Many-body Landau-Zener Physics in Ultracold Atomic Gases

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"You are in a maze of twisty little passages, all alike." -Zork I

Abstract

This thesis will examine a system of bosonic atoms in the p-band on an isotropic optical lattice in 2-dimensions and confined by a trapping potential. By introducing the necessary theoretical framework needed the characteristics of the system is revealed. Among the more important features is the anisotropic tunnelling which is a direct consequence of the p-band physics of the system and the confining trap. By calculating the ground-state the impact of the anisotropic tunnelling is shown, and by utilizing a mean-field approximation a chequerboard pattern will be revealed which will extend throughout the entire lattice. With a change to an anisotropic lattice, the properties will be affected and thus the transition of the ground-state will also be studied. In particular it will be shown how the ground-state transfers from one distribution to another when the lattice parameters are changed.

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Contents

1 Introduction

The subject of a cold atom gas is one that is heavily focused on contemporary research [1]. When sufficiently low temperatures are reached a wide range of quantum phenomena appears, perhaps the most famous one is Bose-Einstein condensation which only appears at temperatures very close to absolute zero (for bosonic particles). Moreover, one of the most commonly used cooling techniques to achieve such a low temperature is laser cooling, together with an atomic trap. As a consequence of the high precision in the cooling processes, atomic gases is one of the best candidates when it comes to the study of mesoscopic quantum phenomena[1] and simulation of other quantum phenomena in the field of condensed matter theory.

This thesis will concern the examination of neutral atoms in a two-dimensional (2D) periodic potential confined by a harmonic potential; these atoms will be restricted to the first excited band of the periodic potential (known as the p-band). As a consequence of the restriction to the first lattice band, a double quasi-degeneracy will be introduced in the 2D case, which directly affect the physical properties of the system. These properties include tunnelling and the distribution of atoms in the system as a whole. In order to capture the properties of the system, the goal for this thesis will first be to obtain the ground-state wave function for an isotropic 2D lattice and from there make further predictions. When the ground-state is obtained, an inhomogeneity will be introduced in the lattice. This inhomogeneity will affect the state (population) and by utilizing numerical methods, the time evolution of the ground-state (and population) will be mapped out. Before proceeding, some clarifications will be made on the basic physics of the system as well as introduce some future notifications.

The periodic potential can be approximated by utilizing the harmonic approach (if the lattice potential is sufficiently deep this approximation is valid). In this approximation each site is treated as containing a single isolated harmonic oscillator. The harmonic oscillator has the known energy

$$E = \hbar\omega(n_x + n_y + 1), \quad n_x, n_y = 0, 1, 2, 3, ... \tag{1}$$

steaming from the Schrödinger equation

[1] Mesoscopic can be seen as an intermediate length scale, the scale between atoms and materials measured the micrometer scale.

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle \tag{2}$$

with the Hamiltonian on the form of

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2), \tag{3}$$

where the oscillator exist in 2D. From Eq.(1) it becomes apparent that the energy corresponding to the first excited energy level is double degenerated where either n_x or n_y can be 1 while the other is 0. From here on, the atoms with wave functions with $(n_x, n_y) = (1, 0)$ will be denoted *x-flavoured* and those with $(n_x, n_y) = (0, 1)$ will be denoted *y-flavoured*. Important to notice is that the flavour do not refer specifically to the spatial coordinates x and y, but to the quantum number n_x and n_y, it will be possible for an x-flavourd atom to tunnel in the y-direction and vis versa. Up to this point each site in the lattice has been treated as an isolated harmonic oscillator. This however cannot capture the tunnelling aspect of the system. Each site is connected by tunnelling to one another and therefore it is not correct to treat each site as an isolated oscillator. The Hamiltonian in the harmonic approximation would for a system with tunnelling take the form of

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2) + \hat{t}_{tun} \tag{4}$$

where $\hat{t}_{tun}$ indicate some type of tunnelling contribution and will be explained in detail later. With this additional term the energy given above becomes invalid and the quantum numbers n_x and n_y cease to be good quantum numbers. This leads to a split in the total energy level for the periodic potential, as a consequence of the superposition principle applied to each and every lattice points energy function. Thus the p-band is the arrange of energy levels corresponding to the superposition of every-site in the harmonic approximation (in the first excited level), when tunnelling between sites are allowed. This approach is what is usually called the *Tight-binding model*[2].

This thesis is based on the work of [2] and will revisit many of the same topics that where discussed in the original paper. One exception being the coverage of further studies on how an initial state evolves in time when subjected to a change in the lattice parameters. Furthermore, even though this

[2]Note that the Tight-binding model and the Tight-binding approximation not are the same thing, even though they are related.

thesis will revisit most of the same topics as the original paper so will they not necessarily be discussed in a similar manner.

1.1 Outline

This thesis is aimed at students on a level corresponding to the end of a bachelors program. Many of the important conclusions stem from theoretical models, methods and tools that are beyond the grasp of the bachelors program. This includes foremost concepts from *Quantum field theory* and the treatment of many-body quantum mechanics, but even other aspects such as the *split-operator method* and *imaginary time propagation* ought to be something that the reader is not familiar with on that level. Furthermore, the vital *mean-field approximation* in the form that is being used in this thesis will also be unfamiliar for most readers. As a consequence most of the theoretical framework will not be reviewed in a completely rigorous way, instead a more approachable style will be favoured. Thus, the emphasis will be on explaining the theoretical framework from a starting-point relating to the problem being treated. As of that, the necessary tools will only be presented and seldom defined in a strict general mathematical fashion. Rather, an intuitive explanation will be given along with a motivation of the necessity in the using of a certain tool[3].

The thesis will consists of four parts (including the introduction) that serves to explain and declare important parts of the project. First a theoretical discussion will follow in which most of the theoretical framework will be outlined. The section starts by further explaining the system and specifying the course of action. After the theoretical section comes the results of the thesis. This will mostly be in the form of graphs and figures showing important relations between flavours as well as other important features of the system (this could include some amount of theory discussion concerning the non-symmetric lattice). Finally there is a conclusion section to accommodate for any final words along with a discussion of the results in the previous sections.

[3]The word tool here refers to any theoretical method or model, these can include for example the split-operator method or the mean-field approximation.

2 Theory

In the introduction there was a brief discussion about the system being treated in this thesis. For further use, so will the system now be specified more in detail. The system is composed firstly of a 2D optical square lattice. The lattice is created by utilizing interference of coherent laser beams travelling in opposite directions. By fine tuning these lasers it is possible to change the two most important parameters of the lattice, the *well depth* (lattice depth) and the *periodicity*. These have a direct effect on the tunnelling ability of the stored atoms. Along with these parameters are the occurrence of energy band in the lattice. In this thesis the particles are restricted to the first excited band, the p-band. This is in contrast to the more commonly treated system where the particle are residing on the s-band, the lowest energy band. Secondly there is an applied harmonic trapping potential, which can be applied by utilizing a number of different effects in real life settings [3]. Because of this potential the atoms are confined in a certain area of the lattice. Lastly are the particles, in this case neutral bosonic atoms which are indistinguishable from one another. This entire contraption forms the system, and is what will be treated in this thesis. In figure (1) a schematic picture of the two potentials is shown.

To study the properties of the atomic flavours in the lattice a wave function must first be obtained. In the low temperature limit most of the particles should be in the available ground-state of the p-band. Therefore the goal should further be to first obtain the ground-state wave function and thereafter begin to make predictions. This section's goal will thus be to obtain the wave function for the ground-state in the optical lattice with an applied confining trap.

In the following subsections the basic cornerstones of the theory involved in the acquirement of the ground-state wave function will be outlined. As mention beforehand, the purpose is to achieve the ground-state wave function, and on the way several other important aspects will be discussed. Furthermore, several vital expressions will be established which in themselves makes predictions on the physics of the system. The outline is as follows for the rest of the section.

First the Hamiltonian for the system is derived from the *second quantized formalism* by introducing the creation and the annihilation operators. Secondly, the equations of motion will be derived utilizing *the Heisenberg equations* as well as the mean-field approximation. In the following section the

split-operator method along with imaginary time propagation is explained with a starting point stemming from the system. Lastly is a more in depth treatment of the mean-field approximation and the consequences it has on the system.

Before proceeding some clarifications on the notation will be made. In the following treatment of the theory, operators will not be written as symbols with a hat. Instead it will be apparent from the context which parameters that are operators and which are not. The hat notation will only be used if there is some chance for confusion. Furthermore, the indices will foremost account for the flavour (x or y) and the position in the lattice, where i refers to the lattice locations in the x-direction and where j refers to the lattice locations in the y-direction in the instances where both are occurring at the same time.

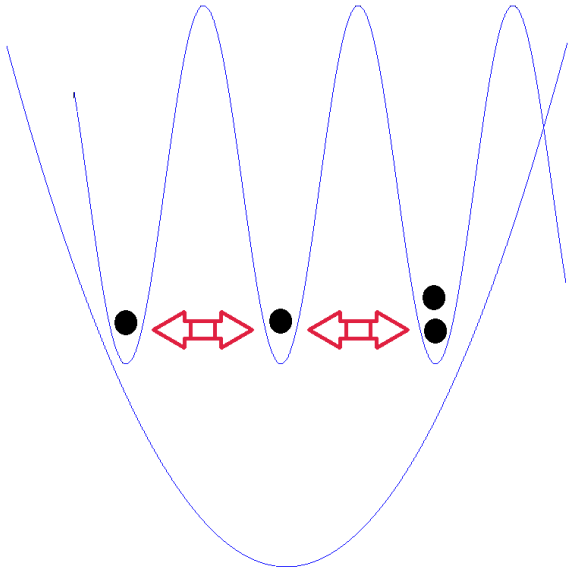

Figure 1: A simplified picture of the system as seen from the side, consisting of a periodic potential, a harmonic potential and some particles (atoms). The red arrows indicate tunnelling processes and there directions.

2.1 Derivation of the second quantized Hamiltonian

In order to describe the system and make any qualified predictions its dynamics should be described. A proper way to do this is by utilizing the Hamiltonian formulation. The system that is being examined in this thesis lends itself to be described in the terms of the field operators $\Psi^\dagger(\vec{r})$ and $\Psi(\vec{r})$ which create or destroy a particle in a the position $\vec{r}$. In this way the tunnelling nature of the particles in the lattice can be captured in the sense that the tunnelling process is described by the destruction of the particle in one location and the creation of it in another location. The formulation of the Hamiltonian with these field operators are what is called *the second quantized Hamiltonian* [4] [5] and is the starting point for this paper. For this system, in addition to the standard dynamics usually attributed to a single particle system, there is also a interparticle interaction term accounting for particle interactions in the many-body case. The many-body Hamiltonian for this system take the form of

$$H = \int d\vec{r} \left(\Psi^\dagger(\vec{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\vec{r}) \right] \Psi(\vec{r}) + \frac{\tilde{U}_0}{2} \Psi^\dagger(\vec{r}) \Psi^\dagger(\vec{r}) \Psi(\vec{r}) \Psi(\vec{r}) \right), \quad (5)$$

where m is the mass of the particles and U_0 is the strength of the interparticle interaction. $V(\vec{r})$ is in this case the combined effects of the applied potentials and is on the form of $V(\vec{r}) = V_{latt}(\vec{r}) + V_{trap}(\vec{r})$ where the lattice potential is given by

$$V_{latt}(\vec{r}) = V_x \sin^2(kx) + V_y \sin^2(ky), \quad (6)$$

where V_α is the amplitude of the potential in a certain direction ($\alpha \in [x, y]$), and k the wave vector $k = 2\pi/\lambda$, with λ being the wavelength of the lasers used to create the lattice potential; moreover the trap part of the potential is given by

$$V_{trap(\vec{r})} = \frac{m\tilde{\omega}^2}{2} \left(x^2 + y^2 \right), \quad (7)$$

which describes a harmonic potential trap with a characteristic frequency of $\tilde{\omega}$. Because of the nature of the system with a periodic potential it is favourable to change basis from the generic field operator $\Psi^\dagger(\vec{r})$ and $\Psi(\vec{r})$ which can create or destroy a particle anywhere in space to one which is

restricted to only target locations with in the lattice. The wave function of the particle must thus be located at a certain lattice site i.

The first step should be to find the wave functions that satisfy the Schrödinger equation and for the periodic given potential. The solutions will be eigenfunctions of the energy associated with the period potential and they will account for all the different energy levels, i.e. the band structure (as previously mentioned the atoms in this thesis are exclusively restricted to the p-band). The eigenfunctions that satisfy these conditions are the so called *Bloch states* which are a practical basis for the expansion of the field operators $\Psi^\dagger(\vec{r})$ and $\Psi(\vec{r})$. The field operators $\Psi^\dagger(\vec{r})$ and $\Psi^\dagger(\vec{r})$ can be expressed in terms of the Bloch functions as

$$\Psi^\dagger(\vec{r}) = \sum_{\nu q} \phi^*_{\nu q}(\vec{r})\hat{b}^\dagger_{\nu q}, \tag{8}$$

$$\Psi(\vec{r}) = \sum_{\nu q} \phi_{\nu q}(\vec{r})\hat{b}_{\nu q}, \tag{9}$$

where $\phi_{\nu q}(\vec{r})$ is the Bloch state with quasimomentum q in the ν:th energy band, and where $b_{\nu q}$ and $b^\dagger_{\nu q}$ are bosonic operators which annihilate or create a particle of certain quasimomentum q in the ν:th energy band. The quasi momentum q is restricted to the first *Brillouin zone*, i.e. $-\pi/\lambda \leq q \leq +\pi/\lambda$, and where λ is the wave length of the applied laser to create the optical lattice. But this does not entirely solve the original concerns. The wave functions should practical describe the scenario where particles are only (up to a certain amount of uncertainty) allowed to populate sites within the lattice. A base to expand $\Psi(\vec{r}')$ in that has these properties are the known *Wannier functions*

$$\Psi^\dagger(\vec{r}) = \sum_{\nu j} W^*_{\nu R_j}(\vec{r})a^\dagger_{\nu j}, \tag{10}$$

$$\Psi(\vec{r}) = \sum_{\nu j} W_{\nu R_j}(\vec{r})a_{\nu j}, \tag{11}$$

where $a^\dagger_{\nu j}$ and $a_{\nu j}$ are the creation and annihilation operators for bosons that creates or destroys a particle at site j in the lattice, and $W_{\nu R_j}$ is the site localized Wannier wave function. For a complete picture it is also noteworthy to state that the Wannier functions are related to the Bloch state in the following manner

$$W_{\nu R_j} = \sum_{q \in Bz} e^{-iq \cdot R_j} \phi_{\nu q}(\vec{r}) \tag{12}$$

with notation as before and where Bz indicates the first Brillouin zone. From here it also becomes apparent that the Wannier functions themselves are not solutions to the original Schrödinger equation for the periodic lattice, in contrast to the Bloch states $\phi_{\nu q}(\vec{r})$ and $\phi^{\dagger}_{\nu q}(\vec{r})$.

The properties of the Wannier functions depend on which excited band the system is populating (can be seen from the above relation). In this thesis only the p-band is allowed for the particles and as such the Wannier functions for the different flavours take the form

$$\begin{aligned} W_{xj}(\vec{r}) &= W_{1j_x}(x) W_{0j_y}(y) \\ W_{yj}(\vec{r}) &= W_{0j_x}(x) W_{1j_y}(y) \end{aligned} \tag{13}$$

where j_α indicates a site with a certain wave function in the $\alpha = \{x, y\}$ direction. The number before j_α indicates the number of nodes for the wave function which means it contains information of how the wave function looks. The structure of the wave function is akin to the ones which appears in the harmonic oscillator[4] where the wave function for the secondary stationary state is more elongated then that of the first ground-state. This directly determines the shape and moreover the physical properties for the two flavours, namely the tunnelling properties in different directions.

For further use, it is preferable to define dimensionless parameters. This is done by scaling with a suitable quantity. The energy is scaled by the recoil energy $E_r = \hbar^2 k^2 / 2m$ and every parameter with the unit length is scaled by $l = \lambda / 2\pi$. This results in that the frequency for the harmonic trap becomes $\omega = \sqrt{2} m \tilde{\omega} / \hbar k^2$ and the expression $V_{trap} = \omega^2 (x^2 + y^2)$ where now $x = kx$ and $y = ky$ is the dimensionless position values.

By expanding the field operator $\Psi(\vec{r})$ in terms of the localized Wannier functions it will enable the possibility to determine tunnelling properties between neighbouring sites in the lattice. This is simply accomplished by substituting in the expression for the Wannier functions into the Hamiltonian. The resulting calculations can however be somewhat bothersome and therefore some clarifications will be made. The first thing to do in order to ease the calculation should be to write out more explicitly the expansion

[4] Se [6] page 58.

$$\Psi^\dagger(\vec{r}) = \sum_j \sum_\nu \left(W^*_{\nu,x,j}(\vec{r}) a^\dagger_{\nu,x,j} + W^*_{\nu,y,j}(\vec{r}) a^\dagger_{\nu,y,j} \right), \tag{14}$$

in the case for the creation operator. Furthermore, any of the resulting integrals with an odd number of Wannier functions (regarding a specific flavour) should be equal to zero in the case of a symmetric integral interval (which is exactly the case in a periodic potential). In that way, most of the resulting terms will vanish and the remaining calculations should be considerable simplified. The only remaining thing to comment is the appearance of the number operator in the final result. At one point in the calculation, in order to obtain the Hamiltonian below the use of commutator is necessary. The relation used can be found in the next section if there is any uncertainty for the reader[5]. The resulting Hamiltonian can be written as, if only tunnelling to the nearest neighbouring site is allowed (this is called the *tight binding-approximation*)

$$H = H_0 + H_{nn} + H_{FD}, \tag{15}$$

where the parts are as follow

$$H_0 = -\sum_{\alpha,\beta} \sum_{\langle \mathbf{ij} \rangle_\beta} t_{\alpha\beta} a^\dagger_{\alpha,\mathbf{i}} a_{\alpha,\mathbf{j}} + \sum_\alpha \sum_{\mathbf{j}} V_{trap}(R_{\mathbf{j}}) n_{\alpha,\mathbf{j}}\,, \tag{16}$$

$$H_{nn} = \sum_\alpha \sum_{\mathbf{j}} \frac{U_{\alpha\alpha}}{2} n_{\alpha,\mathbf{j}}(n_{\alpha,\mathbf{j}} - 1) + \sum_{\alpha\beta,\alpha\neq\beta} \sum_{\mathbf{j}} U_{\alpha\beta} n_{\alpha,\mathbf{j}} n_{\beta,\mathbf{j}}\,, \tag{17}$$

$$H_{FD} = \sum_{\alpha\beta,\alpha\neq\beta} \sum_{\mathbf{j}} \frac{U_{\alpha\beta}}{4} \left(a^\dagger_{\alpha,\mathbf{j}} a^\dagger_{\alpha,\mathbf{j}} a_{\beta,\mathbf{j}} a_{\beta,\mathbf{j}} + a^\dagger_{\beta,\mathbf{j}} a^\dagger_{\beta,\mathbf{j}} a_{\alpha,\mathbf{j}} a_{\alpha,\mathbf{j}} \right), \tag{18}$$

where $n_{\alpha\mathbf{j}} = a^\dagger_{\alpha\mathbf{j}} a_{\alpha\mathbf{j}}$ is the number operator that counts the number of particles of a certain flavour and $\sum_{\langle \mathbf{ij} \rangle_\alpha}$ is the sum over the nearest neighbours in the lattice in the direction $\alpha\,(\alpha, \beta = x, y)$; the tunnelling coefficients are given by

[5]The relation can be summarized by formulating it as $\left[a_{\mu,j}, a^\dagger_{\nu,i}\right] = \delta_{i,j}\delta_{\mu,\nu}$ where i and j are different sites, ν and μ are different lattice bands and $\delta_{i,j}$ as well as $\delta_{\mu,\nu}$ are the Kronecker delta.

$$t_{\alpha\beta} = -\int d\vec{r} W^*_{\alpha,\mathbf{j}}(\vec{r})[-\nabla^2 + V_{latt}(\vec{r})]W_{\alpha,\mathbf{j}+\mathbf{1}_\beta}(\vec{r}) \tag{19}$$

and the interaction parameters by

$$U_{\alpha\beta} = U_0 \int d\vec{r} |W_{\alpha,\mathbf{j}}(\vec{r})|^2 |W_{\beta,\mathbf{j}}(\vec{r})|^2, \tag{20}$$

where $j + 1_\beta$ is a notation for the sum over the neighbouring site j in the direction of β. At this point an important feature appears when Eq.(13) is combined with Eq.(19). The tunnelling coefficient depends on the physical form of the Wannier function. Seen from Eq.(13) the physical form differs in each direction, the consequence of this is that for tunnelling in a direction orthogonal to the node, results in that the Wannier function for the first band ($W_{1j_\alpha}(\alpha)$) will determine the tunnelling coefficient. On the other hand, when tunnelling happens in the direction of the node, the Wannier function for the second band ($W_{2j_\alpha}(\alpha)$) will determine the coefficient. This directly means that tunnelling in the x-direction for an x-flavour atom has an larger probability then tunnelling in the y-direction, and vice-versa is true for the y-flavoured atoms.

By observing the characteristics of the various parts of the Hamiltonian, the effect from each becomes apparent. H_0 is the energy associated with tunnelling and the trapping potential. In the first part, the sum counts every different case of tunnelling for the two flavours by destroying a particle on one site and creating it on another. The result are four different terms accounting for tunnelling of the two flavours in the two available directions. The second part shifts the energy on each site due to the trapping potential and the number of particles. This is done by utilizing the number operator $n_{\alpha\beta}$ which counts the number of particles of each flavour. H_0 usually denotes the ideal part because the lack of any terms depending on inter-particle interactions, and can because of that be compared to the physics of a single particle.

H_{nn} accounts for what will be called the density-density contribution of the energy. The first term takes into consideration the energy build-up in each site with an increase amount of particles. This can easily be seen from the factor $n_{\alpha,j}(n_{\alpha,j} - 1)$. If there is only one particle in the lattice site then the factor becomes zero as a consequence of $(n_{\alpha,j} - 1)$, meaning that this term only gives a contribution when there are several particles at the site. Important to notice is that this term only counts the number

of particles of the same flavour. The second term accounts for the inter-particle's interaction between the different flavours by simply counting the number of particles of both flavours.

The last part of the Hamiltonian, H_{FD}, is responsible solely for what will be known as the inter-flavour conversion. This interaction accounts for the changing of particle's flavour. This change take place within a single site j. It is important to notice that tunnelling and change of flavour is not allowed within the same process, thus a particle cannot tunnel *and* change its flavour at the same time. The two terms in the sum accounts for both cases, two particles changing flavour from y to x, and two particles changing flavour from x to y. The energy of this process depends on the interaction strength $U_{\alpha\beta}$, meaning that a stronger interaction leads to higher energy required to change the flavour. Hence, this process can be viewed as two identical particles colliding within the same site and thereafter scattering into the other.

2.2 Arriving at the equations of motion

With the Hamiltonian known it is possible to calculate the equations of motion of what will be the *order parameter* ψ. This can be achieved by making use of the Euler-Lagrange equation or Heisenberg's equation of motion. In this thesis the later one will be used[6]. The operators of interest are the annihilation/creation operators which in the mean-field approximation (more detail on this approximation will follow) are replaced by the complex numbers ψ. Heisenberg's equation of motion takes the following form for the two operators of the x-flavour (the y-flavour ones are identical except the indices),

$$\dot{a}^\dagger_{x,i} = \frac{i}{h}\left[a^\dagger_{x,i}, H\right] = \frac{i}{h}\left(\left[a^\dagger_{x,i}, H_0\right] + \left[a^\dagger_{x,i}, H_{nn}\right] + \left[a^\dagger_{x,i}, H_{FD}\right]\right), \tag{21}$$

$$\dot{a}_{x,i} = \frac{i}{h}\left[a_{x,i}, H\right] = \frac{i}{h}\left(\left[a_{x,i}, H_0\right] + \left[a_{x,i}, H_{nn}\right] + \left[a_{x,i}, H_{FD}\right]\right). \tag{22}$$

Here, H_0, H_{nn} and H_{FD} are all given in the previous section. Because of the similarity when calculating the motion of the two operators only one of them will be calculated in this thesis, the other ones follow in a similar

[6]This is mainly done to differentiate this thesis from the work of [2].

manner. Moreover the operators $a^\dagger$ and a contain the same information and only differ by hermite conjugation. Hence, it is sufficient to calculate the motion for only one of them. The commentator can be calculated by parts and so with H_0

$$\frac{i}{h}\left[a^\dagger_{x,i}, H_0\right] = \frac{i}{h}\left[a^\dagger_{x,i}, \left(-\sum_{\alpha,\beta}\sum_{(ij)_\beta} t_{\alpha\beta} a^\dagger_{\alpha,i} a_{\alpha,j} + \sum_\alpha \sum_j V_{trap}(R_j) n_{\alpha,j}\right)\right]. \tag{23}$$

To more clearly see the nature of the Hamiltonian it can be useful to explicitly write out each part of the tunnelling. Each term will correspond to tunnelling in a certain direction for some flavour. Important to notice is the only terms that correspond to tunnelling to a neighbour site will be allowed in accordance with the tight-binding approximation. Furthermore, the number operator has in this case reverted back to its definition to simplify the calculations. Explicitly the commentator take the form of

$$\begin{aligned}\Big[a^\dagger_{x,i}, \Big\{ &-t_{xx}\left(a^\dagger_{x,i+1}a_{x,i} + a^\dagger_{x,i-1}a_{x,i} + a^\dagger_{x,i}a_{x,i+1} + a^\dagger_{x,i}a_{x,i-1}\right) \\ &-t_{xy}\left(a^\dagger_{x,j+1}a_{x,j} + a^\dagger_{x,j-1}a_{x,j} + a^\dagger_{x,j}a_{x,j+1} + a^\dagger_{x,j}a_{x,j-1}\right) \\ &-t_{yx}\left(a^\dagger_{y,i+1}a_{y,i} + a^\dagger_{y,i-1}a_{y,i} + a^\dagger_{y,i}a_{y,i+1} + a^\dagger_{y,i}a_{y,i-1}\right) \\ &-t_{yy}\left(a^\dagger_{y,j+1}a_{y,j} + a^\dagger_{y,j-1}a_{y,j} + a^\dagger_{y,j}a_{y,j+1} + a^\dagger_{y,j}a_{y,j-1}\right) \\ &+\sum_\alpha\sum_j V_{trap}(R_j)a^\dagger_{x,j}a_{x,j}\Big\}\Big].\end{aligned} \tag{24}$$

To evaluate this commutator the following relations are used

$$\left[a_{\alpha,i}, a^\dagger_{\alpha,i}\right] = 1, \left[a^\dagger_{\alpha,i}, a_{\alpha,i}\right] = -1, \tag{25}$$

$$\left[a^\dagger_{\alpha,i}, a^\dagger_{\beta,i}\right] = \left[a^\dagger_{\alpha,i}, a_{\beta,i}\right] = 0, \tag{26}$$

$$[a^\dagger_{\alpha,i}, a^\dagger_{\alpha,j}] = 0. \tag{27}$$

The last two of these are trivial if one just consider each site of the lattice to belong to its own Hilbert space (and thus commute). The first one is

the well known relation between the bosonic creation/annihilation operators and follows from the fact that the creation/annihilation operator change the eigenvalue of the number operator by one. Along with these relations it is also necessary to use the following identity for the commutators

$$[A, BC] = [A, B]C + B[A, C], \tag{28}$$

where A, B and C are operators.

With these relations and the identity for the commutator it is possible to evaluate Eq.(24). In this case where the motion of an x-flavour operator is wanted, only the terms with t_{xx} and t_{xy} and the term stemming from the potential trap will give a non-zero contribution. The calculation of the remaining commutators are trivial if the above mentioned relations are used. The result of the calculation is

$$\frac{i}{h}\left[a^\dagger_{x,i}, H_0\right] = -\sum_{\beta\in x,y} t_{x\beta}(a^\dagger_{x,j+1_\beta} - 2a^\dagger_{x,j} + a^\dagger_{x,j-1_\beta}) + \frac{\omega^2}{2}(x_j^2 + y_j^2)a^\dagger_{x,j}, \tag{29}$$

where the expression for the potential trap has been used. Also the term with the factor of two has been added on the tunnelling terms for future use. The adding of the factor two does not change the final expression because it only amounts to an overall energy shift.

The two remain parts of the Hamiltonian (responsible for the interaction) can together be written explicitly as

$$\begin{aligned} H_U = H_{nn} + H_{FD} = &\frac{U_{xx}}{2}a^\dagger_{x,j}a^\dagger_{x,j}a_{x,j}a_{x,j} + \frac{U_{yy}}{2}a^\dagger_{y,j}a^\dagger_{y,j}a_{y,j}a_{y,j} \\ &+U_{xy}a^\dagger_{x,j}a_{x,j}a^\dagger_{y,j}a_{y,j} + U_{yx}a^\dagger_{y,j}a_{y,j}a^\dagger_{x,j}a_{x,j} \\ &+\frac{U_{xy}}{2}(a^\dagger_{x,j}a^\dagger_{x,j}a_{y,j}a_{y,j} + a^\dagger_{y,j}a^\dagger_{y,j}a_{x,j}a_{x,j}) \\ &+\frac{U_{yx}}{2}(a^\dagger_{x,j}a^\dagger_{x,j}a_{y,j}a_{y,j} + a^\dagger_{y,j}a^\dagger_{y,j}a_{x,j}a_{x,j}), \end{aligned} \tag{30}$$

where the number operator has been replaced by the creation/annihilation operator. The calculations of the commutators follows in a similar way as before, where the known relations for the creation/annihilation operators are used along with the identity for the commutator. The only real difference in

the calculation process is the appearances of commutators with four operators. Still this is easily solved by once again utilizing the operator identity[7]. The result of the calculation is

$$\frac{i}{h}\left[a^{\dagger}_{x,i}, H_U\right] = (U_{xx}a^{\dagger}_{x,j}a_{x,j} + (U_{xy}+U_{yx})a^{\dagger}_{y,j}a_{y,j})a^{\dagger}_{x,j} + \left(\frac{U_{xy}+U_{yx}}{2}\right)a^{\dagger}_{y,j}a^{\dagger}_{y,j}a_{x,j}. \tag{31}$$

Putting everything together, along with replacing the operator $a^{\dagger}$ with (in the spirit of the mean-field approximation) the complex number ψ^* yields[8]

$$\begin{aligned} -i\frac{\partial \psi^*_{x,j}}{\partial t} &= -\sum_{\beta \in x,y} t_{x\beta}(\psi^*_{x,j+1_\beta} - 2\psi^*_{x,j} + \psi^*_{x,j-1_\beta}) + \frac{\omega^2}{2}(x_j^2 + y_j^2)\psi^*_{x,j} \\ &+ (U_{xx}|\psi_{x,j}|^2 + (U_{xy}+U_{yx})|\psi_{y,j}|^2)\psi^*_{x,j} + \left(\frac{U_{xy}+U_{yx}}{2}\right)(\psi^*_{y,j})^2\psi_{x,j}, \end{aligned} \tag{32}$$

where $\psi_{x,j} = a_{x,j}$. For completeness the motion for ψ^*_y is also presented below, obtained in a completely analogous way

$$\begin{aligned} -i\frac{\partial \psi^*_{y,j}}{\partial t} &= -\sum_{\beta \in x,y} t_{y\beta}(\psi^*_{y,j+1_\beta} - 2\psi^*_{y,j} + \psi^*_{y,j-1_\beta}) + \frac{\omega^2}{2}(x_j^2 + y_j^2)\psi^*_{x,j} \\ &+ (U_{yy}|\psi_{y,j}|^2 + (U_{xy}+U_{yx})|\psi_{x,j}|^2)\psi^*_{y,j} + \left(\frac{U_{xy}+U_{yx}}{2}\right)(\psi^*_{x,j})^2\psi_{y,j}. \end{aligned} \tag{33}$$

The normalizing condition is given by

$$N = N_x + N_y = \sum_j |\psi_{x,j}|^2 + \sum_j |\psi_{y,j}|^2, \tag{34}$$

where N is the total number of atoms in the lattice and where $|\psi_{\alpha,j}|^2$ is the density of the flavour given by $n_{\alpha,j} = |\psi_{\alpha,j}|^2$ which tells the number of atoms of a certain flavour α in site j.

The equations of motion for the x- and y-flavour are at first sight very similar to one another, in the sense that each x-flavoured term is replaced by

[7]The identity is uses such as [A,BCD]= [A,BC]D+BC[A,D].

[8]The two resulting equations of motion are usually called *Gross-Pitaevskii equations*. A Gross-Pitaevskii equation is a form of non-linear Schrödinger equation.

a y-flavoured one in the case of ψ_y. Important to notice however is again the presence of the tunnelling coefficient which strongly depends on the overlap of the Wannier functions. Any change to the periodic potential will affect the motion of ψ. In order to determine the behaviour of the flavours these two equations of motion have to be solved for what now is the total order parameter $\psi = (\psi_{x,j}, \psi_{y,j})$ (that is to say that the order parameter possess a *spinor* character). In the following section one of the possible way to solve these equations will be discussed, namely the *split-operator method*.

2.3 Solving the equations

With the equations of motion now known the task has come to try and solve them in a sufficiently effective manner. As usual there is always the option of solving the equations by employing purely numerical methods (like some form of Runge–Kutta method) but this would in this case require a more substantial amount of computer power and also be less elegant. Instead of using more traditional methods this thesis will opt to use the split-operator method[9] (which is also a numerical method). In the following calculations the equations of motion for ψ_x and ψ_y will be used instead of ψ_x^* and ψ_y^*, ψ and ψ^* are related by an hermitian conjugate as said previously. To continue with the calculations, a continuum approximation will be invoked to reduce the terms related to the tunnelling to

$$\psi_{\alpha,j+1_\beta} - 2\psi_{\alpha,j} + \psi_{\alpha,j-1_\beta} \to \frac{\partial^2}{\partial\beta^2}\psi_\alpha(\alpha,\beta), \tag{35}$$

which is possible because of the manually added factor of two from previously. This has to be done in order to make way for the ability to diagonalize the Hamiltonian later on. In the continuum approximation the kinetic energy is transformed from a form depending on the lattice to a form more akin to that of a free particle. This approximation is not exact but can however convey some of the aspects of the physical dynamics of the system while simplifying the calculations. Later in this section the discrete model (where the continuum approximation is relaxed) will be discussed but until then the continuum model will be used. By defining the matrix elements

[9]The notations used here will be similar to the ones used by Fernanda Pinheiro in her licentiate thesis, the author takes no credit for the formulation of the method here.

$$H_{11} = -t_{xx}\frac{\partial^2}{\partial x^2} - t_{xy}\frac{\partial^2}{\partial y^2} + U_{xx}|\psi_{x,j}|^2 + (U_{xy} + U_{yx})|\psi_{y,j}|^2, \tag{36}$$

$$H_{22} = -t_{yx}\frac{\partial^2}{\partial x^2} - t_{yy}\frac{\partial^2}{\partial y^2} + U_{yy}|\psi_{y,j}|^2 + (U_{xy} + U_{yx})|\psi_{x,j}|^2, \tag{37}$$

$$H_{12} = (\frac{U_{xy} + U_{yx}}{2})\psi_{y,j}\psi^*_{x,j}, \tag{38}$$

$$H_{21} = (\frac{U_{xy} + U_{yx}}{2})\psi_{x,j}\psi^*_{y,j}, \tag{39}$$

the equations of motion (32) and (33) can then be rewritten as

$$i\frac{\Psi_j}{\partial t} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \Psi_j \tag{40}$$

where $\Psi_j = \begin{bmatrix} \psi_{xj} \\ \psi_{yj} \end{bmatrix}$. This has the non-trivial general solution

$$\Psi_j = e^{-iHt}\Psi'_j, \tag{41}$$

where Ψ'_j is the solution at time 0. Moving on, use that the evolution operator obeys

$$U(dt) = e^{-iHdt} = exp\left(-i\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} dt\right) =$$
$$exp\left(-i\left\{\begin{bmatrix} H_{11} & 0 \\ 0 & H_{22} \end{bmatrix} + \begin{bmatrix} 0 & H_{12} \\ H_{21} & 0 \end{bmatrix}\right\} dt\right).$$

Matrix multiplication is non commutative but for small dt:s ($\lim\ dt \to 0$) the following approximation is valid

$$U(dt) \approx e^{-idt\begin{bmatrix} H_{11} & 0 \\ 0 & H_{22} \end{bmatrix}} e^{-idt\begin{bmatrix} 0 & H_{12} \\ H_{21} & 0 \end{bmatrix}} = U_1(dt)U_2(dt). \tag{42}$$

This is the essence of the split-operator method. At this point $U_2(dt)$ can be Taylor expanded (as dt is small). The expansion is given by

$$e^{-idtA} = \sum_{n=0}^{\infty} \frac{(-idt)^n}{n!}A^n = 1 - idtA + \frac{(-idt)^2}{2}A^2 + \frac{(-idt)^3}{6}A^3 + \dots, \tag{43}$$

where $A = \begin{bmatrix} 0 & H_{12} \\ H_{21} & 0 \end{bmatrix}$. Reviewing the expansion subsequent it is noticed that for even and odd powers the following is true (if $\kappa = \frac{U_{xy}+U_{yx}}{2}$)

$$\frac{(-idt)^n}{n!}A^n = \frac{(-idt)^{n-1}}{n!}|\psi_{xj}|^{n-1}|\psi_{yj}|^{n-1}\kappa^{n-1}\begin{bmatrix} 0 & -idt\kappa\psi_{yj}\psi_{xj}^* \\ -idt\kappa\psi_{xj}\psi_{yj}^* & 0 \end{bmatrix} \tag{44}$$

for odd terms (where n is an odd number) and

$$\frac{(-idt)^n}{n!}A^n = \frac{(-idt)^n}{n!}\kappa^n|\psi_{xj}|^n|\psi_{yj}|^n\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{45}$$

for even terms (n is an even number). An example of the two cases is given by

$$\begin{bmatrix} 0 & H_{12} \\ H_{21} & 0 \end{bmatrix}^2 = \begin{bmatrix} \kappa^2|\psi_{xj}|^2|\psi_{yj}|^2 & 0 \\ 0 & \kappa^2|\psi_{xj}|^2|\psi_{yj}|^2 \end{bmatrix} \tag{46}$$

and

$$\begin{bmatrix} 0 & H_{12} \\ H_{21} & 0 \end{bmatrix}^3 = \kappa^3|\psi_{xj}|^2|\psi_{yj}|^2\begin{bmatrix} 0 & \psi_{yj}\psi_{xj}^* \\ \psi_{xj}\psi_{yj}^* & 0 \end{bmatrix}, \tag{47}$$

both which are contained in the more general form given above. At this point it is noticed that the resulting terms from the expansion that are even are the same as those from the expansion of $\cos x$ where x is the argument of expansion, likewise the terms from the expansion that are odd are the same as those from the expansion of $\frac{\sin x}{x} = \operatorname{sinc} x$. Thus it is possible to write U_2 as

$$U_2(dt) = \begin{bmatrix} \cos(\kappa dt\,|\psi_{xj}||\psi_{yj}|) & -idt\kappa\operatorname{sinc}(\kappa dt\,|\psi_{xj}||\psi_{yj}|)\psi_{yj}\psi_{xj}^* \\ -idt\kappa\operatorname{sinc}(\kappa dt\,|\psi_{xj}||\psi_{yj}|)\psi_{xj}\psi_{yj}^* & \cos(\kappa dt\,|\psi_{xj}||\psi_{yj}|) \end{bmatrix}. \tag{48}$$

To proceed, the purpose of the method is to form $\Psi(dt) = U_1(dt)U_2(dt)\Psi' = U_1(dt)\tilde{\Psi}$ where $\tilde{\Psi} = U_2(dt)\Psi'$. With this the equation takes the form of

$$\begin{bmatrix} \psi_{xj} \\ \psi_{yj} \end{bmatrix} = \begin{bmatrix} e^{-idtH_{11}} & 0 \\ 0 & e^{-idtH_{22}} \end{bmatrix}\begin{bmatrix} \tilde{\psi}_{xj} \\ \tilde{\psi}_{yj} \end{bmatrix}. \tag{49}$$

With closer inspection of the expression for H_{11} and H_{22} it becomes apparent that another split-operator is needed in order to separate the momentum part

from the position part. Thus, the exponentials containing H_{11} and H_{22} are rewritten as

$$e^{-idtH_{11}} = exp\left\{-idt\left(-t_{xx}\frac{\partial^2}{\partial x^2} - t_{xy}\frac{\partial^2}{\partial y^2} + U_{xx}|\psi_{xj}|^2 + (U_{xy}+U_{yx})|\psi_{yj}|^2\right)\right\} \approx$$
$$exp\left\{-idt\left(-t_{xx}\frac{\partial^2}{\partial x^2} - t_{xy}\frac{\partial^2}{\partial y^2}\right)\right\} exp\left\{-idt\left(U_{xx}|\psi_{xj}|^2 + (U_{xy}+U_{yx})|\psi_{yj}|^2\right)\right\} \tag{50}$$

and

$$e^{-idtH_{22}} = exp\left\{-idt\left(-t_{yx}\frac{\partial^2}{\partial x^2} - t_{yy}\frac{\partial^2}{\partial y^2} + U_{yy}|\psi_{yj}|^2 + (U_{xy}+U_{yx})|\psi_{xj}|^2\right)\right\} \approx$$
$$exp\left\{-idt\left(-t_{yx}\frac{\partial^2}{\partial x^2} - t_{yy}\frac{\partial^2}{\partial y^2}\right)\right\} exp\left\{-idt\left(U_{yy}|\psi_{yj}|^2 + (U_{xy}+U_{yx})|\psi_{xj}|^2\right)\right\}, \tag{51}$$

where again the assumption that dt is small has been made. Taking this into consideration, Eq.(49) instead takes the form of

$$\Psi(dt) = u_1 u_2 \tilde{\Psi} \tag{52}$$

where u_1 and u_2 are defined as

$$u_1 = \begin{bmatrix} e^{-idt\left(-t_{xx}\frac{\partial^2}{\partial x^2} - t_{xy}\frac{\partial^2}{\partial y^2}\right)} & 0 \\ 0 & e^{-idt\left(-t_{yx}\frac{\partial^2}{\partial x^2} - t_{yy}\frac{\partial^2}{\partial y^2}\right)} \end{bmatrix} \tag{53}$$

and

$$u_2 = \begin{bmatrix} e^{-idt\left((U_{xx}|\psi_{xj}|^2 + (U_{xy}+U_{yx})|\psi_{yj}|^2\right)} & 0 \\ 0 & e^{-idt\left((U_{yy}|\psi_{yj}|^2 + (U_{xy}+U_{yx})|\psi_{xj}|^2\right)} \end{bmatrix}. \tag{54}$$

In order to obtain the ground-state a guess of a feasible ground-state must first be made. A good guess is a Gaussian wave function.

After making a starting guess the procedure to obtain the true ground-state can begin. The first step is to calculate $u_2\tilde{\Psi}$, where Ψ' is the guessed ground-state at time zero. This is easily done by simple multiplication. The next step is to apply u_1 to $u_2\tilde{\Psi}$ as in Eq.(52). This would however result

in an cumbersome calculation as a consequence of the second derivative in u_1. On the other hand, in momentum space the calculation would simplify greatly as the second derivative would be replaced by P^2 which in momentum space is a diagonal operator. Therefore the resulting calculations would only amount to a simple multiplication. What is left, is to Fourier transform $u_2\tilde{\Psi}$ from position space to momentum space. This is easily done numerically by utilizing the *fast Fourier transformation algorithm*. After the trivial multiplication with u_1, the resulting momentum function is transformed back (by the means of the *inverse Fourier transformation*), yielding the final result. The sequence can be formulated as

$$\begin{bmatrix}\psi_{x,j}(t+dt)\\ \psi_{y,j}(t+dt)\end{bmatrix} = \mathcal{F}^{-1}\left\{\begin{bmatrix} e^{-\left(-t_{xx}\frac{\partial^2}{\partial x^2}-t_{xy}\frac{\partial^2}{\partial y^2}\right)idt} & 0\\ 0 & e^{-\left(-t_{yx}\frac{\partial^2}{\partial x^2}-t_{yy}\frac{\partial^2}{\partial y^2}\right)idt}\end{bmatrix}\mathcal{F}\left\{u_2\tilde{\Psi}\right\}\right\} \tag{55}$$

where $\mathcal{F}$ is the Fourier transform and $\mathcal{F}^{-1}$ is the inverse Fourier transform. The result of the method is the ability to obtain the wave function in a later time dt.

Finally comes the most important factor in how this procedure can give the ground-state. The trick is to propagate in imaginary time which works in the following way [7]. Start with the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi. \tag{56}$$

If the derivative is take with respect to imaginary time the Schrödinger equation takes the form of

$$\frac{\partial\psi}{\partial it} = \frac{-H\psi}{\hbar}, \tag{57}$$

where $\hbar$ will be put to one as previously done. Now expand ψ in eigenfunctions to the Hamiltonian H and make it so that each eigenfunction has the matching energy value E_j, i.e.

$$\psi = \sum_j c_j\psi_j, \tag{58}$$

where

$$H\psi_j = E_j\psi_j. \tag{59}$$

At this point define the imaginary time τ as

$$\tau = -it, \tag{60}$$

then the general solution to the Schrödinger equation will be

$$\psi_j(\tau) = e^{-\tau H_j}\psi_j(0) = e^{-\tau E_j}\psi_j(0). \tag{61}$$

As the imaginary time progresses each of the eigenfunction will decay in an exponentially way. The rate in which it decays will be related to the energy E_j of the eigenfunction and the ground-state will relate to other eigenstate as

$$\frac{\psi_i(\tau)}{\psi_0(\tau)} \propto e^{-\tau(E_j - E_0)}. \tag{62}$$

This gives the indication that states that are not the ground-state will be exponentially suppressed and vanishing quicker then that of the ground-state. For completeness the original wave function takes the form of

$$\psi(\tau) = \sum_j c_j\psi_j(\tau) = \sum_j e^{-\tau E_j}\psi_j(0)c_j. \tag{63}$$

Taking the overlap between the ground-state and *any* state gives

$$\lim_{\tau\to\infty} \frac{\langle\psi(\tau)|c_0\psi_0(\tau)\rangle}{\langle\psi(\tau)|\psi(\tau)\rangle} = \lim_{\tau\to\infty} \frac{c_0^2 e^{-2\tau E_0}}{c_0^2 e^{-2\tau E_0} + \sum_{j=1}^{\infty} c_j^2 e^{-2\tau E_j}}. \tag{64}$$

which means that regardless of which wave function is chosen it will in the limit of $\tau \to \infty$ converge to the ground-state because of $E_j > E_0$. Thus

$$\psi(\tau) = c_0 e^{-\tau H}\psi_0(0) + \mathcal{O}\left(e^{-\tau(E_1 - E_0)}\right) \tag{65}$$

is true for any wave function. Moreover, if the initial wave function is chosen is such a way that the overlap c_0 between the chosen wave function and the ground-state wave function is non-zero the the ground-state can be explicitly calculated using

$$\psi_0(0) = \lim_{\tau\to\infty} \frac{\psi(\tau)}{\sqrt{\langle\psi(\tau)|\psi(\tau)\rangle}}. \tag{66}$$

To summarize, the split-operator method together with the Imaginary Time Propagation is able to yield the ground-state for the system. This whole process will be carried out by a computer and with sufficiently small time steps to keep the approximation in the split operator method valid. With the ground-state known it becomes possible to make predictions on the physics of the system.

2.3.1 The discrete model

Previously the equations of motion where solved by applying the continuum approximation to the term responsible for what can be thought on as the kinetic energy of the system. This approximation can however not capture every part for the physical system. Thus instead of approximating the kinetic energy as a continuum, the tunnelling part has to be treated as a discreet phenomena. This is done by transforming the terms responsible for the kinetic energy from position space to momentum space. In momentum space the free Hamiltonian H_0 will be diagonalizable and the problem will be solvable. To obtain the discrete model of the Hamiltonian, a discrete Fourier transformation will be made. This transformation will only be made on H_0 of the full Hamiltonian that in the continuum approximation is replaced by the second derivative, the part that leads to

$$-\sum_{\beta\in x,y} t_{x\beta}(a^\dagger_{x,j+1_\beta} - 2a^\dagger_{x,j} + a^\dagger_{x,j-1_\beta}). \tag{67}$$

The part that is responsible for this term is the tunnelling

$$-\sum_{\alpha,\beta}\sum_{\langle ij\rangle_\alpha} t_{\alpha\beta}a^\dagger_{\alpha\mathbf{i}}a_{\alpha\mathbf{j}}, \tag{68}$$

in the Hamiltonian. Therefore $a^\dagger$ and a will be transformed, from position space to momentum space by the use of a discrete Fourier transformation. To carry out this transformation the following relations has to be known

$$\sum_i e^{-i\chi_i(k'-k)} = \delta_{k'k}, \tag{69}$$

where $\delta_{k'k}$ is the Kronecker delta; and where the relation between the creation and annihilation operator for position space to momentum space is

$$a_{x,i} = \sum_k e^{ik\chi_i} a_{xk}, \tag{70}$$

where[10] x is the index that as usually denote the flavour, χ is the notation for distance in the x-direction in the lattice (to avoid confusion with the flavour notation) and where k indicates the discrete momentum index. In Eq.(69) it was used that k and χ are related by the discrete Fourier transform. Writing out the tunnelling term for two neighbouring sites[11] gives

$$-t_{xx} \sum_i (a^\dagger_{x,i+1} a_{x,i} + a^\dagger_{x,i} a_{x,i+1}), \tag{71}$$

accounting for the tunnelling between two neighbouring sites. By employing the momentum expression for $a^\dagger$ and a, the tunnelling term takes the form

$$-t_{xx} \sum_i \left(\sum_{k'} e^{-ik'\chi_{i+1}} a^\dagger_{x,k'} \sum_k e^{ik\chi_i} a_{x,k} + \sum_k e^{-ik\chi_i} a^\dagger_{x,k} \sum_{k'} e^{ik'\chi_{i+1}} a_{x,k'} \right) \tag{72}$$

with $a^\dagger_{x,i} = \sum\limits_k e^{-ik\chi_i} a^\dagger_{xk}$.

To proceed with the calculations the position distance χ_{i+1} is rewritten as $\chi_i + s$, where s is the distance between two neighbouring sites in the lattice. With this, the expression becomes

$$-t_{xx} \sum_i \left(\sum_{k',k} e^{-ik'(\chi_i+s)} a^\dagger_{x,k'} e^{ik\chi_i} a_{x,k} + \sum_{k,k'} e^{-ik\chi_i} a^\dagger_{x,k} e^{ik'(\chi_i+s)} a_{x,k'} \right), \tag{73}$$

where $\sum\limits_{k',k}$ and $\sum\limits_{k,k'}$ are the sum over both k and k'. This can be written as

$$\begin{aligned} -t_{xx} &\left(\sum_{k',k} \sum_i e^{-i\chi_i(k'-k)} e^{-ik's} a^\dagger_{x,k'} a_{x,k} + \sum_{k,k'} \sum_i e^{-i\chi_i(k-k')} e^{iks} a^\dagger_{x,k} a_{x,k'} \right) \\ &= -t_{xx} \left(\sum_{k',k} \delta_{k',k} e^{-ik's} a^\dagger_{x,k'} a_{x,k} + \sum_{k,k'} \delta_{k,k'} e^{iks} a^\dagger_{x,k} a_{x,k'} \right). \end{aligned} \tag{74}$$

[10] As previously, the calculation will only be carried out for one flavour (x here), the other one follow analogously.

[11] Here the sites $i+1$ and i are considered, any two sites with the different of one will give the same result with same kind of calculations.

Now the Kronecker delta will eliminate every term expect the one where $k' = k$, thus

$$-t_{xx} \sum_k \left(e^{-iks} a^\dagger_{x,k} a_{x,k} + e^{iks} a^\dagger_{x,k} a_{x,k} \right) = -t_{xx} \sum_k 2\cos(ks) n_{x,k} \,, \tag{75}$$

where as before $a^\dagger_{x,k} a_{x,k} = n_{x,k}$ and $\cos(ks) = (e^{-iks} + e^{iks})/2$. So the tunnelling factor is transformed by

$$-t_{xx} \sum_i (a^\dagger_{x,i+1} a_{x,i} + a^\dagger_{x,i} a_{x,i+1}) \to t_{xx} \sum_k 2\cos(ks) n_{x,k} \tag{76}$$

from position space to momentum space. Note that $a_{x,k}$ annihilates an atom with quasimomentum k in the x-flavour, and $n_{x,k}$ counts the number of atoms with quasimomentum k. With the Hamiltonian now diagonalized the same process as before can be applied (split-operator method along with imaginary time propagation) to obtain the ground-state for the discreet model. In the result part the discreet model is the one that will be used.

2.4 Mean-field and the chequerboard pattern

Up until now the mean-field approximation has not been discussed in any detail. In this section the mean-field approximation will be discussed and more importantly, the consequences of it will be revealed. Important to notice is that this discussion is carried out in the absent of the confining trap. When the trap is present the behaviour of the system (in the mean-field approximation) will be modified. Previously the mean-field approximation was used to replace the creation/annihilation operators with complex numbers. The argument why this is possibly can be given more or less in detail. This thesis will try to given an somewhat intuitive explanation[12].

It is known that the dynamics in each lattice site i depend on the number of atoms in the site. By minimizing the uncertainty in the number of atoms for every lattice site one can argue that the most "classical" state is obtained. In order to do this, a corresponding state must be found which minimize the uncertainty for the number operator $\hat{n}_{\alpha,j}$. For the harmonic oscillator only the ground-state corresponding to $n_x = n_y = 0$ (the quantum number n

[12]None of the claims made to explain this will be proven or motivated in any detail, the focus will be on motivating the use of the mean-field approximation.

and the number operator $\hat{n}_{\alpha,j}$ are not the same) fulfils this condition, this is obviously not an option for this thesis because every site is assumed to contain a large number of atoms. However, it is possible to form a linear combination of *Fock states* $|n\rangle$ that still fulfils the uncertainty condition, this is known as a *coherent state*. Moreover, a coherent state is an eigenfunction to the creation/annihilation operator

$$\hat{a}_{\alpha,j} |\Psi\rangle = \psi_{\alpha,j} |\Psi\rangle \tag{77}$$

where $\psi_{\alpha,j}$ can be any complex number. So by making a coherent states ansatz it is possible to exchange the creation/annihilation operators by complex numbers $\psi_{\alpha,j}$. Furthermore it is known that the amplitude to a coherent state evolve with time as

$$\psi_{\alpha,j}(t) = e^{-i\omega t}\psi_{\alpha,j}, \tag{78}$$

where ω is the frequency of the harmonic oscillator. This relation can only be strictly true for a system described solely by the Hamiltonian corresponding to the harmonic oscillator. In the presence of tunnelling terms the expression will be affected. This is foremost an illustration of the fact that ψ is a parameter that evolves in time. With this in mind, $\psi_{\alpha j}$ can be seen as an order parameter for the system. The mean-field approximation is thus to make the ansazts that each state in every site can be taken as a coherent state which minimize the uncertainty in the number of atoms. This can however only be the case when it is possible to regard the interaction contribution from each of the particles (and potentials) as steaming from a single source[13], this is essentially what the mean-field approximation is. Another way to see the mean-field approximation is that the typical, average behaviour, a value is assigned to the system as a whole, in this case it would mean that every site is take to be in a coherent state regardless of the site index j or the number statistics of particles present at the site.

As stated before, the mean-field approximation is equivalent to assigning a complex number ψ^* to each available operator $a^\dagger$ in each site i. It is also known that to every complex number there exist a analogous polar representation. Therefore, the mean-field approximation can be seen as

$$a^\dagger_{x,i} \to |\psi_{x,i}| e^{i\theta_{x,i}}, \tag{79}$$

[13]The harmonic approximation does not take into account the full effect of the periodic potential.

$$a^{\dagger}_{y,i} \rightarrow |\psi_{y,i}| e^{i\theta_{y,i}}, \tag{80}$$

where $\theta_{x,i}$ is some angel, or *phase*. Substituting these expressions into the Hamiltonian for the first part H_0, yields

$$\begin{aligned} H_0 = &-t_{xx}\left(|\psi_x|^2 e^{i(\theta_{x,i+1}-\theta_{x,i})} + |\psi_x|^2 e^{i(\theta_{x,i-1}-\theta_{x,i})} + |\psi_x|^2 e^{i(\theta_{x,i}-\theta_{x,i+1})} + |\psi_x|^2 e^{i(\theta_{x,i}-\theta_{x,i-1})}\right) \\ &-t_{xy}\left(|\psi_x|^2 e^{i(\theta_{x,j+1}-\theta_{x,j})} + |\psi_x|^2 e^{i(\theta_{x,j-1}-\theta_{x,j})} + |\psi_x|^2 e^{i(\theta_{x,j}-\theta_{x,j+1})} + |\psi_x|^2 e^{i(\theta_{x,j}-\theta_{x,j-1})}\right) \\ &-t_{yx}\left(|\psi_y|^2 e^{i(\theta_{y,i+1}-\theta_{y,i})} + |\psi_y|^2 e^{i(\theta_{y,i-1}-\theta_{y,i})} + |\psi_y|^2 e^{i(\theta_{y,i}-\theta_{y,i+1})} + |\psi_y|^2 e^{i(\theta_{y,i}-\theta_{y,i-1})}\right) \\ &-t_{yy}\left(|\psi_y|^2 e^{i(\theta_{y,j+1}-\theta_{y,j})} + |\psi_y|^2 e^{i(\theta_{y,j-1}-\theta_{y,j})} + |\psi_y|^2 e^{i(\theta_{y,j}-\theta_{y,j+1})} + |\psi_y|^2 e^{i(\theta_{y,j}-\theta_{y,j-1})}\right) \\ &+\sum_{\alpha}\sum_{j} V_{trap}(R_j)|\psi_{\alpha,j}|^2, \end{aligned} \tag{81}$$

where it is assumed that the population is the same for the two flavours in all directions (so that $|\psi_x|$ and $|\psi_y|$ are the same for all sites), for example $|\psi_{\alpha,i/j}| = |\psi_{\alpha,i/j+1}| = |\psi_{\alpha,i/j-1}|$ and where i/j indicate either the i direction of the j direction. In the above expression, each term, except one, has a phase relation which is between the different sites. The exception being the term originating from the trapping potential which is phase independent. This should come as no surprise because as previously stated, the effect of the trap is not taken into consideration when making the approximation.

For the ground-state is the energy minimized (in this case the Hamiltonian) and therefore it is possible to determine a restriction on the phase relation between different sites. In order to determine the phase relation, the exponentials are rewritten as

$$e^{id} = \cos(d) + i\sin(d)$$

where d is the relative phase difference between two sites (i.e. $\theta_{x,i+1} - \theta_{x,i}$). Depending on the sign of the tunnelling parameter $t_{\alpha\beta}$ the following conditions minimize the kinetic Hamiltonian (or more specific H_0)

$$t_{xx} < 0 \rightarrow \theta_{x,i+1} - \theta_{x,i} = \pi, \tag{82}$$

$$t_{xx} > 0 \rightarrow \theta_{x,i+1} - \theta_{x,i} = 0. \tag{83}$$

In the above cases, the tunnelling are for x-flavoured atoms in different sites, all the remaining cases follow identically. By inspecting, from the definition of the tunnelling parameter (19) it becomes evident that $t_{xx}, t_{yy} < 0$ and $t_{xy}, t_{yx} > 0$.

In a similar manner, (79) and (80) are substituted in into H_{nn} and H_{FD}, resulting in

$$H_{nn} = \frac{U_{xx}}{2}|\psi_{x,j}|^4 + \frac{U_{yy}}{2}|\psi_{y,j}|^4 + (U_{xy} + U_{yx})|\psi_{x,j}|^2|\psi_{y,j}|^2 \tag{84}$$

and

$$H_{FD} = \left(\frac{U_{xy} + U_{yx}}{2}\right)|\psi_{x,j}|^2|\psi_{y,j}|^2 2\cos(2(\theta_{x,j} - \theta_{y,j})) \tag{85}$$

for the density-density part and for the interflavour interaction respectively. It is apparent that H_{nn} does not contain any information about phase locking within the sites. However, H_{FD} does contain such information, which is vital in determining the phase relation between the two flavours. As all parameters in H_{FD} are larger then zero, the only minimizing condition left is

$$\theta_{x,i} - \theta_{y,i} = \pm\frac{\pi}{2}, \tag{86}$$

meaning that the two flavour's phases are perpendicular to one another in every site. Consequently the mean-field approximation introduces a phase locking between different sites and different flavours in the entire lattice.

Moreover by substituting (79) and (80) into the expansion of the field operator (10) and (11) it takes the form

$$\psi_{\pm}(\mathbf{x}) = |\psi_{x,i}|e^{i\theta_{x,i}}W_{x,i}(\mathbf{x}) + |\psi_{y,i}|e^{i\theta_{y,i}}W_{y,i}(\mathbf{x}) = |\psi|(W_{x,i}(\mathbf{x}) \pm iW_{y,i}(\mathbf{x})) \tag{87}$$

where the phase relation between the two flavours has been used and where $\pm$ in the index indicates the two possible values corresponding to either a phase shift of $\pi/2$ or $-\pi/2$. Furthermore, $|\psi_x|$ is taken to be equal to $|\psi_y|$ (which is feasible for periodic potential without any confining trap) and are consequently replaced by $|\psi|$. By now employing the harmonic approximation for the Wannier functions

$$W_x \propto xe^{\frac{-(x^2+y^2)}{2\sigma^2}}, \tag{88}$$

$$W_y \propto ye^{\frac{-(x^2+y^2)}{2\sigma^2}}, \tag{89}$$

which is valid for a deep periodic potential (at which point every site can be thought on as possessing an independent harmonic oscillator). With this Eq.(87) can be written as

$$\psi_{\pm}(\mathbf{x}) = |\psi|(xe^{\frac{-(x^2+y^2)}{2\sigma^2}} \pm iye^{\frac{-(x^2+y^2)}{2\sigma^2}}). \tag{90}$$

This is a modified Gaussian which is only zero at the origin. If the above result is squared it yields

$$|\psi_i(\mathbf{x})|^2 = |\psi|^2(W_{x,i}^2(\mathbf{x}) + W_{y,i}^2(\mathbf{x})) = |\psi|^2(x^2+y^2)e^{\frac{-(x^2+y^2)}{\sigma^2}}, \tag{91}$$

but $|\psi_i(\mathbf{x})|^2$ is the population of atoms at site i and location x (the location x is taken within the lattice site i), meaning that the atoms in every lattice point is allocated in a circle around the origin (as seen from above in 2D). This can easily be seen by using polar coordinates

$$|\psi_i(\mathbf{x})|^2 = |\psi|^2(x^2+y^2)e^{\frac{-(x^2+y^2)}{\sigma^2}} = [x = r\cos(\Theta); y = r\sin(\Theta)] = |\psi|^2 r^2 e^{\frac{-r^2}{\sigma^2}} \tag{92}$$

where r depends on x and y and therefore give rise to a circular motion (if this is not taken into account the graph would be the same as for the first excited state in the harmonic oscillator).

What is left to study is the dynamics of the distribution of the atoms in the lattice. This can be done by calculating the angular momentum for the particles in a lattice site. The z-angular moment is given by

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \tag{93}$$

where the indices refer to the derivatives in the momentum operator. Applied to $\psi_{\pm}$ it results in

$$\hat{L}_z\psi_{\pm}(\mathbf{x}) = (\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)\psi_{\pm}(\mathbf{x}) \tag{94}$$

$$\hat{L}_z\psi_{\pm}(\mathbf{x}) = \pm\hbar|\psi|(xe^{\frac{-(x^2+y^2)}{2\sigma^2}} \pm iye^{\frac{-(x^2+y^2)}{2\sigma^2}}) = \pm\hbar\psi_{\pm}(\mathbf{x}). \tag{95}$$

The result of the calculation is a net unit angular momentum in one of the two directions resulting from the phase difference. Hence, the conclusion is that in each site the particles (atoms) are aligned in a circle like pattern which is rotating either clockwise or anticlockwise. In that sense each lattice site possess a vortex or antivortex. This depends on the phase between each site and will therefore lead to a alternating pattern akin to a chequerboard pattern. In figure (2) the chequerboard pattern is schematically demonstrated.

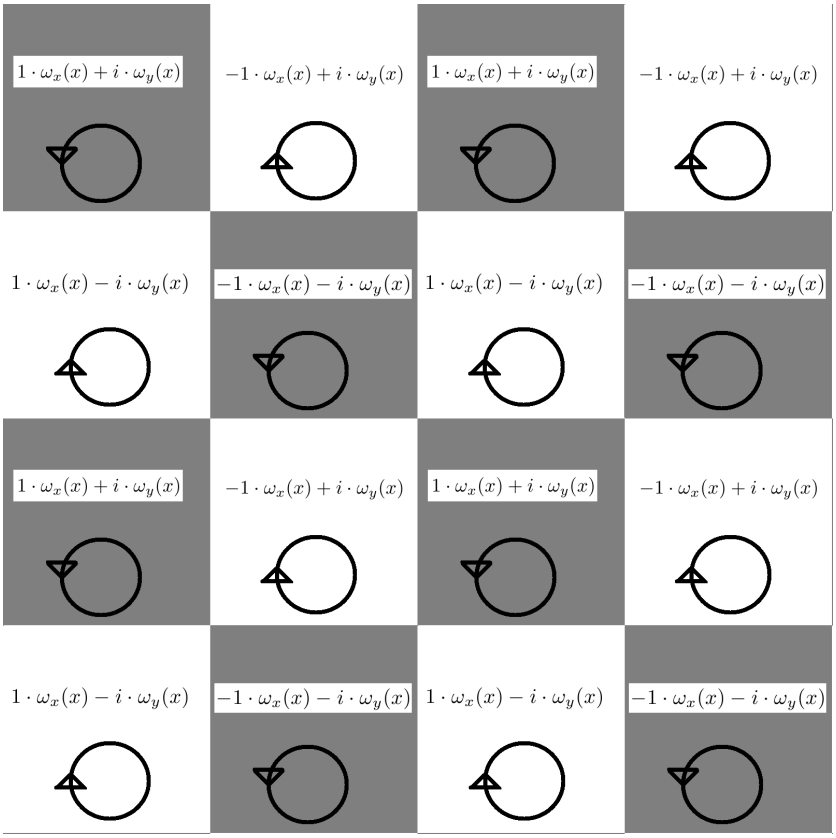

Figure 2: A simplified picture of the chequerboard pattern.

3 Results

With all the necessary theoretical tools now known, the ground-state can be calculated and its properties mapped out. Up until this section only a symmetrical lattice has been considered. This is however only one of the cases which will be studied in this paper. This section will explore the consequences of an anisotropic lattice on the condensate. Worth mentioning is that the harmonic potential is present in all the following results.

The outline for this section will be as follow. First the properties of the ground-state are presented along with the chequerboard pattern. In the subsection that succeeds, the *Landau-Zener formula* will be discussed, which will play a significant roll in the understanding of the evolution of weakly excited states in the anisotropic case. Lastly, the results from the ground-state

propagation in the case of an asymmetric lattice will be revealed. Important to notice is the theoretical discussion which will commence in the second subsection.

3.1 Properties of the ground-state

By utilizing every tools mentioned in the theoretical section the following four graphs are obtained. They depict the characteristics of the ground-state in the system as a whole. In figure (3) and (4) the population of the ground-state in the system is illustrated. As suspected from previously, the x-flavoured atoms tend to tunnel more strongly in the x-direction, creating the broadening structure seen in the picture (and vice versa for the y-flavour and its distribution). In figure (5) the difference between the two flavours is displayed, to further illustrate how the tunnelling difference helps to broaden the distribution. Finally in figure (6) the chequerboard pattern is shown with its alternating properties. For the following figures the dimensionless parameters are: $V_x = V_y = 17$, $\omega = 0.007$ and $U_0 N = 1$.

Important to notice is that the anisotropic tunnelling is only possible because of the confining trap as seen in the above figures. Without the trap there would be no preferred direction for the tunnelling resulting in an isotropic distribution that appears throughout the lattice. With the ground-state sufficiently examined, the concern now changes to the anisotropic lattice and the time evolution of the ground-state.

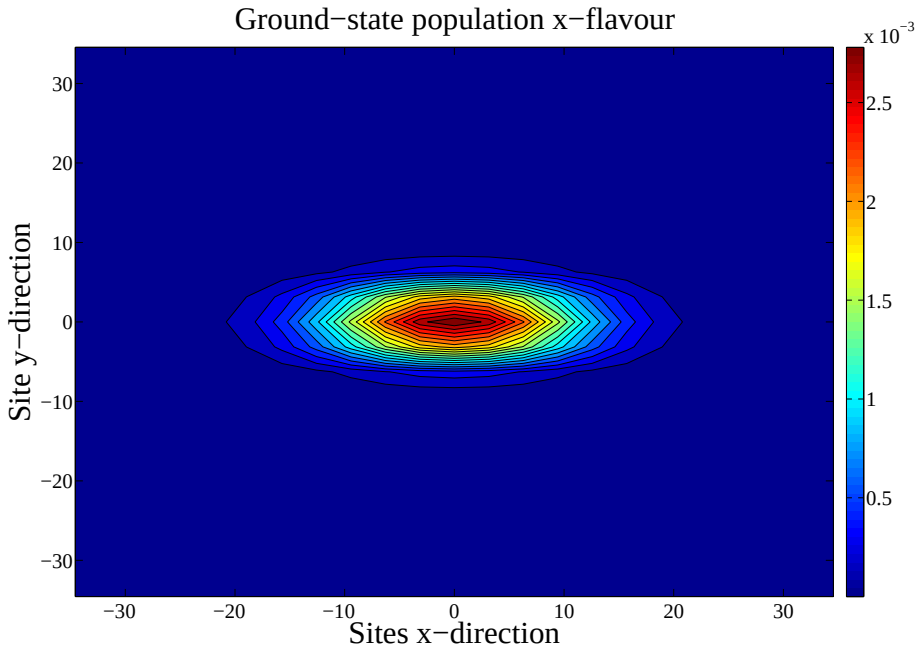

Figure 3: The population of x-flavoured atoms $|\psi_{x,i}|^2$ in the isotropic lattice. The colour indicates how populated each site is by the named flavour.

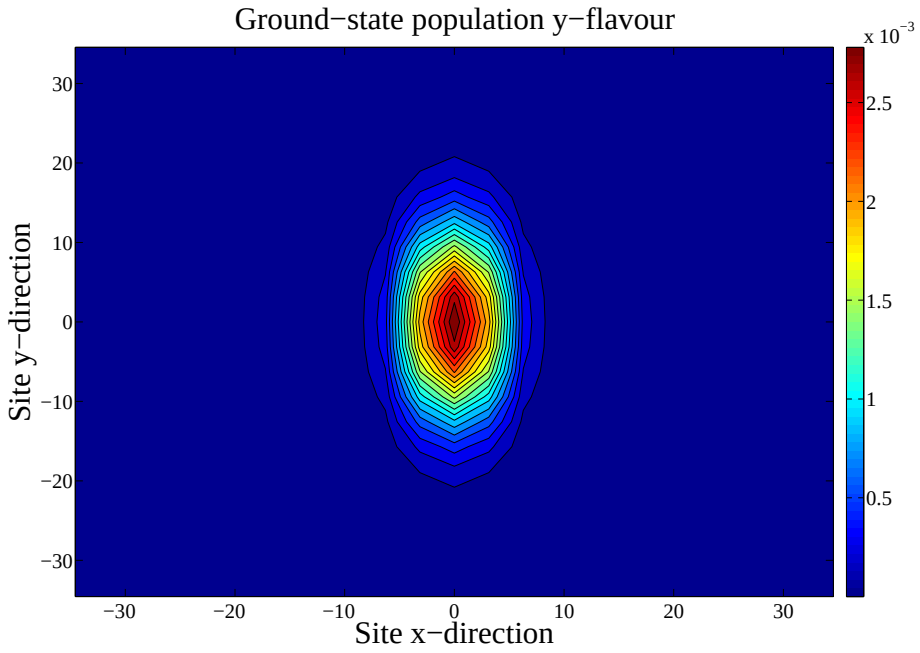

Figure 4: The population of y-flavoured atoms $|\psi_{y,i}|^2$ in the isotropic lattice. The colour indicates how populated each site is by the named flavour.

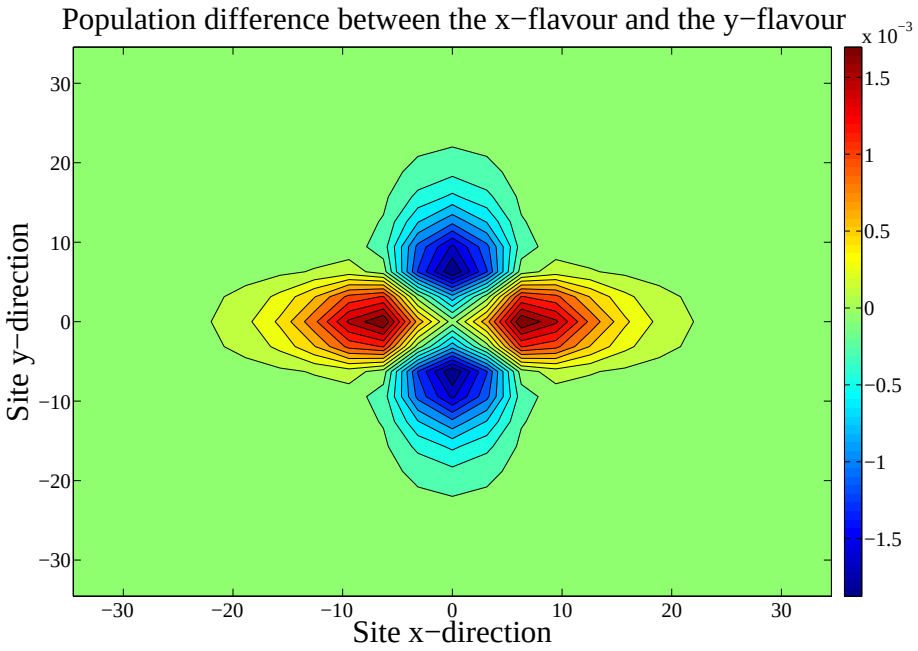

Figure 5: The population difference between the two flavours at different sites in the isotropic lattice. A red colour indicate a surplus of x-flavour atoms and a blue colour a surplus of y-flavour atoms.

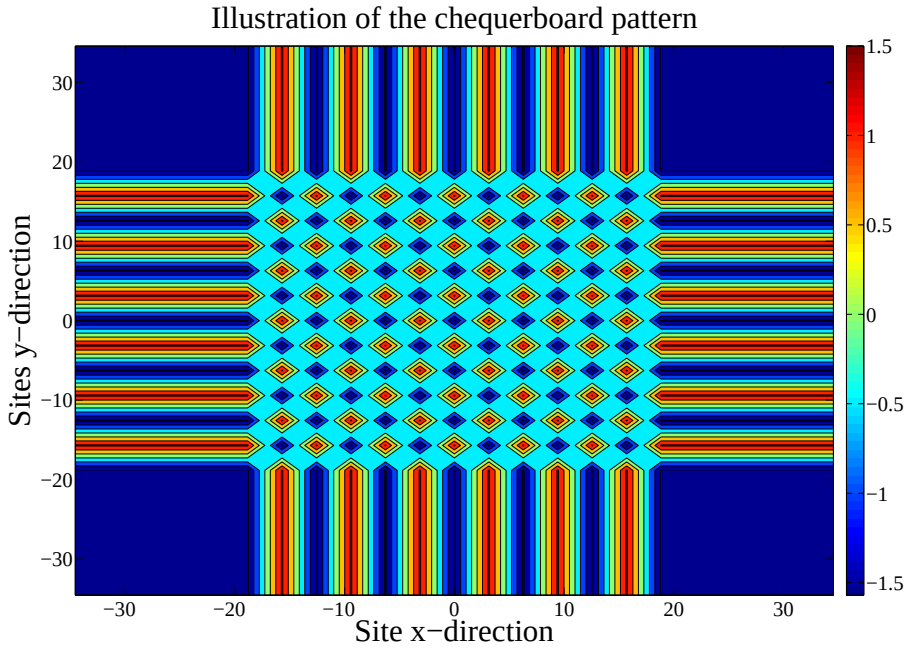

Figure 6: A picture of the phase difference between sites, which demonstrates the chequerboard pattern existing in the isotropic lattice. Note the alternating colour between sites and how it is not an indication of the flavour population but of the phase in each site. At the edge of the lattice it is also shown how the chequerboard pattern breaks down as a consequence of the confining trap. Here the population of one or both flavours is approximately zero and cannot define a phase relation between the two flavours.

3.2 The Landau-Zener formula

From here on only the case in which the lattice is asymmetric will be studied. More precisely the case in which the lattice is changed in time is considered, i.e. the lattice potential becomes time-dependent. From the definition of the periodic potential there are two ways to make it asymmetric, changing either the wave vectors k_x and k_y, or amplitudes V_x and V_y. In this thesis the amplitudes will be varied to create the asymmetry.

By introducing an asymmetry in the lattice the previously discussed degeneracy will be lifted. Furthermore, by changing the amplitude for the potential the tunnelling ability for the atoms will be affected as seen from the definition of the tunnelling parameter. A particle will be less likely to tunnel in a direction where the amplitude is higher. Also in order to minimize the energy the distribution of atoms in the lattice should resemble the flavour which match the direction in which the potential is smaller, so if the potential amplitude is lower in the x-direction (V_x) for example the distribution should look like the distribution of atoms with x-flavour only but now for every atom. Now by changing the amplitudes of the potential is should be possible to cause a shift in the distribution of particle from the x-distribution to the y-distribution. This can be seen as a phase transition from one quantum phase to another in the case of a very weak harmonic trap[14]. However, if the amplitude of the potential is changed by a large value very suddenly there is no guaranty that the ground-states properties will be preserved. Even worse, it is not even certain that the ground-state would still be populated, in the processes some of the atoms can be excited to a higher energy level and thus destroying the condensate properties completely (if a large amount of atoms are excited). So in order to map the time evolution, from one distribution to another, the change has to be moderate to keep the ground-state properties maintained. Another way to formulating it is that the change of the Hamiltonian describing the system has to happen sufficiently slow to keep the properties of the system preserved. When formulating like this it resembles what is called the *Adiabatic theorem* or the *Adiabatic approximation*. The Adiabatic theorem can be formulated like [8]

The Adiabatic theorem. *If a system starts in the eigenstate of the initial Hamiltonian and if the time perturbation acting on it is slow or small enough,*

[14]Strictly it is not possible with a phase transition in a finite system, when there is no trap there is however no restriction to the extent of the system and thus a phase transition can take place.

it will after some time t end in the corresponding eigenstate to the final Hamiltonian.

Proof. Consider a time-dependent Hamiltonian and the related Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle, \tag{96}$$

and where the Hamiltonian has the instantaneous eigenvectors $|\Psi_n(t)\rangle$ according to

$$\hat{H}(t)|\psi_n(t)\rangle = E_n(t)|\psi_n(t)\rangle \tag{97}$$

where the eigenvalue $E_n(t)$ is a function of the instantaneous time t and a consequence of the time-dependence of the Hamiltonian. Furthermore, it is possible to define an orthogonal base in the case of instantaneous eigenstates,i.e.

$$\langle\psi_n(t)|\psi_m(t)\rangle = \delta_{nm}. \tag{98}$$

The general solution can be expressed in terms of $|\Psi_n(t)\rangle$ as

$$|\Psi(t)\rangle = \sum_n c_n(t)e^{i\theta_n(t)}|\psi\rangle, \tag{99}$$

where θ_n is the *dynamic phase*, given by

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt'. \tag{100}$$

Using the expanded expression for the general solution in the Schrödinger equation yields

$$i\hbar\sum_n(\dot{c_n}|\Psi_n(t)\rangle + c_n|\dot{\Psi}_n(t)\rangle + ic_n|\Psi_n(t)\rangle\dot{\theta_n})e^{i\theta_n} = \sum_n c_n\hat{H}|\Psi_n(t)\rangle e^{i\theta_n}, \tag{101}$$

but since $\dot{\theta}_n$ is only $-E/\hbar$ it follows that the third term on the left cancels out with the single term on the right (if the eigenstate relation for the Hamiltonian is used), thus the following is obtained

$$\sum_n \dot{c_n}\psi_n e^{i\theta_n} = -\sum_n c_n\dot{\psi_n}e^{i\theta_n}. \tag{102}$$

To evaluate this expression, the inner product is taken with *another* instantaneous eigenvector, $|\psi_m(t)\rangle$, resulting in

$$\dot{c}_m(t) = -\sum_n c_n \langle \psi_m | \dot{\psi_n} \rangle e^{i(\theta_n - \theta_m)} \tag{103}$$

where every term in the sum on the left hand side of Eq.(97) was zero except when $m = n$ as a consequence of δ_{mn}. To evaluate $\langle \psi_m | \dot{\psi_n} \rangle$, the time derivative of the eigenvalue equation is taken

$$\dot{\hat{H}} |\psi_n(t)\rangle + \hat{H} |\dot{\psi}_n(t)\rangle = \dot{E}_n + E_n |\dot{\psi}_n(t)\rangle. \tag{104}$$

Now by taking the inner product again with $|\psi_m(t)\rangle$ yields

$$\langle \psi_m | \dot{\psi_n} \rangle (E_n - E_m) = \langle \psi_m | \dot{\hat{H}} | \psi_n \rangle, \; m \neq n. \tag{105}$$

Substituting into (103) the result becomes

$$\dot{c}_m(t) = \sum_n c_n \frac{\langle \psi_m | \dot{\hat{H}} | \psi_n \rangle}{E_m - E_n} e^{i(\theta_n - \theta_m)}. \tag{106}$$

If now the initial state is chosen to be one of the instantaneous eigenvectors $|\Psi(0)\rangle = |\psi_n(0)\rangle$ and taken to also fulfil that $c_n(0) = 1$ and $c_m(0) = 0$ (this can only be true when $m \neq n$). Then the above expression can be approximated by

$$\dot{c}_m(t) \approx \frac{\langle \psi_m | \dot{\hat{H}} | \psi_n \rangle}{E_m - E_n} e^{i(\theta_n - \theta_m)}. \tag{107}$$

To obtain $c_m(t)$, the above expression is integrated (it is important at this point to remember the time-dependence of the parameters). The result is, if the time dependence of $\langle \psi_m | \dot{\hat{H}} | \psi_n \rangle$ and $E_m - E_n$ are assumed to be slow,

$$c_m(t) \approx -i\hbar \frac{\langle \psi_m | \dot{\hat{H}} | \psi_n \rangle}{(E_m - E_n)^2} (e^{i(E_m - E_n)t/\hbar} - 1), \tag{108}$$

where $e^{i(\theta_n - \theta_m)}$ has been approximated by $e^{i(E_m - E_n)t/\hbar}$ which again should be valid for a slowly varying Hamiltonian. The physical interpretation of $c_m(t)$ is only meaningful when it is squared. When formulated like this, $|c_m(t)|^2$ tells the probability of transition from one state to another. But

if the time-dependence in (108) is slow (the Hamiltonian is slowly varying with time) then the time derivative of the Hamiltonian should be small and $\langle\psi_m|\dot{\hat{H}}|\psi_n\rangle$ would approach zero, consequently $c_m(t)$ should be able to be arbitrary small. Moreover, if the energy difference between E_m and E_n is large $(E_m - E_n)$ then the population of any other state will be less likely because of the wider energy gap. So the amplitude for the transition processes $|c_m|^2$ is close to zero meaning that the system should *not* populate any other states. Hence, a system that starts in some initial state (with some initial Hamiltonian) which is a instantaneous eigenvector, will end in a corresponding instantaneous eigenvector to the final Hamiltonian provided a slow enough time-dependence. If the energy of the two states should be equal $E_n = E_m$ it would cause the procedure to fail because there would not be any preferred state which minimize the energy of the system.

□

The adiabatic theorem says that if the amplitude of the potential is varied slowly over a time interval the distribution should change while keeping the system in the ground-state.

A model which describes the transition from one quantum state to another is the *Landau-Zener model* or *Landau-Zener formula* [9]. The Landau-Zener model considers a time-depending Hamiltonian and a two-level quantum system. In this case the two levels correspond to the energy difference attributed to the two flavours. More clearly, one of the levels corresponds to the state W_x and the other equals the state for W_y. The model will illustrate how it is possible to transfer population from one of the states to an other as long as the processes is adiabatic. Important to notice is that the Landau-Zener formula for this system is an approximation as it does not take into consideration the full form of the Hamiltonian as well as the presence of other sites[15].

In the Landau-Zener model, the Hamiltonian is take to be

$$H = \begin{bmatrix} \lambda t & g \\ g & -\lambda t \end{bmatrix} \tag{109}$$

where λ is the rate of change and is related to how adiabatic the process is, t the time and g the separation of the energy levels at the cross point, i.e. the

[15]The system in this paper can be thought of as a **many-body Landau-Zener model** where each site contains one realization of a Landau-Zener model.

coupling strength. In figure (7) the notifications is further explained. Solving the time-dependent Schrödinger equation with this Hamiltonian is non-trivial and require some complex calculations. Therefore, the time-dependence in the Hamiltonian will be suppressed when solving for the eigenvalues (t is treated just as an ordinary parameter which corresponds to applying the adiabatic approximation). With the Hamiltonian on the form given above and the time dependence suppressed, the corresponding eigenvalues are calculated to be

$$\Gamma(t) = \pm\sqrt{\lambda^2 t^2 + g^2}. \tag{110}$$

Figure (7) displays the eigenvalues as a function of the time t and for different g:s.

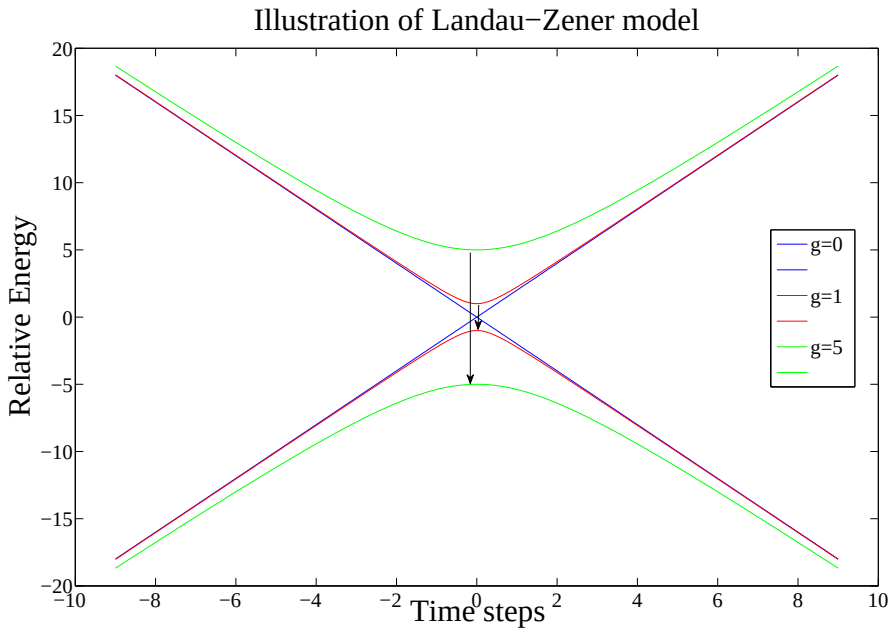

Figure 7: An illustration of the Landau-Zener model. The graphs show $\Gamma(t)$ for different values of g. The arrows indicate the width of the gap and is equal to g (or more exact $2g$). By staying adiabatic it is possible to follow either of the red or green curves from start to finish thus changing the state.

From the definition of g it becomes apparent that a large value for g equals a wider gap and thus a larger energy difference between the two states. But

a larger energy difference should mean that it is easier to stay adiabatic because small disturbances will have a harder time changing the instantaneous eigenstates at each location. In addition, it is common to define the adiabaticity parameter

$$\Lambda = \frac{2\pi g^2}{\hbar \lambda} \tag{111}$$

which is a measurement on how adiabatic the Landau-Zener processes is; a large value on Λ indicates a more adiabatic process. Before proceeding a final remark will be made, to connect the Landau-Zener model with the system being exterminated in this thesis. In order for the system to change from an x-distribution to a y-distribution the flavour has to be changed. This can only be done by the use of the term H_{FD} in the Hamiltonian. Thus it can be thought upon that $g \sim H_{FD}$, meaning that energy gap g is related to the interflavour conversion interaction. This is not the entire truth but it is a good way to visualize how the model relates to the system and what g is.

If the Landau-Zener model is solved for the explicit time-dependence the following is obtained

$$P_{exc} = e^{-\Lambda} = e^{-\frac{\gamma}{\lambda}}, \tag{112}$$

where γ is defined as $\frac{2\pi g^2}{\hbar}$. This expression gives of the probability for excitation, which is the exact opposite of what is wanted in this thesis. However, the particles in a two-level system has to do something of the two things, either *not be* excited or *be* excited . Therefore, the probability for a particle to not be excited should be

$$P_{non} = 1 - P_{exc}. \tag{113}$$

This expression will be used in the subsequent section in order to compare the Landau-Zener model with the system being investigated.

In the following section the result of the evolution in the case of an asymmetric lattice will be presented. As of that, no more theoretical tools will be introduced from here on.

3.3 Properties of the anisotropic lattice and its resulting time-evolution

Before the results from the state propagation in the case of an anisotropic lattice is presented a recap of the procedure will be made. First the ground-state will be obtained using methods discussed previously. Once obtained, a change in the lattice amplitude will be introduced. With the change in the lattice the system will go to the lowest energy level and thus the distribution will be stretched out in the direction of the lowest amplitude. Now the relative amplitude will be changed again, making the direction with the previously lowest amplitude the one which is the largest (the amplitudes will switch values). This change will be made slowly over time to ensure that the system stays quasiadiabatic. The expected results should be that the distribution change its spatial direction 90 degrees (going from x-flavour distribution to a y-flavour distribution) while remaining in the ground-state. The results will be presented in the form of figures below. As earlier the split-operator method will be used for the propagation, i.e. the propagation will be carried out in real time once the ground-state has been obtained. As previously it is important for the time-steps to be sufficiently small for the split-operator method to be valid. Furthermore it is also important for the adiabatic theorem that the time change is small.

The following figures will address a number of things. These are the affects of an anisotropic lattice on the population of flavours, the sensitivity of the propagation on the number of time steps, the fluctuation appearing in the propagation of the ground-state , and the initial and final distribution.

In the coming figures the starting dimensionless parameters will have the following value: $V_x = 17$, $V_y = 16.98$, $\omega = 0.007$ and $U_0 N = 1$ unless otherwise specified. During the process the potential amplitudes are changed step by step till they reach the final values of $V_x = 16.98$ and $V_y = 17$,at which point they have the opposite values they had at the start. By stating these parameters it is also established that the condensate starts in the y-direction. The results will be discuses in the figure-captions.

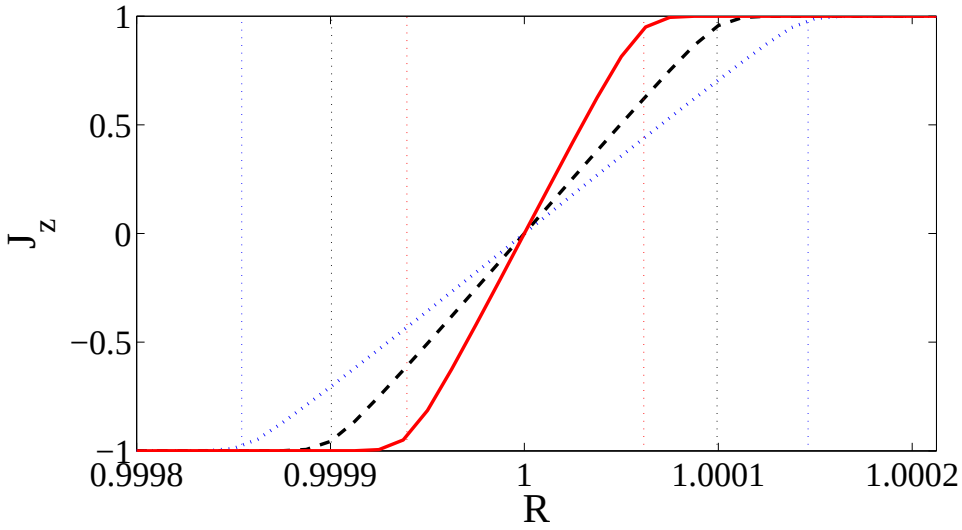

Figure 8: Demonstration of how the population of the ground-state is affected by an asymmetric lattice. Note that this is for the ground-state and is not related to any state evolution. J_z is defined as $\sum_i |\psi_{x,i}|^2 - |\psi_{y,i}|^2$ and R as V_x/V_y. In the figure J_z can be seen as a function of R. The red line corresponds to $\omega = 0.003$, the black to $\omega = 0.005$ and the blue to $\omega = 0.007$. Note how the red curve which corresponds to an weaker trap is the one with the steepest slope, this relates to how a phase transition only can take place in an infinite system. The picture is taken from [2].

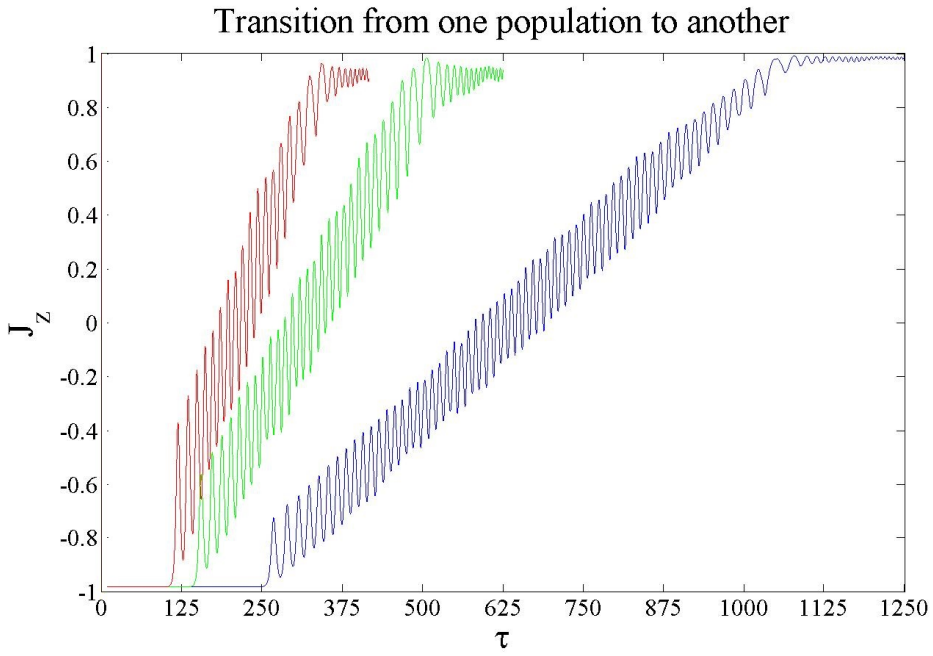

Figure 9: This figure presents the transition process as a function of the dimensionless time τ for three different ramp velocities λ. The ramp velocity λ is define as $\lambda = \frac{\Delta V}{\Delta \tau}$ where $\Delta V = V(\tau_{final}) - V(\tau_{initial})$ and $\Delta \tau = \tau_{final} - \tau_{initial}$ indicates the difference between the initial value and the final value of the potential amplitude and dimensionless time. Depending on how many time steps are taken the process is more or less adiabatic. Note how the red and green ones fails to reach to the same population level as the blue. Note also how the occurring fluctuations are more severe in the red and green ones compared to the blue. Thus, small λ's results in a more adiabatic process as expected.

Figure 10: The figure depict how the population transition depends on λ (as define earlier). The red curve is the calculated points for the transition process with different λ's. The black doted line is the fitting made from the Landau-Zener models prediction Eq.(113) with the adibaticity parameter Λ as a fitting parameter. Note how for larger λ the process is less adiabatic and thus how fever particles change from the starting state to the end state. Additionally, note how the fitting fails to capture the entire nature of the population transition processes. The figure is for the population difference $p_x - p_y$ but as previously stated most of the particles should be in p_x therefore making $p_y \approx 0$ and the notation on the y-axis valid.

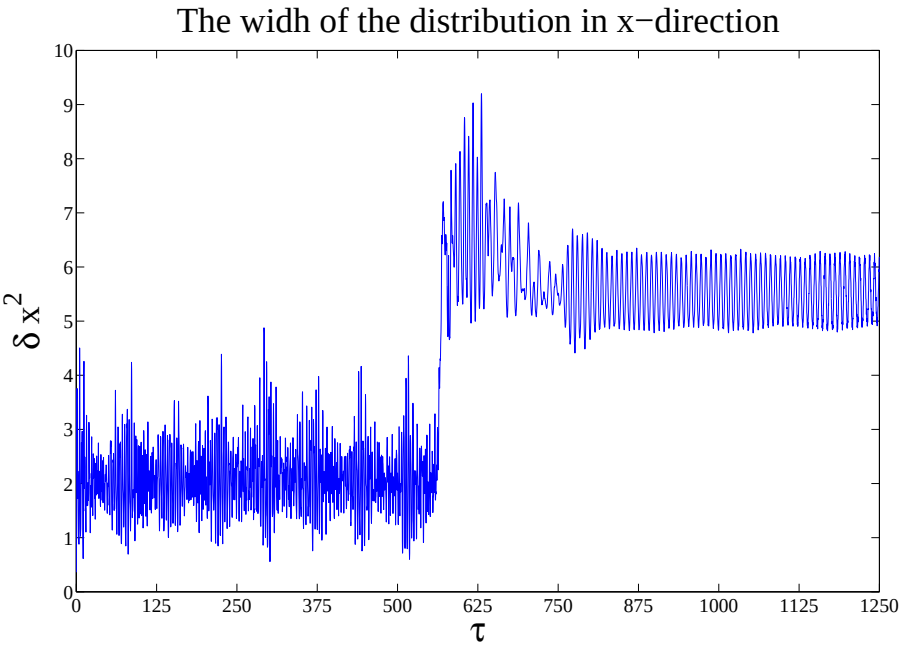

Figure 11: The width of the distribution in the x-direction as a function of τ. The value of the ramp velocity λ is $1.1 \cdot 10^{-9}$. δx^2 is defined as $\langle x^2 \rangle - \langle x \rangle^2$ where $\langle x \rangle$ is the expectation value of the position of the distribution. Note the occurring fluctuations before and after the transition. The fluctuations in the shape of the distribution imply some level of excitation of the atoms.

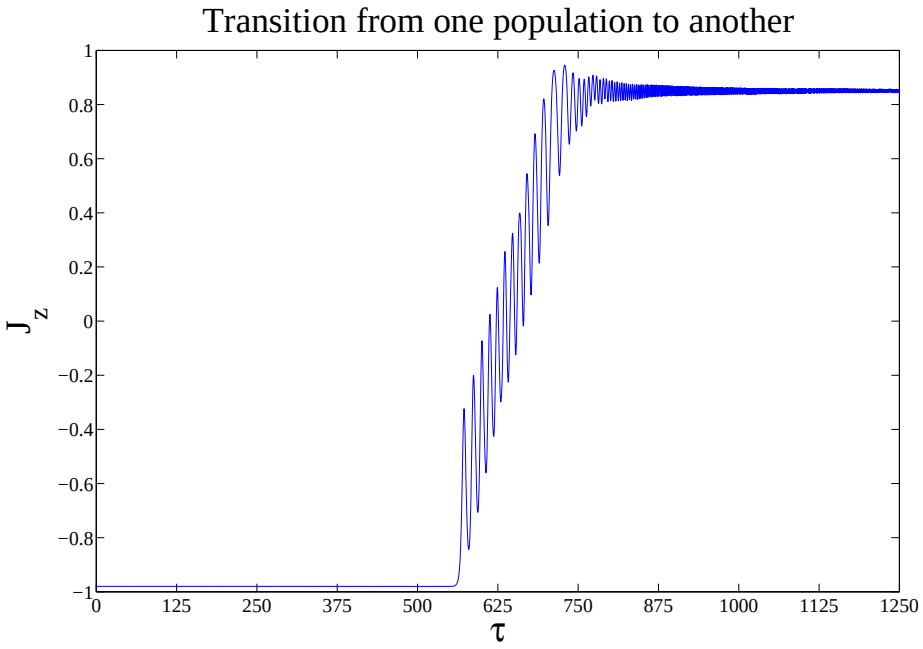

Figure 12: The transition process as a function of the number of steps. The value of the ramp velocity λ is $1.1 \cdot 10^{-9}$. Note how the fluctuations appears to die out after the transition indicating how the processes seems to be adiabatic. However, as seen in figure 11 the width of the distribution in x-direction in not constant, but fluctuating. This indicates again how the processes is not entirely adiabatic even though in appears to be when viewing the population transition.

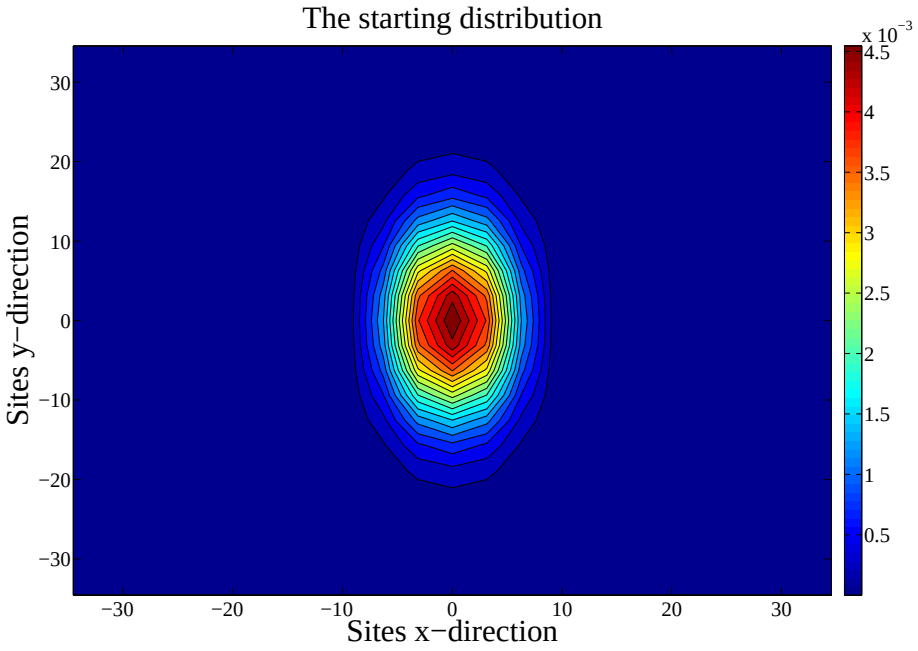

Figure 13: The starting distribution, when $V_y < V_x$. The value of the ramp velocity λ is $1.1 \cdot 10^{-9}$. Note the similarity to the figure 4, depicting the y-flavour distribution.

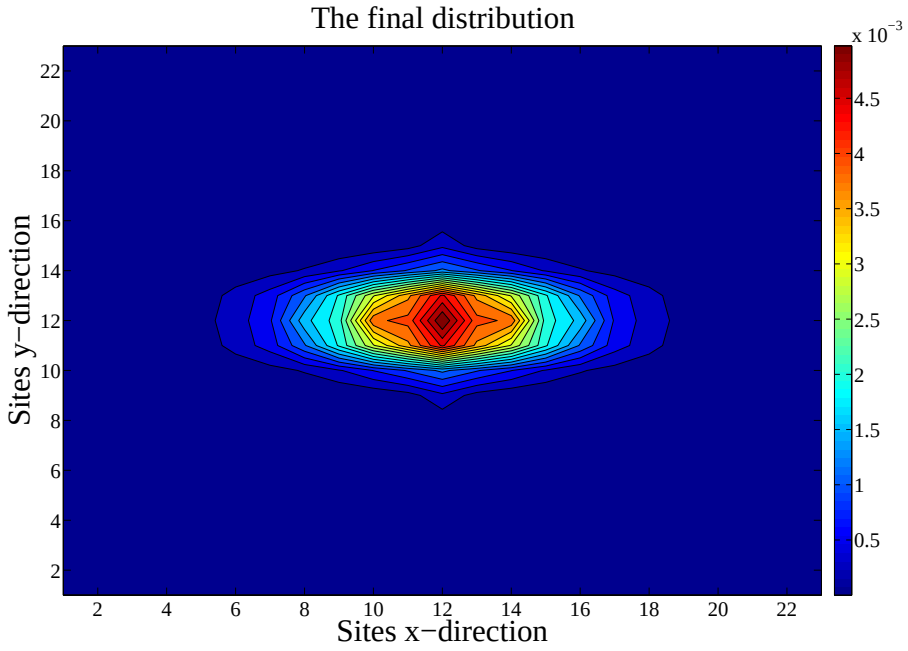

Figure 14: The resulting distribution after the evolution. At this point $V_y > V_x$. The value of the ramp velocity λ is $1.1 \cdot 10^{-9}$. Note how the population still has some width in the y-direction. The resulting conclusion must be that the process is not entirely adiabatic, if it were then the result should be the same as figure 13, only turned 90°. The change in the distributions appearance indicates some type of excitation process.

4 Conclusion

This thesis has examined the properties of a system consisting of bosonic atoms in a the p-band of an optical lattice confined by a harmonic trapping potential. The examination has been carried out in the case of a 2D optical lattice. The analysis of the system was made using the mean-field approximation and the equations of motion where solved by the use of the split-operator method. Is was shown that restriction of the atoms to the p-band in the lattice lead to anisotropic tunnelling even if the lattice was symmetric. The result of the anisotropic tunnelling was also shown in the distribution of atoms in the lattice by a wider distribution in one of the two directions for the two flavours. It was also shown that by using the mean-field approximation a phase relation or phase locking was introduced between the different flavours and sites. The phase locking resulted in alternating pattern of wave functions with vortex like properties (there was also a physical rotation of atoms in each site, alternating in direction between sites) on the lattice which where refereed to as a chequerboard pattern because of its organized structure.

In the case of an asymmetric lattice it was shown how the properties for the system dramatically changed as a consequence of the broken degeneracy. It was indicated how the distribution in the ground-state was wider in the direction with the lowest lattice amplitude and also that the system started in this position with every atom in that distribution. It was also shown how the system behaves when evolving depending on how adiabatic the processes were. Lastly the fluctuations where examined in the transition processes.

In the previous sections there has been some subjects which where omitted to later, they will now be discussed.

During the calculations of the population transfer in the case of an asymmetric lattice the mean-field approximation was used just as in the section before it. However, when utilizing the split-operator method it turned out that nothing changed, the distribution stayed in the original direction. Physically there is nothing to hinder the fact that every atom starts in one way and then proceed to change to the other. Consequently, this must be a shortcoming with some aspect of the theoretical framework. The answer to why this happened is that the mean-field approximation does not take into account any quantum fluctuations. In a real physical system every particle could start (theoretical) in one state in a strongly asymmetrical lattice and there would still be some which would be found in the other state later on. This is

precisely the kind of effect which is omitted in the mean-field approximation, the vacuum fluctuations. Hence, to be able to calculate the evolution of the ground-state it must be assumed that some of the atoms start off in the other state corresponding to the direction with an higher optical lattice amplitude. One way to demonstrate the change that the mean-field brings is to examine the commentator (25), for operators this relation is valid but when the mean-field approximation is made the relation becomes zero, numbers always commute. From this, one can get an idea of how the mean-field approximation in some sense destroys the complete quantum picture, instead bringing it more close to the classical picture (where operators commute). Moreover an possible entanglement between particles is utterly destroyed by the mean-field approximation. Still in order to be able to calculate and predict any of the properties of the system, some simplification and approximation has to be made and in that sense mean-field is a subtle choice.

In the figures from the previous section, where the starting state and the state after the evolution are depicted there is an anomaly in the figure for the state after the evolution. From studying the figure it becomes apparent that the figure differ from the depicting of the x-flavour population. But as the amplitude for the potential changes to a larger value for y the population should shift from y to x uniformly. This is obviously not the case in the figure for the state after the time propagation. The most forthcoming explanation to why this happens must be that some of the atoms have been excited and thus no longer are in the ground-state. This was one of the reasons for why the time propagation should be carried out with small ramp velocities in accordance with the adiabatic theorem. This illustrates the challenge to stay completely adiabatic. It should however be possible to further improve the end result by propagating even longer. Worth to notice is that a larger system will always mean that the time propagation has to go on longer because of the difficulties in staying adiabatic for a larger system.

There are two natural continuations that can be studied with an starting-point from this system. Further studies of the process involved in the excitation of atoms could be of interest. The excitation could be seen as both affecting the ground-state in a certain site as well as affecting the condensate as a whole. Additional studies into the case of a 3-dimensional lattice could also be of interest. In 3-dimensions the system can no longer be consider for the two-state Landau-Zener model and the orientation of the condensate can be affected depending on how the ratio of the amplitudes are varied. Generally though, most of the results obtained in this paper can without any

major difficulties be generalized to 3-dimensions.

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