneously, in order that (7.17) is satisfied and the system is still in the HD regime. In this case the equilibrium equation is

$$\frac{1}{2}r^2\psi + 2\pi\psi^2 = \mu\psi. \quad (7.39)$$

In either case we get an equilibrium equation of the form

$$v_{\text{eff}}(r)\psi = \mu\psi, \quad (7.40)$$

with

$$v_{\text{eff}}(r) = \frac{1}{2}r^2 + C_\alpha\psi^\alpha, \quad (7.41)$$

where $\alpha = 2$, $C_2 = 2\pi$ corresponds to the low dipole-interaction regime, and $\alpha = 3$, $C_3 = C_{dd}$ corresponds to the large dipole-interaction regime.

Equation (7.40) has the ground-state solution

$$\psi_0(r) = \begin{cases} \left(\frac{R^2-r^2}{2\pi\alpha}\right)^{\frac{1}{2}}, & r < R, \\ 0, & r \geq R, \end{cases} \quad (7.42)$$

where $R = \sqrt{2\mu}$ is the TF radius and is fixed by normalising the density. Therefore,

$$R = \left(\frac{N}{2\pi} \frac{(4 + 2\alpha)}{\alpha} (2C_\alpha)^{\frac{2}{4+2\alpha}}\right)^{\frac{1}{4+2\alpha}}. \quad (7.43)$$

This is clearly seen in Fig. 7.5, even for intermediate $C_{dd}$, but particularly for larger values where the only deviation is in the extreme low density region, $r \gtrsim R$.

The function $f$ defined in (7.22) is now only made up of the fluctuating effective potential, so is given by

$$f = \alpha C_\alpha\psi^{\alpha-1}\delta\psi. \quad (7.44)$$
If we introduce the ansatz for the mode functions as
\[ \delta \psi(r, \theta) = u(r)e^{im\theta}, \] (7.45)
then the position dependence of the velocity field is given by
\[ \mathbf{v} \propto -\nabla f = x^{\frac{1}{2}(m-1)}(1-x)^{-\frac{1}{2}} \left( m\alpha (1-x)u(x)(\hat{r} + \hat{\theta}) 
- 2(\alpha - 1)u(x)\hat{r} + 2\alpha x(1-x)u'(x)\hat{r} \right), \] (7.46)
where we have introduced \( x = r^2/R^2 \) for convenience. The velocity field must be analytic at \( x = 1 \) (i.e. \( r = R \)) in order that the outgoing particle velocity be zero at the surface of the gas. It can immediately be seen that the \( \theta \)-component of the velocity field is only analytic at \( x = 1 \) if \( u(x) \) takes the form
\[ u(x) = \psi_0(x)^{1-\alpha}y(x), \] (7.47)
and \( y(x) \) is analytic at \( x = 1 \). The velocity field then takes the form
\[ \mathbf{v} \propto x^{\frac{1}{2}(m-1)} \left( my(x)(\hat{r} + \hat{\theta}) + 2xy'(x)\hat{r} \right), \] (7.48)
and the \( r \)-component is also analytic at \( x = 1 \) if \( y'(x) \) is analytic at \( x = 1 \) as well.

Inserting this new ansatz into the eigen-equation (7.25), and rearranging, we arrive at the ODE
\[ x(1-x)y''(x) + \left[ m + 1 - \left( m + \frac{2}{\alpha} + 1 \right)x \right] y'(x) - \frac{m - \omega^2}{\alpha}y(x) = 0, \] (7.49)
which has the form of Gauss’ Hypergeometric Equation
\[ x(1-x)y''(x) + [c - (a + b + 1)x] y'(x) - aby(x) = 0, \] (7.50)
when we specify the constants
\[ a = \frac{m\alpha + 2 + \sqrt{(m\alpha)^2 + 4\alpha\omega^2 + 4}}{2\alpha} \] (7.51)
\[ b = \frac{m\alpha + 2 - \sqrt{(m\alpha)^2 + 4\alpha\omega^2 + 4}}{2\alpha} \] (7.52)
\[ c = m + 1. \] (7.53)

For \( m \geq 0 \), this has only one solution that is finite on \( x \in (0,1) \),
\[ y(x) = _2F_1(a, b, c; x), \] (7.54)
a hypergeometric function. The derivative is

\[ y'(x) = \frac{ab}{c} \, {}_2F_1(a+1, b+1, c+1; x). \]  

(7.55)

Gauss’ Hypergeometric Theorem states that, as \( R\{(c+1) - (a+1) - (b+1)\} = -\frac{2}{\alpha} < 0 \) for \( \alpha > 1 \), then \( y'(x) \) is only analytic at \( x = 1 \) if \( y'(x) \) is polynomial. Therefore, \( y(x) \) must also be polynomial which only occurs if \( a \) or \( b \) is a negative integer. Solving this condition results in the spectrum

\[ \omega_{m,n} = \sqrt{m + \alpha mn + 2n + \alpha n^2}, \]  

(7.56)

which, it should be noted, is independent of the TF radius, \( R \), and the interaction strength, \( C_\alpha \).

For the \( C_{dd} \to 0 \), HD limit, setting \( \alpha = 2 \) results in the spectrum

\[ \omega^K_{m,n} = \sqrt{m + 2mn + 2n + 2n^2}, \]  

(7.57)

and the \( C_{dd} \to \infty \) limit, with \( \alpha = 3 \) has the spectrum

\[ \omega^{dd}_{m,n} = \sqrt{m + 3mn + 2n + 3n^2}. \]  

(7.58)

This matches the rule observed in a previous section for \( n = 0 \). In Fig. 7.15 and Fig. 7.16, we have plotted the limiting values as dashed lines on the \( n = 1 \) and \( n = 2 \) frequency plots shown previously. The analytics agree excellently with the numerically calculated results.

### 7.3.5 The Nodeless Modes

In Fig. 7.17 we have plotted the numerically obtained quadrupole mode \((m = 2, n = 0)\) frequencies for a range of particle numbers. For the lower particle numbers, the frequency starts at a value larger than \( \sqrt{2} \), and decays to \( \sqrt{2} \) as the dipole interaction strength increases. For the larger particle numbers, the starting value is closer to \( \sqrt{2} \) and the decay is much faster. In fact, for \( N \geq 10^3 \) (the previously calculated lower limit for the HD regime), there is hardly any noticeable dispersion in the frequency, and the results for the lower particle numbers do not have an obvious physical meaning. Note that the noisy fluctuation in the results for the higher particle numbers is due to the basis cut-off.

We have established that the Kohn mode has a frequency fixed at \( \omega_{0,1} = 1 \) for any interaction, however, the other \( n = 0 \) modes also appear to be flat in the HD limit.
Figure 7.15: The $n = 1$ collective mode angular frequencies (solid lines) for a spin-polarised, dipole, fermi gas with $N = 1000$ particles vs. dipole interaction strength. Analytically calculated limiting value for $C_{dd} \rightarrow \infty$ (dashed lines). The naming convention in the labels is $(m, n)$.

Figure 7.16: The $n = 1$ collective mode angular frequencies (solid lines) for a spin-polarised, dipole, fermi gas with $N = 1000$ particles vs. dipole interaction strength. Analytically calculated limiting value for $C_{dd} \rightarrow \infty$ (dashed lines). The naming convention in the labels is $(m, n)$.
Figure 7.17: The quadrupole mode angular frequencies for a spin-polarised, dipole, fermi gas vs. dipole interaction strength for a range of particle numbers.

The analytical results above show that the frequency is fixed to $\omega_{m,0} = \sqrt{m}$ in the $C_{dd} \to 0, N \to \infty$ limit and in the $C_{dd} \to \infty$ limit. This fixes the endpoints at $C_{dd} = 0$ and $C_{dd} = 100$ for the $N \geq 10^3$ curves in Fig. 7.17. However, there is no a priori reason why the dispersion is flat in between.

At either endpoint, the mode density of the $n = 0$ modes has the form

$$\delta \rho_{m,0}(r, \theta) = 2\psi_0(r)\delta \psi_{m,0}(r, \theta) = 2\psi_0(r)^2 - \alpha e^{im\theta} r^m$$

which is proportionally independent of $\alpha$. In the interim systems, the non-local energy contributions are still negligible (i.e. $\lambda_{vW} = 0$), therefore the equilibrium condition is

$$\left. \frac{d \epsilon_{\text{loc}}[\rho]}{d \rho} \right|_{\rho = \rho_0} + \frac{1}{2} r^2 = \mu,$$

where $\epsilon_{\text{loc}}[\rho]$ is the local interaction energy functional. By employing (7.59) as an ansatz for the $n = 0$ modes, we get

$$f = \left( \frac{d^2 \epsilon_{\text{loc}}[\rho]}{d \rho^2} \right) \bigg|_{\rho = \rho_0} \delta \rho$$

$$= \frac{d}{dr} \left( \frac{d \epsilon_{\text{loc}}[\rho]}{d \rho} \right) \bigg|_{\rho = \rho_0} e^{im\theta} r^{m-1}$$

$$= -e^{im\theta} r^m$$
which, when inserted into the eigen-equation, (7.25), gives

\[
\omega^2 \delta \rho + \nabla \cdot (\rho_0 f) = \omega^2 \frac{d\rho}{dr} e^{im\theta} r^{m-1} - \rho_0 \nabla^2 (e^{im\theta} r^m) - \nabla \rho_0 \cdot \nabla (e^{im\theta} r^m) = 0,
\]

(7.62)

and hence (7.59) is a solution of (7.25) with the eigen-frequency \(\omega_{m,0} = \sqrt{m}\). We emphasise that this is a general result for harmonic confinement, as we have not explicitly defined the local interaction energy functional, \(\epsilon_{\text{loc}}[\rho]\).

### 7.3.6 The Breathing Mode

Another mode of particular interest in cold-atom systems is the \((m = 0, n = 1)\) breathing mode, characterised by the cylindrically symmetric expansion and contraction of the gas. Pitaevskii and Rosch\cite{102} show that for a Bose gas, the frequency of this mode is pinned to \(\omega_{0,1} = 2\). Furthermore, they show that this is due to a hidden SO(2,1)-symmetry that is found in systems with an interaction potential that scales as

\[
V(\lambda r) = \lambda^{-2} V(r).
\]

(7.63)

This includes a 2D bose gas with point-like s-wave interactions. The TF term with its \(\rho(r)^2\) contribution to the energy has this scaling, and so we expect the frequency of the breathing mode to be 2 in the \(C_{\text{dd}} \rightarrow 0\) limit. However, the dipole interaction, with its \(\rho \frac{\partial}{\partial r}\) contribution, does not obey this scaling, and hence, the symmetry is broken and the frequency is not pinned to 2 for \(C_{\text{dd}} > 0\). Indeed, we observe this both analytically and numerically as the frequency is exactly 2 in the low dipole, HD limit, and grows to \(\sqrt{5}\) in the large dipole limit (Fig. 7.15).

### 7.4 Conclusions

In this section we have applied the Thomas-Fermi-von Weizsäcker theory in the Hydrodynamic regime to a 2D spin-polarised fermionic system in a cylindrically symmetric harmonic potential. We have developed a scheme to numerically calculate the low-level collective excitation frequencies and found, in particular, that they are dispersionless in the HD limit with respect to dipole interaction strength. Furthermore, we have shown analytically that this is a general result for any interaction potential, dependent \textit{locally} on the particle density.
Chapter 8

A Thomas-Fermi-von Weizäcker-like Theory

The TFvW method offers a density functional scheme that is much less computationally expensive than the Kohn-Sham scheme. To do this, it sacrifices all the non-local properties of the system. Furthermore it requires an exact ground-state energy to be known in order to find the optimal von Weizsäcker parameter. We seek a scheme that captures the simplicity of the TFvW scheme, but without any need for a fit parameter.

8.1 The Average Density Approximation

The Average Density Approximation (ADA), is a scheme first proposed by Alonso et al. [103] and Gunnarsson et al. [104] in the late 1970’s for calculations of the exchange and correlation energies of non-uniform electron systems. Later, these ideas were applied for the construction of the non-local kinetic energy functionals in 1D [105–107] and 3D [108–113] systems.

In the 2D analogy to these works, we specify the non-local kinetic energy as,

\[ T_{nl}[\rho(r)] = \int d^2r \rho(r) t(\bar{\rho}(r)), \]  

(8.1)

in terms of the kinetic energy of the uniform system, \( t(x) \), and the average density defined as

\[ \bar{\rho}(r) = \int d^2r' \rho(r')w(r - r'; \rho(r)). \]  

(8.2)

The non-local nature of the kinetic energy is then captured in the non-local weight function, \( w(x; \rho) \), which is normalised according to

\[ \int d^2x w(x; \rho) = 1. \]  

(8.3)
The weight function is fully specified when the second functional derivative, when evaluated for a uniform system of density, \( \rho_0 \), leads to the exact static linear response function,

\[
\mathcal{F} \left[ \frac{\delta^2 T_{\text{nl}}[\rho]}{\delta \rho(r) \delta \rho(r')} \right]_{\rho(r) = \rho_0} = -\frac{1}{\chi_0(k)}, \tag{8.4}
\]

where \( \mathcal{F} \) denotes the Fourier transform from \( r - r' \) to \( k \). In a circularly symmetric system, this evaluates to

\[
2t'(\rho_0)w(k; \rho_0) + \rho_0 t''(\rho_0)w(k; \rho_0)^2 + 2\rho_0 t'(\rho_0) \frac{dw(k; \rho_0)}{d\rho_0} = -\frac{1}{\chi_0(k)}, \tag{8.5}
\]

where \( w(k; \rho_0) \) is the Fourier transform of \( w(|r - r'|; \rho_0) \).

Note that this weight function gives the exact linear response for a system with uniform density, whether this provides a good description for the inhomogeneous system is yet to be seen.

For a uniform 2D Fermi gas with density \( \rho_0 \), the exact linear response function is given by [114]

\[
\chi_0(\eta) = \begin{cases} 
-\frac{1}{\pi}, & \eta < 1 \\
-\frac{1}{\pi} \left( 1 - \sqrt{1 - \eta^{-2}} \right), & \eta \geq 1
\end{cases}, \tag{8.6}
\]

where \( \eta = k/(2k_F) \) is the scaled wavenumber and \( k_F = \sqrt{2\pi \rho_0} \) is the Fermi wavenumber. The kinetic energy per particle is

\[
t(\rho_0) = \frac{\pi}{2} \rho_0. \tag{8.7}
\]

Therefore, (8.5) reduces to the first-order ODE,

\[
w(k; \rho_0) + \rho_0 \frac{dw(k; \rho_0)}{d\rho_0} = F(\eta), \tag{8.8}
\]

where, for convenience, we have defined

\[
F(\eta) = -\frac{1}{\pi \chi(\eta)} = \begin{cases} 
1, & \eta < 1 \\
\eta^2 \left( \sqrt{1 - \eta^{-2}} + 1 \right), & \eta \geq 1
\end{cases}. \tag{8.9}
\]

Since \( F(\eta) \) is only dependent on \( \eta \), we will assume that the weight function also has a similar dependence, i.e. \( w(k; \rho_0) = w(\eta) \), and hence,

\[
w(\eta) - \frac{\eta}{2} w'(\eta) = F(\eta). \tag{8.10}
\]

The solution to (8.10) can be shown to be

\[
w(\eta) = \begin{cases} 
1 + c_1 \eta^2, & \eta < 1 \\
-4\eta^2 \ln \eta + 2\eta^2 \sqrt{1 - \eta^{-2}} - 2\eta^2 \ln \left[ 1 + \sqrt{1 - \eta^{-2}} \right] + c_2 \eta^2, & \eta \geq 1
\end{cases}. \tag{8.11}
\]
The function must be continuous at $\eta = 1$, so we require that the integration constant $c_1 = c_2 - 1$. We are then free to choose the $c_2$ at our convenience.

In the limit that $\eta \to \infty$, the weight function reduces to

$$w(\eta) \approx -4\eta^2 \ln \eta + (2 - \ln 4 + c_2)\eta^2.$$  \hspace{1cm} (8.12)

The $\eta^2$ divergence may be removed by setting $c_2 = \ln 4 - 2$. The remaining term comes from the corresponding divergent behaviour of $F(\eta)$. It can be removed if we instead look for the weight function, $w_0(\eta)$, that is the solution of the ODE

$$w_0(\eta) - \frac{\eta}{2}w_0'(\eta) = F(\eta) - 2\eta^2.$$  \hspace{1cm} (8.13)

The solution to (8.13) is then

$$w_0(\eta) = \begin{cases} 1 + \eta^2 (\ln 4 - 3 + 2\ln \eta^2), & \eta < 1 \\ 2\eta^2 \left(\sqrt{1 - \eta^{-2}} - 1 + \ln 2 - \ln \left[1 + \sqrt{1 - \eta^{-2}}\right]\right), & \eta \geq 1, \end{cases}$$

which exhibits no divergent behaviour.

In order to use this new weight function, we need to include a term in the kinetic energy functional, $T_{nl}[\rho]$, that results in a $2\pi \eta^2$ term when inserted into (8.4). The von Weizsäcker functional, used in the last chapter, has this property, therefore we rewrite the kinetic energy functional as

$$T_{nl}[\rho] = \frac{\pi}{2} \int d^2r \int d^2r' \rho(r') w_0(r - r'; \rho(r)) \rho(r) + T_{vW}[\rho],$$

where

$$T_{vW}[\rho] = \frac{1}{8} \int d^2r \frac{|\nabla \rho(r)|^2}{\rho(r)}.$$  \hspace{1cm} (8.15)

In Fig. 8.1 is plotted the weight function, $w_0(\eta)$, in Fourier space. It approaches a value of $-\frac{1}{2}$ as $\eta \to \infty$, and hence there will be a singularity at $x = 0$ in real space. The singularity may be removed by defining

$$\tilde{w}_\frac{1}{2}(\eta) = \frac{2}{3} \left(w_0(\eta) + \frac{1}{2}\right),$$

where the tilde indicates that the weight function has been scaled so that the normalisation condition (8.3) is still met, i.e. $\tilde{w}_\frac{1}{2}(0) = 1$. This weight function is plotted in Fig. 8.2, where, $x = 2k_F(r)r$, is the dimensionless spatial coordinate. Of course, a term must be explicitly added to the kinetic energy functional to balance the change in weight function. It is easily seen that this term is proportional to the TF functional.

Note, however, that the numerical calculation is unaffected by removing the singularity, as the calculation is performed in Fourier space. Hence, we use the $w_0(\eta)$ form as it is slightly easier to implement.
Figure 8.1: The weight function in Fourier space. The vertical line indicates the cusp of the piecewise function and the horizontal line is the $\eta \to \infty$ asymptote.

Figure 8.2: The weight function in real space. The real space variable on the horizontal axis is $x = 2k_F(r)r$. 
8.1.1 Ground-State of a General 2D system

The total energy given by
\[
E[\rho] = T_{\text{nl}}[\rho] + E_{\text{int}}[\rho] + \int d^2r \, v_{\text{ext}}(r)\rho(r),
\] (8.18)
is minimised w.r.t. \( \rho(r) \), under the normalisation constraint
\[
N[\rho] = \int d^2r \rho(r) = N_0,
\] (8.19)
when
\[
\frac{\delta E[\rho]}{\delta \rho(r)} - \mu = 0,
\] (8.20)
where, \( \mu \), is a Lagrange multiplier that insures the constraint. If we introduce the wavefunction, \( \psi(r) = \sqrt{\rho(r)} \), and the Fermi wavefunction, \( k_F(r) = \sqrt{2\pi\rho_0(r)} \), then (8.20) may be written in the convenient form
\[
-\frac{1}{2} \nabla^2 \psi(r) + v_{\text{eff}}(r)\psi(r) = \mu \psi(r),
\] (8.21)
where
\[
v_{\text{eff}}(r) = \phi(r) + v_{\text{ext}}(r) + \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(r)},
\] (8.22)
\[
\phi(r) = \frac{\pi}{2} \int \frac{d^2k}{(2\pi)^2} \int d^2r_1 \, e^{ik(r-r_1)} \left[ \Omega_0 \left( \frac{k}{2k_F(r)} \right) + w_0 \left( \frac{k}{2k_F(r_1)} \right) \right] \rho(r_1),
\] (8.23)
and
\[
\Omega_0(\eta) = w_0(\eta) - \frac{\eta}{2} w'_0(\eta) = F(\eta) - 2\eta^2.
\] (8.24)
To proceed further, we would require an explicit definition of the external potential and the interaction energy functional.

8.1.2 Ground-State of a Harmonically Trapped, Ideal Fermi gas

In this section we test the obtained functionals in a 2D harmonic oscillator potential,
\[
v_{\text{ext}}(r) = \frac{1}{2} r^2,
\] (8.25)
where \( r \) is the radial coordinate, scaled by the harmonic oscillator length \( l_{\text{osc}} = \sqrt{\hbar/m\omega} \).

In the ideal gas, the interaction energy is zero and the exact ground-states density calculated via the Kohn-Sham method, is given by \([79, 80]\)
\[
\rho_{\text{ex}}(r) = \frac{2}{\pi} \sum_{n=0}^{M} (-1)^n(M-n+1)L_n(2r^2)e^{-r^2},
\] (8.26)
where \( L_n(x) \) is the \( n^{th} \) Laguerre polynomial and \( M + 1 \) is the number of filled shells. The total particle number is related to the filled shell number via

\[
N(M) = (M + 1)(M + 2).
\]  

The kinetic energy can also be calculated exactly and is given by

\[
T_{ex} = \frac{N}{6} \sqrt{1 + 4N}.
\]  

The cylindrical symmetry of the trapping potential transforms the Fourier transforms in (8.23) into Hankel transforms. The effective potential is then

\[
v_{\text{eff}}(r) = \phi(r) + \frac{1}{2} r^2,
\]  

\[
\phi(r) = \frac{\pi}{2} \int dk \int dr_1 \left[ \Omega_0 \left( \frac{k}{2k_F(r)} \right) + w_0 \left( \frac{k}{2k_F(r_1)} \right) \right] \rho(r_1) J_0(kr_1) J_0(kr). \]  

These equations can be easily implemented into the ITP method, using the discretisation scheme provided by the DHT. The integrals of the piecewise functions, \( \Omega_0(\eta) \) and \( w_0(\eta) \), are then evaluated by a small modification of the DHT.

The number of momentum space sample points must be quite high in order to effectively sample the cusp in \( \Omega_0(\eta) \) and \( w_0(\eta) \). We find that it takes \( \sim 10000 \) sample points to achieve this. If we then want \( \sim 1000 \) real space points to get a smooth and continuous looking result and sufficiently accurate integral properties, then we must store a \( 1000 \times 10000 \) matrix to perform the transform. This is manageable except that the ITP method requires thousands if not tens of thousands of matrix multiplications to sufficiently converge. The CG method proves to be far superior in this case.

In our variant of the CG method we minimise the functional

\[
G[\psi] = E[\tilde{\rho}] + \frac{1}{4} (N[\psi] - N_0)^2,
\]  

w.r.t. \( \psi \), where \( \tilde{\rho} = \frac{N_0 \psi^2}{N[\psi]} \) is the normalised density and

\[
N[\psi] = \int d\mathbf{r} \psi(\mathbf{r})^2,
\]  

is the total particle number functional. For this we will require the SD direction, the negative of the functional derivative. The functional derivative of \( G[\psi] \) can be written in the convenient form

\[
\varphi(r) = \frac{\delta G[\psi]}{\psi(r)} = f(r) + (N[\psi] - N_0 - F[\psi]) \psi(r),
\]  

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where
\[
f(r) = \frac{N_0}{N[\psi]} \left[ -\nabla^2 \psi(r) + r^2 \psi(r) + 2 \tilde{\phi}(r) \psi(r) \right], \tag{8.34}
\]
\[
F[\psi] = \frac{1}{N[\psi]} \int dr_1 f(r_1) \psi(r_1), \tag{8.35}
\]
and \( \tilde{\phi}(r) \) is the \( \phi(r) \) in (8.30) but with \( \rho \) replaced with \( \tilde{\rho} \).

The line minimisations do not have as clean an implementation as in the TFvW method. This is because \( G[\psi + \epsilon \varphi] \) is not polynomial in \( \epsilon \). We instead employ the *reguli falsi* or false position method, which can be thought of as Newton's method except that the derivative (second derivative of \( G \)) is unknown or not easily calculable. In this method, the initial bracketing of a minimum is only a guess, so care must be taken to insure that it is indeed the first minimum, else the algorithm could get stuck in an infinite loop where it is jumping between two valleys.

The CG method implemented with these equations only requires tens, or at most a few hundred, iterations to converge, proving much more efficient than the ITP. The trade-off is the more difficult implementation and it can be much less stable if care is not taken for the initial bracketing in the *reguli falsi* section.

![Figure 8.3: Ground-state density of an spin-degenerate, ideal Fermi gas in a cylindrically symmetric 2D harmonic potential, calculated via the ADA method.](image)

In Fig. 8.3 is plotted the ground-state density calculated via the ADA method. The total particle numbers are chosen from the set that has filled shells (i.e. integer \( M \)). The densities have the basic form found from the TF approximation, but with an
Figure 8.4: Ground-state density of an spin-degenerate, ideal Fermi gas with $N = 30$ particles in a cylindrically symmetric 2D harmonic potential, calculated via the ADA method (blue). This is compared to the same system calculated by the exact KS scheme (green). The inset shows a blow up near where the density decays to zero, on a log scale.

exponentially decaying tail that is expected for a finite particle, physically realisable result. These exponential tails occur in the ADA method without any need for a fitting parameter as was the case in the TFvW method.

There is also evidence of bunching and anti-bunching of the density that suggests the desired oscillating structure in a harmonically trapped Fermi gas. These density oscillations become less important as the particle number increases, as does the exponential tail as the ADA solution converges to the expected TF solution in the infinite particle number limit.

In Fig. 8.4 we directly compare the exact density, calculated via the Kohn-Sham method, to the ADA ground-state density for $N = 30$ particles. The inset shows a blow-up of the tail region on a logarithmic scale. There is excellent agreement with the exact result in the tail region, however, the density oscillations of the ADA result are $\pi$ radians out of phase and have lesser amplitude than the density oscillation in the exact result. Even so, they have a similar wavelength which is a promising result.

This result carries through in the larger particle numbers (Fig. 8.5), and as the particle number grows, the difference becomes less significant.

From (8.15) we can calculate the total kinetic energy in the ADA density. In Table
Figure 8.5: Ground-state density of an spin-degenerate, ideal Fermi gas with: a) \( N = 90 \), b) \( N = 132 \), c) \( N = 182 \), d) \( N = 420 \) particles in a cylindrically symmetric 2D harmonic potential, calculated via the ADA method (blue). This is compared to the same system calculated by the exact KS scheme (green).
we compare this to the exact kinetic energy defined in (8.28). The last column of
the table gives the relative percentage error (RPE) between these results. The RPE is
very small in all cases and improves with increasing particle number.

\begin{table}[h]
\centering
\begin{tabular}{cccc}
\hline
$N$ & $T_{\text{ex}}$ & $T_{\text{nl}}[\rho_{\text{sc}}]$ & RPE \\
\hline
30 & 55 & 54.25 & 1.3 \\
90 & 285 & 283.00 & 0.64 \\
132 & 506 & 503.28 & 0.47 \\
182 & 819 & 815.52 & 0.35 \\
420 & 2870 & 2863.53 & 0.12 \\
\hline
\end{tabular}
\caption{Comparison of the exact kinetic energy with the non-local kinetic energy
calculated via the ADA method. The last column gives the relative percentage error
(RPE) between $T_{\text{ex}}$ and $T_{\text{nl}}[\rho_{\text{sc}}]$.}
\end{table}

As a diagnostic check of the convergence of the densities in our implementation
of the ADA method, we can also calculate the total external potential energy. The
equipartition theorem requires that, for a cloud in equilibrium, the total energy is
shared equally between the kinetic and potential energies. In Table 8.2 is presented
the relative percentage error of the kinetic and potential energies. The $\text{RPE}_{\text{eq}}$ is ex-
tremely small for all particle numbers thus ensuring that the chosen numerical grids
are sufficient for the task.

\begin{table}[h]
\centering
\begin{tabular}{c@{\hspace{1cm}}c}
\hline
$N$ & $\text{RPE}_{\text{eq}}$ \\
\hline
30 & $1.4 \times 10^{-5}$ \\
90 & $3.5 \times 10^{-6}$ \\
132 & $6.2 \times 10^{-6}$ \\
182 & $1.2 \times 10^{-6}$ \\
420 & $4.7 \times 10^{-6}$ \\
\hline
\end{tabular}
\caption{The relative percentage error ($\text{RPE}_{\text{eq}}$) between $T_{\text{nl}}[\rho_{\text{sc}}]$ and $V[\rho_{\text{sc}}]$.}
\end{table}

8.1.3 Other External Potentials

As a further test of the ADA method we present the ground-state densities in some
higher order external potentials. The first is the quartic potential

\begin{equation}
\nu_{\text{ext}}(r) = \frac{1}{2} r^4,
\end{equation}

(8.36)
where \( r \) is now in quartic oscillator units \( l_4 = \left( \frac{\hbar^2}{mV_4} \right)^{\frac{1}{8}} \) and \( V_4 \) is the quartic potential strength parameter.

The KS ground-states are calculated by solving (5.10) with the ansatz

\[
\psi_{m,n}(r, \theta) = \psi_{m,n}(r)e^{im\theta},
\]

(8.37)

for a set of \( m > 0 \) and \( n > 0 \). This involves using the Laplacian matrix from the DHT, and employing MATLAB’s eig() to get the first \( n_{\text{MAX}} \) eigenstates for each \( m < m_{\text{MAX}} \). One must ensure that \( m_{\text{MAX}} \) is sufficiently large that \( \epsilon_{m_{\text{MAX}},0} \) is larger than the Fermi energy. One then sorts the energies from smallest to largest and sums the orbital densities to get the particle density. Note that (5.10) is the same for \( \pm m \) so only the positive angular modes need be calculated, the \( m > 0 \) densities are doubled as two particles are placed in each mode. Also, since the gas is spin-degenerate, two particles are placed in each orbital, i.e. two fermions in the \( m = 0 \) orbitals and for in each of the \( m > 0 \) orbitals, up to the total of \( N \).

The ADA ground-state density (see Fig. 8.6 and Fig. 8.7) again shows excellent agreement in the low density tail of the gas. However, the ADA fails to replicate the oscillations near the centre of the gas. The disagreement is even worse than for the HO potential. In spite of this, the total kinetic energies agree surprisingly well (see Table 8.3). The RPE decreases as the particle number increases.

<table>
<thead>
<tr>
<th>( N )</th>
<th>( T_{\text{ex}} )</th>
<th>( T_{\text{nl}}[\rho_{\text{sc}}] )</th>
<th>RPE</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>30.99</td>
<td>29.44</td>
<td>5.0</td>
</tr>
<tr>
<td>20</td>
<td>93.83</td>
<td>91.59</td>
<td>2.4</td>
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<td>428.8</td>
<td>419.8</td>
<td>2.1</td>
</tr>
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<td>60</td>
<td>578.7</td>
<td>568.9</td>
<td>1.7</td>
</tr>
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<td>800</td>
<td>43050</td>
<td>42930</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Table 8.3: Comparison of the exact kinetic energy calculated via the Kohn-Sham scheme with the non-local kinetic energy calculated via the ADA method for a spin-degenerate ideal Fermi gas in a \( v_{\text{ext}}(r) = \frac{1}{2}r^4 \) potential. The last column gives the relative percentage error (RPE) between \( T_{\text{ex}} \) and \( T_{\text{nl}}[\rho_{\text{sc}}] \). The energy units are in quartic oscillator energy units \( \epsilon_4 = ml_4^2/\hbar^2 \).
Figure 8.6: Ground-state density of a spin-degenerate, ideal Fermi gas with $N = 50$ particles in a $v_{\text{ext}}(r) = \frac{1}{2} r^4$ external potential, calculated via the ADA method (blue) and the Kohn-Sham scheme (green). The length units are in quartic oscillator units $l_4$ (see text).

Figure 8.7: Ground-state density of a spin-degenerate, ideal Fermi gas with $N = 600$ particles in a $v_{\text{ext}}(r) = \frac{1}{2} r^4$ external potential, calculated via the ADA method (blue) and the Kohn-Sham scheme (green). The length units are in quartic oscillator units $l_4$ (see text).

Next we perform the same calculation for the 6th order potential

$$v_{\text{ext}}(r) = \frac{1}{2} r^6,$$  

(8.38)
where $r$ is in sextic oscillator units $l_6 = (\hbar/mV_6)^{1/2}$ and $V_6$ is the sextic potential strength parameter.

Again there is excellent agreement in the tails (see Fig. 8.8 and Fig. 8.9), however, the oscillations have even less agreement than with the quartic potential. This is not reflected in the total kinetic energies, however, as the RPE is not any worse than the quartic potential (see Table 8.4).

<table>
<thead>
<tr>
<th>$N$</th>
<th>$T_{ex}$</th>
<th>$T_{nl}[\rho_{sc}]$</th>
<th>RPE</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>36.85</td>
<td>35.06</td>
<td>4.9</td>
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<td>116.98</td>
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<td>570.67</td>
<td>556.99</td>
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<td>780.77</td>
<td>765.80</td>
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<tr>
<td>300</td>
<td>12929.28</td>
<td>12832.18</td>
<td>0.8</td>
</tr>
<tr>
<td>600</td>
<td>43431.52</td>
<td>43231.63</td>
<td>0.5</td>
</tr>
<tr>
<td>700</td>
<td>56869.87</td>
<td>56635.55</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Table 8.4: Comparison of the exact kinetic energy calculated via the Kohn-Sham scheme with the non-local kinetic energy calculated via the ADA method for a spin-degenerate ideal Fermi gas in a $v_{ext}(r) = \frac{1}{2}r^6$ potential. The last column gives the relative percentage error (RPE) between $T_{ex}$ and $T_{nl}[\rho_{sc}]$. The energy units are in sextic oscillator energy units $\epsilon_6 = ml_6^2/\hbar^2$. 

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Figure 8.8: Ground-state density of a spin-degenerate, ideal Fermi gas with $N = 50$ particles in a $v_{\text{ext}}(r) = \frac{1}{2}r^6$ external potential, calculated via the ADA method (blue) and the Kohn-Sham scheme (green). The length units are in sextic oscillator units $l_6$ (see text).

Figure 8.9: Ground-state density of a spin-degenerate, ideal Fermi gas with $N = 600$ particles in a $v_{\text{ext}}(r) = \frac{1}{2}r^6$ external potential, calculated via the ADA method (blue) and the Kohn-Sham scheme (green). The length units are in sextic oscillator units $l_6$ (see text).
8.2 Conclusions

In this chapter we have developed the 2D ADA method, a scheme to calculate the ground-state of a trapped, spin-degenerate Fermi gas, and applied it in a cylindrically symmetric harmonic trap as well as some higher order external potentials.

The ADA ground-state densities show excellent agreement in the tail region on the surface of the cloud, when compared with the equivalent Kohn-Sham densities for an ideal gas. This agreement in the tail region occurs automatically without any need for a fitted parameter as is the case with the TFvW method. The ADA densities also exhibit oscillations that are completely absent in the TFvW treatment, however, these oscillations do not match with the oscillations in the exact density. Despite this the total kinetic energies match surprisingly well.

We then repeated these calculation in a quartic and sextic potential. The ADA performs just as well with these higher order external potentials, although it is even worse at reproducing the density oscillations.
Chapter 9

Thesis Summary

In this thesis we have explored two aspects of current work in the theory of ultracold atomic gases. We have explored the effect of disorder on a 1D Bose gas in an optical lattice, where the disorder is introduced by the interference between the primary lattice and a second, weaker lattice. We verified, by means of numerical simulation, the results of the Aubry-André model. When the ratio of the lattice wavelengths is incommensurate, there exists a critical disorder strength, beyond which, all eigen-states of the Hamiltonian are localised, and transmission is suppressed. In contrast, if the lattice ratio is commensurate, then the eigen-states are extended and the gas expands ad infinitum. Increasing the secondary lattice strength, decreases the spread rate of the cloud as the bandwidth of the modified Bloch band reduces. However, the transmission is never completely suppressed and there is no transition to localisation.

We demonstrated the effect known as “self-trapping”, where the spreading of the gas is forbidden when the inter-particle interaction energy cannot dissipate, as the maximum kinetic energy is finite and the momentum states have become saturated. Increasing the inter-particle interactions, increases the confinement, and the density that does escape, does so as solitons, wavepackets with finite momentum that hold their shape ad infinitum. The secondary lattice increases the self-trapping effect, as the reduction of the Bloch band’s bandwidth only makes the momentum states saturate sooner.

Next we explored the effect of applying a linear force to the Bose gas in the bichromatic lattice. Such a linear force could be the result of tilting the optical lattice in a gravitational field. In a homogeneous lattice this leads to the well-known Bloch oscillations, where the particle accelerates to the edge of the Brillouin zone in momentum space, and then Bragg scatters of the zone edge. This occurs because of the peri-
odic nature of the band. The result is oscillations in real space, with a well defined period. For the non-interacting Bose gas in a homogeneous lattice, the oscillations are dissipationless. A commensurate secondary lattice reduces the period of the oscillations, even as the amplitude of the centre-of-mass and width are reduced by the decreasing bandwidth. Using a weak, incommensurate bichromatic lattice, the cloud becomes fragmented, however, the oscillations are still present, albeit with many different oscillation periods. The localisation that results in a strong incommensurate lattice, is unbroken by the linear potential, but Bloch oscillations still occur within the virtual transmission zone. When the interactions are strong, the self-trapping resists the oscillations, and looks qualitatively similar to the localised simulation.

In the next chapter we explored the effect of an external magnetic field on charged particles in a 2D disordered lattice. By causing a position dependent shift in the momentum of a Bose gas of neutral atoms, it is possible to manufacture a Hamiltonian identical to that of the charged particles. We again used a secondary lattice to introduce disorder to the optical lattice. In the weak disorder regime, the magnetic field caused the particles in the cloud to move in circular paths, reducing the conductance, exhibiting positive-magneto resistance. The surface of the cloud also exhibited a diamond profile as the cloud expanded, as compared to the normal square profile in the magnetic-field free, square optical lattice. The magnetic field broke the localisation in the strong disordered case, and increasing the magnetic field caused the cloud to spread faster, exhibiting negative magneto-resistance. We also observed negative magneto-resistance when the bichromatic disorder was exchanged for a truly random disorder potential, however, the localisation was not broken by the magnetic field, simply weakened.

In the second half of the thesis we explored the problem of Fermi particles in a harmonic oscillator potential. We employed density functional theory and in particular the Thomas-Fermi-von Weizsäcker method to approximately find the ground-state of the spin-polarised dipolar Fermi gas. Using this method we calculated the collective mode oscillation frequencies in the hydrodynamic regime. We found that the collective frequencies of the surface oscillation modes are dispersionless w.r.t. the dipolar interaction strength. Furthermore, we showed that this is a general result for any interaction potential, dependent locally on the particle density. We developed analytical solutions for the low dipolar interaction strength and high dipolar interaction strength limiting cases. These agreed admirably with the numerically obtained results.

In the final chapter we developed and implemented an average density approxi-
mation method to find the ground state of a spin-degenerate, ideal Fermi gas. The resulting ground-states showed excellent agreement with the exact results, without the need for a fitted parameter as in the TFvW method. The ground-state densities showed density oscillations near the centre of the gas, however, these oscillations did not agree with those in the exact density. In spite of this, the total energies matched surprisingly well.

9.1 Future work

In the future we would like to explore, more, the role of interactions in the disordered system.

We would also like to see if the observations with the disorder and the tilted optical lattice persist when the disorder is caused by a laser speckle pattern.

The algorithms written to perform the simulation in the disorder section can be easily adapted to simulate the effect of speckle disorder in 2D continuous space. We intend to use this to explore the backscattering from a speckle disordered region.

Using the ADA functional and the hydrodynamic equations, we intend to calculate the collective oscillation frequencies of a dipolar gas. We can then directly compare these to the TFvW frequencies we have already calculated.
Appendix A

Line Minimisation Polynomials

With \( \tilde{\psi} = \psi + \epsilon \phi \), let

\[
N(\epsilon) = \int dr \tilde{\psi}^2 = \sum_{k=0}^{2} 2C_k n_k[\psi, \phi] \epsilon^k, \tag{A.1}
\]

\[
B(\epsilon) = \frac{1}{2} \int dr \tilde{\psi} \left[ -\lambda_v \nabla^2 + r^2 \right] \tilde{\psi} = \sum_{k=0}^{2} 2C_k b_k[\psi, \phi] \epsilon^k, \tag{A.2}
\]

\[
C(\epsilon) = 2\pi \int dr \tilde{\psi}^4 = \sum_{k=0}^{4} 4C_k c_k[\psi, \phi] \epsilon^k, \tag{A.3}
\]

\[
D(\epsilon) = \frac{2}{5} C_{dd} \int dr \tilde{\psi}^5 = \sum_{k=0}^{5} 5C_k d_k[\psi, \phi] \epsilon^k, \tag{A.4}
\]

\[
X(\epsilon) = \frac{N_0}{N(\epsilon)}, \tag{A.5}
\]

\[
Y(\epsilon) = \frac{1}{4} (N(\epsilon) - N_0)^2, \tag{A.6}
\]

where \(^nC_k\) is a binomial coefficient, and \( n_k[\psi, \phi], b_k[\psi, \phi], \) etc. are all functionals that evaluate the integrals. After evaluating these functionals via the discrete Hankel quadrature (6.36), the functional (6.13) reduces to a function of one variable

\[
G(\epsilon) = X(\epsilon) \left[ B(\epsilon) + X(\epsilon) \left( C(\epsilon) + \sqrt{X(\epsilon)} D(\epsilon) \right) \right] + Y(\epsilon). \tag{A.7}
\]

To minimise \( G(\epsilon) \), we first find all the stationary points by solving the equation \( G'(\epsilon) = 0 \), given that

\[
G'(\epsilon) = X(\epsilon) \left[ B'(\epsilon) + X(\epsilon) \left( C'(\epsilon) + \sqrt{X(\epsilon)} D'(\epsilon) \right) \right]
+ X'(\epsilon) \left[ B(\epsilon) + X(\epsilon) \left( 2C' + \frac{5}{2} \sqrt{X(\epsilon)} D(\epsilon) \right) \right] + Y'(\epsilon). \tag{A.8}
\]
In the case where $C_{dd} = 0$, this reduces to the 9th order polynomial

\[ N(\epsilon)^3 G'(\epsilon) = 0. \] (A.9)

In the case of finite $C_{dd}$, $G'(\epsilon)$ is a radical function so the stationary points are among the solutions of

\[
4N(\epsilon) \left[ N(\epsilon) (N(\epsilon)B'(\epsilon) + C'(\epsilon)) - N'(\epsilon) (N(\epsilon)B(\epsilon) + 2C(\epsilon)) + N(\epsilon)^2 Y'(\epsilon) \right]^2
- [2N(\epsilon)D'(\epsilon) - 5N'(\epsilon)D(\epsilon)]^2 = 0,
\] (A.10)

a 20th order polynomial of one variable. Only half of the roots of (A.10) are also roots of (A.8), so they must be back substituted to determine the correct set.

The polynomials are solved by finding the eigenvalues of the polynomial’s companion matrix. The result, using a standard eigensolver algorithm, is a set of real and complex double scalars that are near the desired roots. We then discard the imaginary parts and sort the roots from negative to positive. We evaluate (A.8) at each point half-way between each pair of adjacent roots and select the roots that go from negative to positive across this interval. This leaves us with only the minima of (A.7). We then use up to 100 iterations of a hybrid midpoint-Newton method, to refine the minima, and select the least-positive minima. The second derivative, given by

\[
G''(\epsilon) = X(\epsilon) \left[ B''(\epsilon) + X(\epsilon) \left( C''(\epsilon) + 5X(\epsilon)D''(\epsilon) \right) \right]
+ X'(\epsilon) \left[ 2B'(\epsilon) + X(\epsilon) \left( 4C'(\epsilon) + 5X(\epsilon)D'(\epsilon) \right) \right]
+ X'(\epsilon)^2 \left[ 2C(\epsilon) + 15X(\epsilon) \right] D(\epsilon)
+ X''(\epsilon) \left[ B(\epsilon) + X(\epsilon) \left( 2C(\epsilon) + \frac{5}{2} \sqrt{X(\epsilon)}D(\epsilon) \right) \right]
+ Y''(\epsilon),
\]

is required by this method.
Appendix B

List of Acronyms

1D - One Dimensional
2D - Two Dimensional
3D - Three Dimensional
MOT - Magneto-Optical Trap
BEC - Bose-Einstein Condensate
AC - Alternating Current
w.r.t. - with respect to
AA - Aubry-André
gp - Gross-Pitaevskii
RK - Runge-Kutta
RK4 - 4th order Runge-Kutta
EOM - Equation(s) of Motion
FFT - Fast Fourier Transform
CPU - Central Processing Unit
RK4DS - 4th order Runge-Kutta with Double Step error correction
Rms. - Root mean square
HF - Hartree-Fock
DFT - Density Functional Theory
LDA - Local Density Approximation
HK - Hohenberg-Kohn
TF - Thomas-Fermi
KS - Kohn-Sham
SD - Steepest-Descent
CG - Conjugate-gradient
ITP - Imaginary Time Propagation
TFvW - Thomas-Fermi-von Weizsäcker
HD - Hydrodynamic
ODE - Ordinary Differential Equation
ADA - Average Density Approximation
DHT - Discrete Hankel Transform
RPE - Relative Percentage Error
HO - Harmonic Oscillator
Bibliography


