Pinning of Vortex Lattices in Single and Multicomponent Bose-Einstein Condensates by an Optical Potential

Martijn Mink
September 11, 2008

Institute for Theoretical Physics, Utrecht University

Supervisors: Prof.dr. Cristiane de Morais Smith and Dr. Rembert Duine
## Contents

6.3 Determining the Energy Functional ........................................ 62
6.4 Results .............................................................................. 63
6.5 Including an Optical Lattice ................................................ 67
6.6 Phase Diagram .................................................................... 68

7. Conclusions and Outlook ...................................................... 72

8. Acknowledgements ................................................................ 74

9. References ............................................................................ 75
1. ABSTRACT

It is possible to form a Bose-Einstein condensate (BEC) by cooling atoms trapped in a potential down to $\mu$kelvin. By applying rotation to a BEC, vortices appear in the condensate. When the rotation frequency $\Omega$ of a BEC in a radially symmetric trap approaches the (radial) trapping frequency $\omega$ and the interaction between the atoms is weak, the system enters the so-called mean-field lowest Landau level regime. In this regime the macroscopic condensate wave function is completely determined by the position of the vortices. Working in this simplified limit, we determine the vortex lattice structure for single and two-component condensates, both in the presence and in the absence of a regular optical lattice potential, that acts as a pinning potential for the vortices. For the single component case in the absence of the optical lattice, the ground state is the well-known triangular Abrikosov lattice. For the two-component case, the geometry of the lattice depends on the inter- and intra-component interactions. In the presence of pinning, however, we find new vortex lattice structures determined by the competition between vortex interactions and pinning potential. We determine the vortex lattice structure phase diagram as a function of optical-lattice strength and geometry.
2. INTRODUCTION

The control over temperature plays and has played a vital role in condensed-matter-physics research. This is because most novel and interesting quantum phases occur only below a certain temperature, which can be of the order of micro- or nanokelvin. For a long time, systems were cooled by letting them come into contact with another colder system. The Nobel Prize winning discovery of superconductivity by the Dutch physicist Kamerlingh Onnes in 1911 is an example of the use of this technique. During the last decades a revolution has occurred in cooling techniques. Since the temperature of a gas of atoms is determined by the kinetic energy of those atoms, scientists realized that one could use laser light to slow atoms down, thus cooling them. For their contribution to the development of this technique, Steven Chu, Claude Cohen-Tannoudji, and William Phillips were awarded the 1997 Nobel Prize. Using the technique of laser cooling followed by the technique of evaporative cooling, Eric Cornell and Carl Wieman were able to achieve Bose-Einstein Condensation (BEC) of a dilute gas of rubidium atoms, after cooling them to a temperature of about 170 nanokelvin [Cor95]. For this immense experimental achievement they were awarded the Nobel Prize in 2001 together with Wolfgang Ketterle. A BEC is a state of matter that was predicted by Albert Einstein and Satyendra Bose in the beginning of the 20th century, in which, in the case of an atomic Bose gas, all atoms in the gas behave coherently as one single

Fig. 2.1: The momentum distribution of atoms for temperatures higher than (left), around (middle), and lower than (right) the transition temperature. Picture taken from [NIST].
quantum-mechanical wave. A famous picture showing the phase transition to the condensed state is shown in Fig. 2.1 where the momentum distribution of the atoms is shown. In the left picture, the temperature is higher than the transition temperature and the momentum distribution is classical. For temperatures close to the transition temperature, a peak develops at zero momentum (middle diagram). Finally, the right picture, with a temperature smaller than the transition temperature, shows that most atoms have condensed in the zero momentum state.

One of the most remarkable properties of a BEC is its superfluidity. This is demonstrated by its response to rotation, e.g., when it is stirred by laser light. If the rotation speed is above a certain critical velocity, one can observe the formation of a vortex in the BEC [Dal00]. A vortex is a spinning flow of atoms around a center, much like a whirlwind, and is a topological excitation in the BEC. If the rotation velocity is increased further, more and more vortices will appear in the system. Because the vortex-vortex interaction is repulsive, they will, under certain conditions, arrange themselves in a regular lattice, which turns out to have a triangular structure, the so-called Abrikosov lattice [Abr57,Dal00,Ket01]. A vortex lattice with more than 100 vortices was created in the group of Ketterle and can be seen in Fig. 2.2. For a two-component condensate the situation is different. Here, the ground state consists of two interlaced square vortex lattices, where the vortices of the first species are located at centers of the unit cells of the vortex lattice of the second species [Cor04b]. Such an interlaced square vortex lattice is shown in Fig. 2.3, where only the vortices of one component are shown due to the observation technique used. The difference between the two cases is caused by the fact that at the vortex core of a particular atomic species, the density of the other atomic species need not be equal to zero. The interaction energy is minimized by a density distribution that is as uniform as possible. Hence, in the two component case, the interlaced square vortex lattice has a density distribution that is more uniform than a lattice in which the vortices of both species lie on top of each other.
Besides generating a vortex lattice in a BEC in a harmonic magnetic trapping potential, it is also possible to superimpose an optical lattice potential on the trapping potential, load the BEC in it, and then generate vortices. An optical lattice is a regular pattern of potential maxima and minima created by the interference pattern between crossed laser beams. Because of the dipolar interaction of the atoms with the laser light, the atoms want to sit at the positions where the electric field strength is maximal. An example is a 2-dimensional square lattice structure which resembles an egg-box, which is shown in Fig. 2.4 but also other dimensionalities and geometries are possible. In 2006, experimentalists succeeded in creating a rotating optical lattice potential with square geometry, which they applied to a BEC with a vortex lattice [Cor06]. They observed the pinning of vortices at the potential maxima for sufficient optical lattice strength and confirmed the theoretical prediction by Reijnders and Duine [Du04]. An experimental picture of the pinned vortex lattice is shown in Fig. 2.5(c) and, converted to reciprocal space, in Fig. 2.5(f). Vortices are pinned at the potential maxima, since vortices correspond to density minima, and it is thus energetically favorable for them to sit at the maxima of the optical lattice. In this way the optical lattice pushes the vortices in a (e.g.) square lattice structure, which competes with the intrinsic (triangular) ordering tendency of the single component vortex lattice.

In this thesis we will calculate phase diagrams for both single and multicomponent condensates with the optical lattice strength and geometry, as well as the intercomponent interaction strength as parameters. These calculations will be done in the so-called Lowest Landau Level regime (LLL), where the condensate wave function is completely determined by the position of the vortices. The motivation for this procedure is the following: We described above that in the formation of an interlaced square vortex lattice in a two-component condensate the intercomponent interaction inside the vortex core is important. Reijnders and Duine calculated in Ref. [Du05] the
phase diagram for a two component condensate in the presence of an optical lattice potential. However, they use a step-function like ansatz for a vortex, in which the density is zero in the vortex core of some finite size, and is equal to the "global" density outside the vortex core. However, as Reijnders and Duine also state in Ref. [Du05], this ansatz has only limited validity, since it is not suitable to describe the tendency towards a total density distribution inside the vortex cores that is as uniform as possible. In this thesis we use the ansatz that the vortex positions form an infinite regular lattice. This completely specifies the wave function, and we do not need a crude step-function like approximation for the density distribution of a vortex.

This thesis is organized as follows. In Chapter 3 we introduce the concepts which we will need in later chapters. These are the macroscopic wave function of the condensate, vortices and the transformation of the wave function to a rotating frame, and the parameterization of infinite regular lattices. The physics of the LLL is described in Chapter 4. We derive two representations of the LLL wave function and analyze some of its properties. We also calculate the energy of square and triangular vortex lattices directly. In Chapter 5 we use a more sophisticated approach, which assumes a vortex lattice of infinite size. This approach was proposed by Ho in Ref. [Ho01] and we use it to determine the vortex structure of a BEC both in the presence of rotation and an applied optical lattice potential. In Chapter 6 we use an extended version of this approach from Ref. [Ho02] to analyze vortex structures in multi-component condensates. Finally, in Chapter 7 we give our conclusions and an outlook for further research.
3. PRELIMINARIES

3.1 Macroscopic Wave Function

At zero temperature, the Bose-Einstein condensed state is described at the mean-field level by a complex macroscopic wave function $\Psi(\mathbf{r})$ and the energy $E[\Psi]$ is given by

$$E[\Psi] = \int \! d\mathbf{r} \left[ \frac{\hbar^2}{2M} |\nabla \Psi(\mathbf{r})|^2 + V(\mathbf{r})|\Psi(\mathbf{r})|^2 + \frac{1}{2}g|\Psi(\mathbf{r})|^4 \right],$$

(3.1)

where $M$ is the mass of the bosons, $V(\mathbf{r})$ is an external (trapping) potential, and $g = 4\pi\hbar^2a/M$ the two-body transition matrix at low energy, with $a$ the interparticle s-wave scattering length [Peth]. The macroscopic wave function is normalized to the number of particles $N$

$$\int \! d\mathbf{r} \Psi^*(\mathbf{r})\Psi(\mathbf{r}) = N.$$  

(3.2)

We can rewrite $\Psi(\mathbf{r})$ in terms of the particle density $\rho(\mathbf{r}) = \Psi^*(\mathbf{r})\Psi(\mathbf{r})$ and phase $\phi(\mathbf{r})$

$$\Psi(\mathbf{r}) = \sqrt{\rho(\mathbf{r})}e^{i\phi(\mathbf{r})}.$$  

(3.3)

Using this, we rewrite the energy of Eq. (3.1) in a physically clearer form

$$E(\Psi) = \int \! d\mathbf{r} \left[ \frac{1}{2}J(\mathbf{r}) (\nabla \rho(\mathbf{r}))^2 + \frac{1}{2}(M\rho(\mathbf{r}))v^2(\mathbf{r}) + V(\mathbf{r})\rho(\mathbf{r}) + \frac{1}{2}g\rho^2(\mathbf{r}) \right],$$

(3.4)

where we defined the "compressibility" $J(\mathbf{r}) = \hbar^2/4M\rho(\mathbf{r})$ and the velocity field $v(\mathbf{r}) = \frac{\hbar}{M} \nabla \phi(\mathbf{r})$ (below we show that $v(\mathbf{r})$ is indeed the velocity field). The first term in Eq. (3.4) is the "elastic" energy due to variations in the density distribution of the condensate. Note that the stiffness $J \sim 1/\rho$, and thus that density variations are energetically more costly in area's of low density than in areas of high density. The second term is the kinetic energy
of the system and the third corresponds to the coupling of the density to the (single particle) potential. The last term is the interaction energy of the system due to the mutual repulsion (for $g > 0$) of the bosons.

The optimal form of $\Psi(r)$ is that which minimizes the energy functional of Eq. (3.1) subject to the constraint Eq. (3.2). Using the method of Lagrange multipliers, the constraint is enforced by instead minimizing the functional

$$K[\Psi, \lambda] = E[\Psi] - \lambda \left[ \int d^3r \Psi^\dagger(r)\Psi(r) - N \right],$$

(3.5)

with respect to $\Psi$, $\Psi^\dagger$ and $\lambda$, where $\lambda$ is the Lagrange multiplier. Let $\Psi_0(r)$ be the optimal wave function, then the total energy of the system is given by $E_0 \equiv E[\Psi_0]$ (and not $K[\Psi_0]$). The value of the Lagrange multiplier $\lambda_0$ corresponding to $E_0$ is recognized as the chemical potential $\mu$ because it holds that $\lambda_0 = \partial E_0/\partial N = \mu$ [Kar06]. This minimization procedure leads to the well-known Gross-Pitaevskii equation (GPE)

$$-\frac{\hbar^2}{2M} \nabla^2 \Psi(r) + V(r)\Psi(r) + g|\Psi(r)|^2\Psi(r) = \mu \Psi(r),$$

(3.6)

and the constraint Eq. (3.2).

In analogy to the Schrödinger equation, the dynamic behavior of the condensate wave function $\Psi(r, t)$ is determined by the time-dependent GPE

$$-\frac{\hbar^2}{2M} \nabla^2 \Psi(r, t) + V(r)\Psi(r, t) + g|\Psi(r, t)|^2\Psi(r, t) = i\hbar \partial_t \Psi(r, t),$$

(3.7)

where $\partial_t$ denotes differentiation with respect to $t$. By substituting Eq. (3.3) into Eq. (3.7), we arrive at equations for $\partial_t \rho(r, t)$ and $\partial_t \phi(r, t)$. For the density we obtain

$$\partial_t \rho(r, t) = -\nabla \cdot \left[ \rho(r, t) \frac{\hbar}{M} \nabla \phi(r, t) \right],$$

(3.8)

which is a continuity equation for the density field $\rho(r, t)$ and provides the justification of denoting $v(r, t) = \frac{\hbar}{M} \nabla \phi(r, t)$ a velocity field. Note that it holds that $\nabla \times v(r, t) = 0$ wherever the phase of $\Psi$ is well-defined. This shows that only rotation-free velocity profiles are possible. For the time-derivative of the phase we obtain

$$-\hbar \partial_t \phi(r, t) = -\frac{\hbar^2}{2M} \left( \frac{\nabla^2 \rho(r, t)}{2\rho(r, t)} - \frac{(\nabla \rho(r, t))^2}{4\rho^2(r, t)} \right) + \frac{1}{2} M v^2(r, t) + V(r) + g \rho(r, t),$$

(3.9)
which is the Josephson relation in its most general form, and which we will need in Chapter 4. The solutions of Eqs. (3.9) and Eqs. (3.8), when substituted into Eqs. (3.3), provide us with the macroscopic wave function \( \Psi(\mathbf{r}) \) describing the BEC.

### 3.2 Vortices and the Transformation to a Rotating Frame

An important question is in which way a condensate can support angular momentum. This can only happen by (netto) rotation-free movement of atoms around an axis, which we will denote the \( z \)-axis. To make this statement more precise, consider a condensate with the velocity profile \( \mathbf{v}(\mathbf{r}) = f(\mathbf{r}) \hat{\theta} \), where \( r \) and \( \theta \) are the radius and polar angle in cylindrical coordinates. This is the simplest ansatz for a velocity profile with azimuthal symmetry and translation symmetry along the \( z \)-axis. From the condition \( \nabla \times (f(\mathbf{r}) \hat{\theta}) = 0 \) one can deduce that \( f(\mathbf{r}) = C/r \), for some constant \( C \). Thus, the fact that the velocity profile is rotation-free demands that the radial dependence is \( 1/r \).

Now, using the single-valuedness of the macroscopic wave function \( \Psi(\mathbf{r}) \), we show that \( C \) can not be any arbitrary number, but can only take values in a discrete (quantized) set. From the single-valuedness it follows that the phase of the wave function \( \phi(\mathbf{r}) \) must change by a multiple of \( 2\pi \) over a closed contour \( \partial A \) that winds the \( z \)-axis once. Thus, it holds that

\[
2\pi n = \oint_{\partial A} \nabla \phi(\mathbf{r}) \cdot d\mathbf{l},
\]

where \( n \) is a (not necessarily positive) integer, and that

\[
2\pi n = \oint_{\partial A} \frac{MC}{\hbar r} \hat{\theta} \cdot d\mathbf{l} = \frac{MC}{\hbar} \oint_{\partial A} d\theta = \frac{2\pi MC}{\hbar}.
\]

Thus, we obtain \( C = n\hbar/M \) and for the velocity profile \( \mathbf{v}(\mathbf{r}) \)

\[
\mathbf{v}(\mathbf{r}) = \frac{n\hbar}{Mr} \hat{\theta}.
\]

A solution of the GPE Eq. (3.6) with such a velocity profile is called a quantized vortex line of charge \( n \) or simply a vortex. We can take the contour \( A \) to be an arbitrary small circle around the \( z \)-axis, and it follows for \( n \neq 0 \) that the phase of the wave function \( \phi(\mathbf{r}) \) must be singular on the \( z \)-axis, which can only happen when the density vanishes. If we assume that
φ(\(\mathbf{r}\)) only depends on the angular variable \(\theta\), it follows from Eq. (3.10) and the definition of \(\mathbf{v}(\mathbf{r})\) that \(φ(\mathbf{r}) = n\theta\). To obtain the density profile away from the \(z\)-axis, one substitutes the ansatz for a vortex of charge \(n\), being \(Ψ(\mathbf{r}) = \sqrt{ρ(\mathbf{r})} e^{inθ}\), into the GPE Eq. (3.6) and solves it for \(ρ(\mathbf{r})\). This can only be done numerically. In the absence of an external trapping potential the solution for \(ρ(\mathbf{r})\) increases quadratically with \(r\) from the origin, while going to a constant value \(ρ_0\) for large \(r\). The crossover occurs at the so-called healing length \(ξ = ℏ/\sqrt{2M\mu}\), that describes the competition between interaction and kinetic energy. In Fig. 3.1 the density profile \(ρ(r)\) is shown as a function of \(r\) for \(n = 1\). The fact that the phase has a singularity at the vortex core has as a consequence that the vortex state has a topological character. The velocity profiles of vortices of different charge cannot be continuously deformed into each other and a vortex can only enter the condensate from the side.

Now, we turn to the question of the amount of angular momentum carried by a vortex state. If a condensate in a symmetric trapping potential contains a vortex of charge \(n\) and has a particle number density \(ρ(\mathbf{r})\), then by using Eq. (3.10) we find that the angular momentum density \(ρ_L(\mathbf{r})\) is given by

\[
ρ_L(\mathbf{r}) = Mr(\mathbf{r}) \times \mathbf{v}(\mathbf{r}) = ρ(\mathbf{r})nℏ.
\]

Thus, the angular momentum density \(ρ_L(\mathbf{r})\) scales as the number density \(ρ(\mathbf{r})\), i.e. each boson carries an angular momentum \(nℏ\) and the total angular momentum of the vortex state of charge \(n\) is equal to \(Nnℏ\), where \(N\) is the number of particles in the condensate. Note that a vortex centered at an arbitrary position \(a\) does not have a total angular momentum \(Nnℏ\) and for such a vortex it does not hold that \(ρ_L(\mathbf{r}) = ρ(\mathbf{r})nℏ\). In the next chapter we will return to off-center vortices. Note that at the mean field level the total angular momentum in the system is quantized in units of \(Nℏ\) and not in units of \(ℏ\). This fact is caused by the approximate mean field description we are using.

In this thesis we want to investigate the behavior of rotating condensates, both in the presence and in the absence of a co-rotating optical lattice potential. It is convenient to transform the problem to a coordinate frame...
that rotates with the optical lattice, because in that frame the Hamiltonian is time-independent. The question is what the energy functional is in the rotating frame. We will show that this functional is $K - \Omega L_z$, where $K$ is given in Eq. (3.5) and $L_z$ is the $z$-component of the angular momentum, where both are calculated in the non-rotating frame. The Lagrangian density $\mathcal{L}(\Psi^*, \Psi)$ describing the condensate and from which the time-dependent GPE Eq. (3.7) can be derived is

$$\mathcal{L}(\Psi^*, \Psi) = \frac{i\hbar}{2} (\Psi^*(\mathbf{r}, t) \partial_t \Psi(\mathbf{r}, t) - \Psi(\mathbf{r}, t) \partial_t \Psi^*(\mathbf{r}, t)) - \left(\frac{\hbar^2}{2M} |\nabla \Psi(\mathbf{r}, t)|^2 + V(\mathbf{r}, t)|\Psi(\mathbf{r}, t)|^2 + \frac{1}{2} g |\Psi(\mathbf{r}, t)|^4 \right),$$

(3.11)

where the potential $V(\mathbf{r}, t)$ possibly depends on time [Peth]. Now, we transform from the non-rotating laboratory frame $S$ to a frame $S'$, which rotates with constant angular velocity $\Omega$ around the $z$-axis in the anti-clockwise direction. In Chapter 4 we will show that for $\Omega$ close to $\omega$, the energy functional $K - \Omega L_z$ simplifies, making it possible to obtain simple expressions for the basis wave functions. Let $\mathbf{r}$ be a fixed position vector in $S$, then the transformed position vector $\mathbf{r}'$ in $S'$ rotates clockwise and is given by

$$\mathbf{r}' = \begin{pmatrix} \cos \Omega t & \sin \Omega t \\ -\sin \Omega t & \cos \Omega t \end{pmatrix} \mathbf{r} \equiv A(t)\mathbf{r}.$$

From this expression one obtains $r' = r$, $\theta' = \theta - \Omega t$, and $\nabla = A^{-T}(t)\nabla'$. It follows that positional derivatives are transformed trivially, i.e. only by a rotation. Since $\mathbf{r}'$ depends on time, a time-derivative will pick-up an extra term. It holds for the co-rotating optical lattice potential that $V(r, \theta, t) = V(r, \theta - \Omega t) = V(r', \theta')$, i.e., it holds that the optical lattice is time-independent in $S'$. We demand that the wave functions in both frames have the same value for equal physical points in space. Thus, it must hold that

$$\Psi'(\mathbf{r}') = \Psi(\mathbf{r}) \quad \text{and} \quad \Psi = \Psi' \circ A(t).$$

This leads to the following equalities

$$\partial_t \Psi(\mathbf{r}, t) = \partial_t [\Psi'(A(t)\mathbf{r}, t)] = \partial_t (\Psi')(\mathbf{r}', t) + \nabla' \Psi'(\mathbf{r}', t) \cdot \partial_t A(t)\mathbf{r},$$

(3.12)

$$\nabla \Psi(\mathbf{r}, t) = A^{-T}(t)\nabla' \Psi'(\mathbf{r}', t).$$

(3.13)
From $\Psi'(r') = \Psi(r)$, it follows $\rho'(r') = \rho(r)$ and $\phi'(r') = \phi(r)$. It is instructive to write the continuity equation Eq. (3.8) in the new coordinates. Using $\rho = \rho' \circ A(t)$, $\phi = \phi' \circ A(t)$, and $\partial_t r' = \Omega r' \times \hat{z}$ we obtain

$$
(\partial_t \rho')(r', t) = -\nabla' \cdot \left( \rho'(r', t) \left( \frac{\hbar}{M} \nabla' \phi'(r', t) - \Omega r' \hat{\theta} \right) \right). \tag{3.14}
$$

Thus, one finds the result that in the rotating frame the velocity profile $v'(r')$ is not given by $v'(r') = (\hbar/M) \nabla' \phi'(r')$, but by $v'(r') = (\hbar/M) \nabla' \phi'(r') - r' \Omega \hat{\theta}$. The origin of the extra term is of course the time-dependent coordinate transformation and its form is precisely the one which is expected intuitively. An important observation is that the continuity equation Eq. (3.8) changes after a transformation to a (non-inertial) rotating frame, or, in other words, that the velocity profile in $S'$ is not given by $v'(r') = (\hbar/M) \nabla' \phi'(r')$. Note that a vortex of charge $n$ with an anti-clockwise rotation sense in $S$ has an anti-clockwise rotation sense for $r \leq \sqrt{\hbar/M\Omega}$, but a clockwise rotation sense for $r \geq \sqrt{\hbar/M\Omega}$ in $S'$. Now, we substitute $\Psi = \Psi' \circ A(t)$ in Eq. (3.11) to find the Lagrangian density $\tilde{L}(\Psi^*, \Psi')$ in terms of the transformed wave functions $\Psi^*$ and $\Psi'$. From Eq. (3.13), it follows that $|\nabla \Psi(r)|^2 = |\nabla' \Psi'(r')|^2$, and the only extra terms in $\tilde{L}(\Psi^*, \Psi')$ come from the time derivatives. Using Eq. (3.12) one obtains

$$
\tilde{L}(\Psi^*, \Psi') = \frac{i\hbar}{2} (\Psi^*(r', t)(\partial_t \Psi')(r', t) - \Psi'(r', t)(\partial_t \Psi^*)(r', t))
$$

$$
- \left( \frac{\hbar^2}{2M} |\nabla' \Psi'(r', t)|^2 + V(r')|\Psi'(r', t)|^2 + \frac{1}{2} g |\Psi'(r', t)|^4 \right)
$$

$$
+ \frac{i\hbar}{2} \partial_t r' \cdot (\Psi^*(r', t) \nabla' \Psi'(r', t) - \Psi'(r', t) \nabla' \Psi^*(r', t)). \tag{3.15}
$$

Note that the potential $V(r')$ is now time-independent. Next, we use that $\partial_t r' = \Omega r' \times \hat{z}$ and that $\hbar \rho' \nabla' \phi' = (\hbar/2i)(\Psi^* \nabla' \Psi' - \Psi' \nabla' \Psi^*)$ to rewrite the last term of $\tilde{L}(\Psi^*, \Psi')$

$$
\frac{i\hbar}{2} \partial_t r' \cdot (\Psi^*(r', t) \nabla' \Psi'(r', t) - \Psi'(r', t) \nabla' \Psi^*(r', t))
$$

$$
= -\hbar \Omega \rho'(r', t)(r' \times \hat{z}) \cdot \nabla' \phi'(r', t) = -\hbar \Omega \rho(\mathbf{r}, t)(A(t) \mathbf{r} \times A(t) \hat{z}) \cdot A(t) \nabla \phi(\mathbf{r}, t)
$$

$$
= \Omega M \rho(\mathbf{r}, t)(\mathbf{r} \times \mathbf{v}(\mathbf{r}, t)) \cdot \hat{z} \equiv \Omega \rho_{L_z}(\mathbf{r}, t),
$$

where we used $A(t) \hat{z} = \hat{z}$. The function $\rho_{L_z}(\mathbf{r}, t)$ is the angular momentum density in the $z$-direction in the non-rotating frame and is defined as $\rho_{L_z} = \ldots$
ψ^* \hat{L}_z \psi, where \hat{L}_z is the z-component of the angular momentum operator, \( \hat{L}_z = -i\hbar (\mathbf{r} \times \nabla) \cdot \mathbf{\hat{z}} \). The time-dependent GPE in the rotating frame can be derived from \( \mathcal{L}(\Psi'^*, \Psi') \) and is given by

\[
i\hbar \partial_t \Psi'(\mathbf{r}, t) = -\frac{\hbar^2}{2M} \nabla^2 \Psi'(\mathbf{r}, t) + V(\mathbf{r}) \Psi'(\mathbf{r}, t) + g|\Psi'(\mathbf{r}, t)|^2 \Psi'(\mathbf{r}, t) - \Omega \hat{L}_z \Psi'(\mathbf{r}, t).
\]

(3.16)

We can again do the substitution

\[
\Psi'(\mathbf{r}, t) = \sqrt{\rho'(\mathbf{r}, t)} e^{i\phi'(\mathbf{r})},
\]

from which we obtain equation Eq. (3.14) and the transformed form of Eq. (3.9)

\[
-\hbar \partial_t \phi'(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \left( \frac{\nabla^2 \rho'(\mathbf{r}, t)}{2\rho'(\mathbf{r}, t)} - \frac{(\nabla \rho'(\mathbf{r}, t))^2}{4\rho^2(\mathbf{r}, t)} \right) + \frac{\hbar^2}{2m} (\nabla \phi'(\mathbf{r}, t))^2 + V(\mathbf{r}) + g\rho'(\mathbf{r}, t) - \hbar \Omega r \cdot \nabla \phi'(\mathbf{r}, t).
\]

(3.17)

Since the new term in \( \tilde{\mathcal{L}}(\Psi'^*, \Psi') \), namely \( \Omega \rho L_z(\mathbf{r}, t) \), does not depend on the time-derivatives of \( \Psi \) or \( \Psi^* \), the conjugate momenta do not change and we can find the transformed energy functional \( \tilde{E}[\Psi'^*, \Psi'] \) using \( E[\Psi'^*, \Psi'] = (\partial_t \Psi'^*) \partial L / \partial (\partial_t \Psi'^*) + (\partial_t \Psi') \partial L / \partial (\partial_t \Psi') - L[\Psi'^*, \Psi'] \) with \( L[\Psi'^*, \Psi'] = \int d\mathbf{r} \mathcal{L}(\Psi'^*, \Psi') \)

\[
\tilde{E}(\Psi'^*, \Psi') = \int d\mathbf{r} \left[ \frac{\hbar^2}{2M} |\nabla \Psi'(\mathbf{r}, t)|^2 + V(\mathbf{r}) |\Psi'(\mathbf{r}, t)|^2 + \frac{1}{2} g|\Psi'(\mathbf{r}, t)|^4 \right] - \Omega L_z,
\]

(3.18)

where we dropped the prime on the integration (dummy) variable. Note that we again should include a Lagrange multiplier to enforce that \( \int \Psi'^* \Psi' = N \) as we did in Eq. (3.5). The energy functional Eq. (3.18) looks awkward: it contains terms with wave functions \( \Psi' \) in a rotating frame and angular momentum in the non-rotating frame. We now show that Eq. (3.18) is actually very convenient. The first thing to note is that from the manipulations below Eq. (3.15) it follows that

\[
L_z = \int d\mathbf{r} M \rho'(\mathbf{r}, t) \left( \mathbf{r} \times \frac{\hbar}{M} \nabla \phi'(\mathbf{r}, t) \right) \cdot \mathbf{\hat{z}},
\]

(3.19)

i.e., we calculate \( L_z \) in the non-rotating frame by taking \( (\hbar/m) \nabla \phi'(\mathbf{r}, t) \) as the velocity profile. Consider now some wave function in the rotating frame
\( \Psi'_{0}(r, t) \). Its time evolution is given by the transformed time-dependent GPE Eq. (3.16) and as a consequence it will obey the transformed continuity equation Eq. (3.14). The number density of atoms is given by \( \rho'(r, t) \) and the velocity profile in the rotating frame by \( (\hbar/M) \nabla \phi'(r, t) - \Omega r^\theta \). This corresponds to a velocity profile in the non-rotating frame of \( \nabla \phi'(r, t) \). The angular momentum in the non-rotating frame is then given by Eq. (3.19).

Consider now a condensate rotating at some velocity \( \Omega \) around the \( z \)-axis. Assume it has only two states: a state \( \Psi'_0 \) that has energy (the first term of Eq. (3.18)) \( E_0 \) and angular momentum (in the non-rotating frame) 0 and a state \( \Psi'_L \) with energy \( E_L \) and angular momentum \( L \). Then, it follows from Eq. (3.18) that the state \( \Psi'_0 \) will be energetically favorable for \( \Omega \leq \Omega_c \equiv (E_L - E_0)/L \) and the state \( \Psi'_L \) for \( \Omega \geq \Omega_c \). This result can e.g. be used to estimate the critical rotation frequency above which it will be energetically favorable for a vortex to enter the cloud. It also shows that for high \( \Omega \), the condensates will have a large amount of angular momentum, i.e., many vortices. If one calculates the energy of a condensate with a single vortex of charge \( n \), one finds that the energy \( E_n \) of such a state scales as \( n^2 \) [Peth]. Hence, under normal circumstances, a vortex of charge \( n \) will be unstable and will disband into \( n \) separate vortices of charge 1. These vortices will arrange themselves in a triangular lattice structure, the so-called Abrikosov lattice. This lattice structure was predicted by Abrikosov in 1957 in the context of quantized magnetic flux lines in type-II superconductors [Abr57]. An Abrikosov lattice of over 100 vortices was observed experimentally in 2001 in a cold atom system by the group of Ketterle [Ket01], following earlier experiments by the group of Dalibard [Dal00] of lattices with \( \sim \) 10 vortices.
3.3 Regular Lattices

3.3.1 Parameterization of the Unit Cell

In this thesis we will consider regular two-dimensional lattices of vortices. In this section we show how we parameterize these vortex lattices. A regular lattice is determined by two lattice vectors $\mathbf{c}_i$, as shown in Fig. 3.2. We assume $|\mathbf{c}_1| \leq |\mathbf{c}_2|$ and denote the area of the unit cell $\nu$, i.e. $|\mathbf{c}_1 \times \mathbf{c}_2| = \nu$. In addition, we consider lattices which are equal up to a global rotation the same lattice. Then, we can parameterize the unit cell of the lattice by $\nu$, the smallest angle $\theta$ between the two lattice vectors $\mathbf{c}_1$ and $\mathbf{c}_2$, and by the ratio $p$ between the lengths of the largest and smallest lattice vector, $p = |\mathbf{c}_2|/|\mathbf{c}_1|$. Thus, we have $p \geq 1$ and $0 < \theta \leq \frac{\pi}{2}$. Let $c_1$ be the length of $\mathbf{c}_1$, then the lattice vectors are given by $\mathbf{c}_1 = c_1(1, 0)^T$ and $\mathbf{c}_2 = pc_1(\cos \theta, \sin \theta)^T$. From the requirement $\nu = |\mathbf{c}_1 \times \mathbf{c}_2| = p c_1^2 \sin \theta$, we can then eliminate $c_1$ in favor of $\nu$ and write

$$\mathbf{c}_1 = \sqrt{\frac{\nu}{p \sin \theta}} (1, 0)^T$$

and

$$\mathbf{c}_2 = \sqrt{p \nu \sin \theta (\cot \theta, 1)^T}.$$  \hspace{1cm} (3.20)

It is important to note that for a given lattice, there are also other possible choices of lattice vectors, as shown in Fig. 3.3. Indeed, every combination $\mathbf{c}'_i = n'_1 \mathbf{c}_1 + n'_2 \mathbf{c}_2$ will span the lattice, provided that $|\mathbf{c}'_1 \times \mathbf{c}'_2| = \nu$ or $|n'_1 n'_2 - n'_1 n'_2| = 1$. Hence, there are several combinations of $\theta$ and $p$ that represent the same lattice. Throughout this thesis we will calculate the energy of a vortex lattice as a function of $\nu$, $\theta$, and $p$ and this freedom in
choice will enable us to choose $\pi/3 \leq \theta \leq \pi/2$. If, for some choice of lattice vectors $\mathbf{c}_i$, we have $\theta \leq \pi/3$, we can always choose different lattice vectors $\mathbf{c}'_i$ with $\pi/3 \leq \theta \leq \pi/2$, as we explain in the following. It is clear that there must exist a vector $\mathbf{c}_0$, which is the smallest lattice vector, which, together with a lattice vector $\mathbf{c}_s$, spans the lattice, as shown in Fig. 3.4. We consider the vectors $\mathbf{c}_n = \mathbf{c}_s - l_1 \mathbf{c}_0$, with $l_1$ an integer. The point now is that we can choose $l_1$ such that $|\mathbf{x} \cdot \mathbf{c}_n| \leq c_0/2$, i.e. $\mathbf{c}_n$ lies between the two vertical dashed lines. Since we also know that $\mathbf{c}_n$ is not the smallest lattice vector, $\mathbf{c}_n$ must also lie outside the dashed circle. If $\mathbf{c}_n$ lies in area A we choose $-\mathbf{c}_0$ and $\mathbf{c}_n$ as the lattice vectors and if $\mathbf{c}_n$ lies in area B we choose $\mathbf{c}_0$ and $\mathbf{c}_n$ as the lattice vectors. In both cases the new $\theta$ obeys $\pi/3 \leq \theta \leq \pi/2$. Thus, for an arbitrary pair $(p, \theta)$ we can find a new pair $(p_n, \theta_n)$ by choosing different basis vectors, with $\theta_n \geq \pi/3$, and we will choose the pair for which $\theta_n$ is closest to $\pi/2$. To gain some insight in the values of these new lattice parameters $(p_n, \theta_n)$, we plot the functions $p_n(p, \theta)$ and $\theta_n(p, \theta)$ in Fig. 3.5. One observes that for $\theta \to \pi/2$ it holds that $p_n \to p$ and for $\theta \to 0$ that $p_n \to \infty$. Considering $\theta_n$, one observes that both for $\theta \to \pi/2$ and $\theta \to 0$ it holds $\theta_n \to \pi/2$. We will not go into detail about the behavior of $(p_n, \theta_n)$ for non-extremal values of $\theta$, except noting the trend that for high values of $p$ it holds that $\theta_n$ is close to $\pi/2$ for all $\theta$. For later convenience we define the dimensionless lattice vectors as $\tilde{\mathbf{c}}_i \equiv \mathbf{c}_i/\sqrt{v}$. Note that the $\mathbf{c}_i$’s are functions of $\nu$, $p$, and $\theta$, but that the $\tilde{\mathbf{c}}_i$’s do not depend on $\nu$.
3. Preliminaries

3.3.2 The Reciprocal Lattice

Normally, one defines the reciprocal lattice vectors by $K_1 = (2\pi/\nu)c_2 \times \hat{z}$ and $K_2 = -(2\pi/\nu)c_1 \times \hat{z}$. With these definitions, it holds that $|c_i \cdot K_j| = 2\pi \delta_{ij}$ and that

$$K_1 = \frac{2\pi p \sin \theta}{\sqrt{p\nu \sin \theta}} (1, -\cot \theta)^T \quad \text{and} \quad K_2 = \frac{2\pi}{\sqrt{p\nu \sin \theta}} (0, 1)^T. \quad (3.21)$$

However, taking the cross product with $\hat{z}$ amounts to sending $(x, y) \to (y, -x)$, i.e. performing a global rotation over $\pi/2$ in the clockwise direction. Thus, if we would use the alternative definition $K_1^a = -K_2$ and $K_2^a = K_1$, we can go from $c_i$ to $K_i^a$, by performing a global rotation and a scaling by $2\pi/\nu$. From this argument, it is clear that the real space lattice and the reciprocal lattice are identical up to a global rotation and a uniform scaling.

These remarks are important because in Chapter 5 we will have to evaluate summations and products over all reciprocal lattice vectors. We have just shown that instead of the reciprocal lattice vectors, we can also take the vectors in real space as summation or product variables. The advantage is that we have a much better intuition for real space.
4. LLL PHYSICS

4.1 The LLL wave function

In the previous chapter, the energy functional was derived for a condensate of atoms of mass $M$ in a radially symmetric magnetic trap, with trapping frequencies $\omega_z$ and $\omega_\bot \equiv \omega$, loaded in an optical lattice potential $V(r, t)$, in a frame rotating with angular velocity $\Omega$ around the symmetry axis ($z$-axis). In this frame, the energy functional is time-independent. For now, we will ignore the optical lattice potential. Then, the condensate wave function $\Psi(x, y, z)$ is given by minimization of this energy functional, which (in a rewritten form) reads

$$K = \int \! \! d r \Psi^*(r)[h_z + h_\bot - \Omega L_z - \mu] \Psi(r) + \frac{1}{2} g \int \! \! d r |\Psi(r)|^4,$$

where $h_z = -(\hbar^2/2M) \nabla_z^2 + M\omega_z^2 z^2/2$ and $h_\bot = -(\hbar^2/2M) \nabla_\bot^2 + M\omega^2(x^2 + y^2)/2$ are the single particle Hamiltonians. Note that the radial and $z$-direction are decoupled in the single particle part of the Gross-Pitaevskii functional $K$ in Eq. (4.1). Since we will be interested in the arrangement of the vortices in the $xy$-plane, we will assume a step function for the $z$-dependence of the wave function, i.e., we write $\Psi(r) = \psi(x, y)\theta(d_z/2 - |z|)/\sqrt{d_z}$, where $d_z$ is a typical condensate size. We drop the constant contribution from the single particle Hamiltonian $h_z$. It is useful to rewrite $h_\bot - \Omega L_z = \mathcal{H} + (\omega - \Omega)L_z$, where

$$\mathcal{H} = \frac{1}{2M}(-i\hbar \nabla - eA/c)^2/2M,$$

which is the Hamiltonian $(-i\hbar \nabla - eA/c)^2/2M$ of a particle of charge $-e$ moving in the $xy$-plane, subjected to an uniform magnetic field $B\hat{z}$ in the $z$-direction with a vector potential $A = B\hat{z} \times r/2$, with $eB/Mc = 2\omega$. The eigenfunctions of $\mathcal{H}$, $h_{n,m}(x, y)$, have eigenvalues $\epsilon_{n,m} = \hbar\omega(2n + 1)$ [Gir],
where $m$ and $n$ are non-negative integers. The integer $n$ is called the Landau Level index, and $m$ labels the degenerate states within a Landau level $n$. In addition, the $h_{n,m}(x, y)$ are also eigenfunctions of $L_z$ with eigenvalues $\hbar(m - n)$. Combination of these two facts leads to the eigenvalue equation

$$(h_{\perp} - \Omega L_z)h_{n,m}(x, y) = \hbar[(\omega + \Omega)n + (\omega - \Omega)m + \omega]h_{n,m}(x, y).$$ (4.2)

Now, we consider the limit of $\Omega$ close to $\omega$, where the centrifugal force almost cancels the effect of the harmonic trapping potential. Then, the eigenvalue equation for $h_{n,m}$ can be written as

$$(h_{\perp} - \Omega L_z)h_{n,m}(x, y) = \hbar\omega(2n + 1)h_{n,m}(x, y).$$ (4.3)

If the contribution of other terms in the Hamiltonian (e.g. the interaction energy and optical lattice potential) are much smaller than the gap of $2\hbar\omega$, the macroscopic condensate wave function will consist only of orbitals with $n = 0$. This is equivalent to saying that the system resides in the Lowest Landau Level (LLL). The typical interaction energy per particle is $gn_p$, where $n_p$ is the particle density. Thus, to be in the LLL requires that $gn_p \ll 2\hbar\omega$. Ref. [Cor04a] shows that the LLL is attainable experimentally. The (unnormalized) LLL wave functions are given by $h_m(x, y) \equiv h_{0,m}(x, y) = c_m z^m e^{-r^2/2\ell^2}$, where $z$ is the complex position coordinate $z = x + iy$, $r^2 = x^2 + y^2$, $c_m$ is some normalization constant that we will specify later, and $\ell$ is the magnetic length, defined as $\ell = \sqrt{\hbar/M\omega}$ [Gir]. Note that the LLL regime is degenerate, all wave functions in the LLL have the same energy. In Fig. 4.1, the density $\rho_m \equiv h_m^* h_m$ is plotted as a function of the $x$-coordinate for $y = 0$ and $m = 1, 2, 3$. For all $m$ the density goes to zero for $r \to \infty$ or $r \to 0$ and for higher $m$ the radius of the “ring” is larger. We can write the phase of $h_m(x, y)$ (up to a constant) as $\phi(x, y) = \tan^{-1} y/x$. Thus, for the velocity profile $v_m(x, y)$ of $h_m(x, y)$ we find $v_m(x, y) = (m\ell^2\Omega/r)\hat{\theta}$ and it follows that $h_m(x, y)$ represents a quantized vortex at the origin of charge $m$, and $\phi(x, y)$ increases by $2\pi m$ when going around the origin. Note that only non-negative values of $m$ are possible.

It is instructive to calculate the energy of a classical particle of mass $M$ moving in the trapping potential with velocity $v_m(x, y)$. That energy is given by $E = M\omega^2 r^2/2 + Mm^2 \ell^4 \Omega^2/2r^2 = (M\Omega^2 \ell^2/2) \left[\frac{r^2}{\ell^2} + \frac{m^2 \ell^2}{r^2}\right]$, which is minimal at $r = \sqrt{m\ell}$ with $E = mM\Omega^2 \ell^2$. The maximum of the wave function $h_m(x, y)$ is also at $r = \sqrt{m\ell}$ and the standard deviation is equal to $\sigma_r = \ell/2$. 
The general form \( \psi(x, y) \) of the condensate wave function in the LLL is a linear combination of (normalized) LLL basis functions,

\[
\psi(x, y) = \sum_{m=0}^{\infty} \frac{a_m}{\sqrt{\pi m!}} \ell^{m+1} z^m e^{-r^2/2\ell^2} \equiv f(z) e^{-|z|^2/2\ell^2},
\]

where \( f(z) \) is an arbitrary analytic function. It must hold that \( \sum_{m=0}^{\infty} |a_m|^2 = N \) for \( \psi \) to be normalized. In analogy to Chapter 3, where we wrote the wave function in terms of a density and a phase, we write \( f(z) = \sqrt{\bar{\rho}(z)} e^{i\phi(z)} \), where \( \bar{\rho} \) and \( \phi \) are both real functions. The function \( f(z) \) is analytic and obeys the Cauchy-Riemann equations. This leads to the following relations between \( \bar{\rho} \) and \( \phi \),

\[
\partial_x \phi = -\frac{\partial_y \bar{\rho}}{2\bar{\rho}} \quad \text{and} \quad \partial_y \phi = \frac{\partial_x \bar{\rho}}{2\bar{\rho}}.
\]

Now, using these equations we can eliminate \( \phi(x, y) \) from the continuity equation Eq. (3.14) to obtain

\[
\partial_t \bar{\rho}(x, y, t) = (\Omega - \omega)(x\partial_y - y\partial_x)\bar{\rho}(x, y, t) = 0.
\]

In hindsight, this result is obvious since all states in the LLL have the same energy and therefore all states are stationary states (in the rotating frame!). Now, we consider Eq. (3.17) in the LLL with \( g = 0 \). Using the relations Eq. (4.5) we obtain, after some algebra, the result

\[
\partial_t \phi(r, t) = -\Omega.
\]

Thus, the wave function evolves in time as \( e^{-i\Omega t} \), which is consistent with the fact that a state in the LLL is a stationary state with energy \( \hbar\Omega \). Note
that it follows that $\nabla \phi$ is time-independent in the rotating frame. In the non-rotating frame, the wave function (as well as its density distribution and velocity profile) perform an anti-clockwise uniform rotation around the $z$-axis with angular velocity $\Omega$. Using Eq. (4.5) we can deduce that $\nabla^2 n(x, y) = 0$, $\nabla^2 \phi(x, y) = 0$, and $\nabla \phi \perp \nabla \tilde{\rho}$, where $n \equiv \log(\tilde{\rho})$.

Now, we go back to Eq. (4.4) and assume some cut-off $N_v$ such that $a_m = 0$ for $m > N_v$. By the fundamental theorem of algebra, it holds that a complex polynomial of degree $N_v$ is completely determined (up to a constant factor) by the position of its (possibly degenerate) zeros. We assume that the zero’s of $\psi$ are given by the collection of complex numbers $\{\xi_b\}$ and then we can rewrite the wave function $\psi$ as

$$\psi(x, y) = \sqrt{\frac{N}{\pi \ell^2 C}} \prod_{b=1}^{N_v} (z - \xi_b) e^{-|z|^2/2\ell^2},$$

(4.6)

for some normalization factor $C$. It holds that the $\{\xi_b\}$ are precisely the positions of the vortices. Thus, a LLL state is completely determined by the positions of its vortices. This is a very important property of the LLL regime, which can very much simplify the calculations. Note that the cutoff $N_v$ is also equal to the number of vortices in the system.

### 4.2 Calculation of Energy Terms

Now, we will compare the two representations of the wave function $\psi$ in Eq. (4.4) and Eq. (4.6) by calculating the various terms of the energy functional Eq. (3.18) in terms of the $a_m$ of Eq. (4.4) and in terms of the $\xi_b$ of Eq. (4.6). We define

$$K = \frac{\hbar^2}{2M} \int dr |\nabla \Psi(r)|^2, \quad P = \int dr V(r)|\Psi(r)|^2, \quad \text{and} \quad R = L_z,$$

with $V(r) = M\omega^2(x^2 + y^2)/2$. Then, by using the orthogonality of the LLL basis wave functions, one obtains

$$K = P = \frac{1}{2} \hbar \Omega \sum_{m=0}^{N_v} (m + 1)|a_m|^2 \quad \text{and} \quad R = \hbar \sum_{m=0}^{N_v} m|a_m|^2.$$

(4.7)

If we put $g = 0$ the total energy functional from Eq. (3.18) is given by

$$E = K + P - \Omega R = \hbar \Omega \sum_{m=0}^{N_v} |a_m|^2 = \hbar \Omega \sum_{m=0}^{\infty} |a_m|^2 = N\hbar \Omega,$$
where we used the normalization condition for the macroscopic wave function and the fact that we set the $a_m$’s to zero for $m > N_v$. Again, we again obtain the result that the LLL is degenerate. Now, we project the interaction energy $I = (g/2) \int \text{d}r |\Psi(r, t)|^4$ on the LLL. We determine $I$ by substituting Eq. (4.4) for $\psi$ and obtain the result
\[ I = \frac{g}{4\pi d_z \ell^2} \sum_{m=0}^{2N_v} \frac{m!}{2^m} \left| \sum_{r=0}^{m} \frac{a_r}{\sqrt{r!}} \frac{a_{m-r}}{\sqrt{(m-r)!}} \right|^2. \]

Note that $K$, $P$ and $\Omega R$ are single-particle energies, and $I$ is a two-particle energy, as expected. To be able to calculate $K$, $P$, $R$, and $I$ in terms of the vortex coordinates $\xi_b$, we first expand Eq. (4.6) in terms of the LLL basis wave functions. Comparing Eq. (4.4) and Eq. (4.6), one can deduce that
\[ a_m = (-1)^{N_v-m} \sqrt{\frac{N_m!}{C}} P_{N_v-m}(\{\xi\}), \]
where $P_m(\{\xi\}) = \ell^{N_v-m} \sum_{i_1 < i_2 < \cdots < i_m} \xi_{i_1} \xi_{i_2} \cdots \xi_{i_m}. \quad (4.8)$

Following [Gun06] we will denote $P_m(\{\xi\}) \equiv P_m$ the $m$th symmetric polynomial in the variables $\{\xi\}$. It holds that up to some factors the $m$th symmetric polynomial is equal to $a_{N_v-m}$. From the normalization condition, $\sum_{m=0}^{\infty} |a_m|^2 = N$, one obtains an expression for $C$
\[ C = \sum_{m=0}^{N_v} m! |P_{N_v-m}|^2. \]

Now we substitute Eq. (4.8) into the expressions for $K$, $P$, $R$, and $I$, leading to
\[ K = P = \frac{Nh\Omega}{2C} \sum_{m=0}^{N_v} (m+1)m! |P_{N_v-m}|^2, \quad R = \frac{Nh}{C} \sum_{m=0}^{N_v} mm! |P_{N_v-m}|^2, \quad (4.9) \]
and \[ I = \frac{gN^2}{4\pi d_z \ell^2 C^2} \sum_{m=0}^{2N_v} \frac{m!}{2^m} \left| \sum_{r=0}^{m} P_{N_v-r} P_{N_v-(m-r)} \right|^2. \quad (4.10) \]
4. LLL Physics

4.3 Regular Vortex Lattices in the LLL

To gain insight in the LLL we will calculate the above expressions from Eq. (4.9) and Eq. (4.10) numerically for regular square and triangular lattices and compare the results. The set of points of these lattices are denoted by $Sq(x,c)$ and $Tr(x,c)$, respectively, and are given by

$$Sq(x,c) = \{(x_i,x_j)|i,j \in \mathbb{Z} \text{ and } i^2 + j^2 \leq c^2\} \quad \text{and} \quad Tr(x,c) = \{xic_1 + xjc_2|i,j \in \mathbb{Z} \text{ and } |ic_1 + jc_2|^2 \leq c^2\}.$$ 

The parameter $x$ scales the lattice uniformly and $c$ controls the amount of vortices in the lattices, while ensuring a regular structure. The lattice vectors for the triangular case are given by $c_1 = p(1,0)$ and $c_2 = p(1/2, \sqrt{3}/2)$, where $p^2 = 2/\sqrt{3}$ is a normalization factor which ensures that the unit cells of the square and triangular lattices have equal area. The number of vortices in the sets $Sq(x,c)$ and $Tr(x,c)$ is a step function of $c$, increasing at a discrete set of values of $c$. For a given $c$, we minimize $I$ as a function of $x$ and denote the optimal value $x_0$. We carry out this procedure for the square and triangular lattices separately. As an example, we will analyze the case of a triangular lattice with $c = 3.5$. This lattice has 37 vortices and is shown in Fig. 4.2(a). We denote the angular momentum per vortex $R'$, i.e. $R' = R/N_v$. In Fig. 4.2(b) we plot $R'$ in units of $\hbar$ and $I$ in arbitrary units, both as a function of $x$. One observes that the interaction energy $I$ has a minimum around $x_0 = 1.8\ell$ and that around $x_0$ the value of $R'$ drops steeply from $\hbar\omega$ to 0. These characteristics are present also for other vortex numbers, both for the triangular and square lattice structures. Qualitatively, we can understand these observations as follows: Recall that $a_m$ in equation Eq. (4.8) is the coefficient of the $m$-th (normalized) LLL basis wave function $h_m(x,y)$, see equation Eq. (4.4). From Eq. (4.8) it follows that $a_m$ scales with $x$ as $a_m \sim x^{N_v-m}$. Hence, for small (large) values of $x$ the basis wave functions $h_m$ with $m$ close to $N_v$ (0) will be dominant in the wave function $\psi(x,y)$ in Eq. (4.4). In Fig. 4.3 we show a logarithmic plot of the values of $|a_m|^2$ as a function of $m$: for $x = 1.5$ in Fig. 4.3(a) and for $x = 2.1$ in Fig. 4.3(b). Indeed, one observes that for $x < x_0$, the $a_m$’s with $m$ close to $N_v = 37$ are dominant, and that for $x > x_0$, the $a_m$’s with $m$ close to 0 are dominant. Note that most $a_m$ have value zero. The reason for this is that (for the triangular lattice) $P_l = 0$, unless $l$ is a multiple of six. The angular momentum eigenvalue of $h_m$ is $m\hbar$ and this fact explains the observed curve
Fig. 4.2: (a) A regular triangular lattice configuration with 37 vortices. (b) The angular momentum per vortex, $R'$, in units of $\hbar$ and the interaction energy $I$ in arbitrary units, both as a functions of $x$.

Fig. 4.3: Logarithmic plot of the values of $|a_m|^2$ as a function of $m$ (a) for $x = 1.5$ and (b) for $x = 2.1$.

for $R'$: for small values of $x$, the wave function consists for the most part out of basis states with angular momentum close to $Nh$, whereas for large values of $x$, states with angular momentum eigenvalue close to 0 dominate in the wave function. The crossover between these two regimes occurs around $x_0 = 1.8\ell$ and the curve for $R'$ is increasingly steep for higher number of vortices. Now, the density distribution of $h_m$ is a ring of radius $\sqrt{m}\ell$ and (full) width equal to $\ell$. Thus, for small values of $x$ the density is concentrated in the ring of radius $\sqrt{N_v}a$ and for large values of $x$ near the origin. The optimal density distribution will be the one that is as uniform as possible, i.e. near the crossover between regions of small and large angular momentum.
4.4 Results as a function of $N_v$

Now, we extend our analysis to other vortex numbers and calculate first $x_0$, then $I$ and $R$ at $x_0$, for different vortex numbers $N_v$, both for the square and triangular lattices. For vortex numbers higher than 100, the numerical calculations become too lengthy. For both types of lattices and all vortex numbers we find that $x_0 \approx 1.78 \ell$. Thus, it is reasonable to assume that the crossover that we described above occurs for regular lattices at a unit cell area of approximately $1.78^2 \ell^2 = 3.17 \ell^2$. It is interesting to compare this value to the vortex density that is expected classically. The circulation around a closed contour in a 2D system with a velocity profile $v(r)$ is defined as $\Gamma = \oint v(r) \cdot dl$. Consider a fluid with a uniform bulk rotation around the $z$-axis with angular velocity $\Omega$. It holds that $v(r) = \Omega \hat{z} \times r$ and if we choose the contour to be a circle of radius $r$ around the origin, it holds that $\Gamma = 2\pi \Omega r^2$. From Eq. (3.10) one obtains that the circulation around a single vortex is equal to $\hbar/M$, and thus for the total circulation around a circle of radius $r$ around the origin, in a system with a vortex density $n_v$, we obtain $\Gamma = \pi r^2 n_v \hbar/M$. Equating the $\Gamma$ in both cases, we obtain $n_v = \Omega M/\pi \hbar = 1/\pi \ell^2$. Thus, the unit cell area of approximately $3.17 \ell^2$ obtained from our calculations is within our accuracy equal to the classically expected area of $\pi \ell^2$. At the crossover value of $x$, the angular momentum per vortex is approximately $0.55 \hbar$ for both lattices and this value seems to be independent of the number of vortices in the system. Thus, we observe that for our vortex numbers the total angular momentum in the system increases linearly with the vortex number $N_v$.

In Fig. 4.4(a) we plot the interaction energy $I$ in units of $gN^2/d_z \ell^2$ for $x = x_0$ versus the number of vortices $N_v$ in the system for the triangular lattice structure. One observes that $I$ decreases monotonically with $N_v$ and that the value of $I$ seems to converge to a limit value for $N_v \to \infty$. We obtain a similar plot for the square lattice. It is not clear from Fig. 4.4(a) whether this limit is equal to 0 or has a finite value. A little thought, however, shows that $I \to 0$ when the cutoff $N_v \to \infty$. For higher values of $N_v$ the density is able to spread out over a larger area, since basis states $h_m$ of higher quantum number are available, and this causes $I$, which scales as the density squared, to go to 0 for $N_v \to \infty$. In the next section, we will describe how to take the limit $N_v \to \infty$ without unphysical results such as a diverging angular momentum and a vanishing interaction energy. But first, we compare the obtained energies for both lattices to deduce which of the two is the smallest.
In Fig. 4.4(b) we plot the data points of the interaction energy $I$ versus the total angular momentum $L_z$, both at $x_0$, both for the triangular lattice (solid line) and the square lattice (dashed line). The values of $I$ for the square lattice are raised by 0.01 to prevent the curves from falling on top of each other. The lines correspond to a least squares fit to the data points of the function $f(x) = ax^b e^{-cx}$. Because boundary effects are large for small vortex numbers, the first 2 (3) data points were not taken into account for the fit for the triangular (square) lattice. Furthermore, the data points were weighted with the value of $N_v$ for that data point, because boundary effects are smaller for larger vortex numbers.

In Fig. 4.4(c) we plot the difference $\Delta I$ between the fit found for the square and triangular lattice, i.e. $\Delta I = f_{\text{square}} - f_{\text{triangular}}$ versus the angular momentum $L_z$. One observes that for the vortex numbers that we have chosen, the triangular lattice structure is energetically favorable in comparison with the square lattice structure. This result is consistent with the literature and experiment [Abr57,Dal00,Ket01]. On a side note, we remark that we compared the energies of the square and triangular vortex lattices as a function of angular momentum. However, this approach is not exactly the right one. In the gedanken-experiment we use, it is not true that the system has some fixed angular momentum and that we look for a state of minimal energy having that angular momentum. Instead, we should consider the following situation. We apply an anisotropic potential (e.g. pinning potential) to the non-rotating condensate that rotates with an angular velocity $\Omega$ and delivers angular momentum to the condensate. After some time, the condensate reaches rotational equilibrium and the transfer of angular momentum stops. This corresponds to the situation in the presence of pinning that we will consider in the next two chapters. To go the an unpinned situation, one slowly turns the anisotropic potential off, all the time keeping the condensate in rotational equilibrium with the anisotropic potential. One could regard the situation in this chapter as if there was a rotating anisotropic potential of infinitesimal strength that ensures that the condensate is in rotational equilibrium with velocity $\Omega$ and offers the possibility of angular momentum exchange. Hence, instead of comparing energies of vortex lattices at fixed angular momentum, in the next chapter we will compare these energies in the limit of $N_v \to \infty$. The fact that $\Delta I$ decreases with $N_v$ is explained by the observation that both fitting functions $f$ decrease with $N_v$. We used $f(x) = ax^b e^{-cx}$ as a fitting function instead of, e.g., $f(x) = a e^{-cx}$, because the former fits our data points much better. However, making the latter
choice for the fitting function influences the curve of $\Delta I$ shown in Fig. 4.4(c) only for a very small amount. In Fig. 4.4(c) one also observes that $\Delta I \to 0$ when $N_v \to \infty$. In the next section we show how to take the limit $N_v \to \infty$.

4.5 First Order Corrections

We saw in the previous section that the approximate eigenvalue equation Eq. (4.3) has as a consequence that the interaction energy $I$ of a regular vortex lattice and the energy difference $\Delta I$ between square and triangular vortex lattices in the LLL go to 0 when the number of vortices $N_v$ goes to infinity. In the next chapter we want to use an approach by Ho from Ref. [Ho01] that uses this assumption to calculate the interaction energies of vortex lattices. In this section we take into account terms that are first order in the small parameter $\epsilon = (\omega - \Omega)/\omega \ll 1$ in our analysis and investigate the limit $N_v \to \infty$.

We rewrite the exact eigenvalue equation Eq. (4.2) in terms of $\epsilon$

$$(h_{\perp} - \Omega L_z)h_{n,m}(x,y) = \hbar\omega[2n + (m-n)\epsilon + 1]h_{n,m}(x,y).$$

If we again assume that the contribution from other terms in the Hamiltonian is much smaller than $2\hbar\omega$, the wave function $\psi(x,y)$ will consist only of orbitals with $n = 0$ and we arrive at the eigenvalue equation

$$(h_{\perp} - \Omega L_z)h_m(x,y) = \hbar\omega(m\epsilon + 1)h_m(x,y), \quad (4.11)$$

where again $h_m \equiv h_{0,m}$. The difference between Eq. (4.3) and Eq. (4.11) is that in the latter the degeneracy is lifted by the small parameter $\epsilon$ and that it is energetically costly to include orbitals of high angular momentum. Note that since $n = 0$, it still holds that the wave function can be written as the product of an analytic function and a Gaussian, as in Eq. (4.4). Instead of $I$, the energy $E$ which we have to minimize becomes

$$E = I + \epsilon\hbar\sum_{m=0}^{N_v} m|a_m|^2 = I + \epsilon\omega R, \quad (4.12)$$

where we used Eq. (4.7). To be able to rescale to dimensionless quantities we write, using Eq. (4.9) and Eq. (4.10),

$$\omega R = N\hbar\omega\alpha_R \quad \text{with} \quad \alpha_R \equiv \frac{1}{C} \sum_{m=0}^{N_v} mm!|P_{N_v-m}|^2,$$
Fig. 4.4: (a) The interaction energy $I$ in units of $gN^2/d_z \ell^2$ at $x = x_0$ versus $N_v$ for the triangular lattice. (b) $I$ versus the total angular momentum $L_z$ and a fit $f(x) = ax^b e^{-cx}$ for the triangular (solid line) and the square lattice (dashed line). The curve for the square lattice is raised by 0.01 to prevent the curves from falling on top of each other. (c) $\Delta I$ versus $L_z$. 
\[ I = \alpha_I \frac{g N^2}{d_z \ell^2} \quad \text{with} \quad \alpha_I = \frac{1}{4\pi C^2} \sum_{m=0}^{2N_v} \sum_{r=0}^{m} \frac{m!}{2^m} P_{N_v-r} P_{N_v-(m-r)} \left| a_{m-r} \right|^2. \]

Now, if we define \( E' = E d_z \ell^2 / g N^2 \) and \( \beta = \hbar \omega d_z \ell^2 / g N \), it holds for the dimensionless energy \( E' \) that

\[ E' = \alpha_I + \epsilon \beta \alpha_R. \]  

(4.13)

We calculate \( E' \) for the triangular lattice of 37 vortices displayed in Fig. 4.2(a) for several values of \( \epsilon \beta \) and plot the results in Fig. 4.5(a). One observes that if we increase the value of \( \epsilon \beta \) the position \( x_0 \) of the minimum shifts to the right and the value of \( E' \) at \( x_0 \) increases. It also holds that for moderate values of \( \epsilon \beta \) the minimum becomes much deeper, which is caused by the extra contribution from \( R \) at the left part of the curve. For the square lattice and other vortex numbers we find similar results. In Fig. 4.5(b) we plot the minimum of the rescaled energy \( E' \) for the square lattice as a function of the vortex number \( N_v \) for several values of \( \epsilon \beta \), where the lines connecting the data points are guides to the eye. The points for \( \epsilon \beta = 0 \) are (of course) the same as in Fig. 4.4(a), but for higher values of \( \epsilon \beta \) one observes that \( E' \) is constant for \( N_v > 50 \). The explanation for this observation is given in Figs. 4.6(a) and (b). Here we plot the values of \( |a_m|^2 \) for two values of \( m \) versus the number of vortices \( N_v \). We show in Fig. 4.6(a) the values of \( |a_m|^2 \) for \( m = 5 \) and \( m = 9 \) for the square lattice and in Fig. 4.6(b) the values of \( |a_m|^2 \) for \( m = 1 \) and \( m = 7 \) for the triangular lattice. Again, the lines are guides to the eye. One observes that for both lattices \( |a_m|^2 \) goes to a constant non-zero value for \( N_v \to \infty \). This observation also holds for values of \( m \) that are not displayed and has two consequences. The first is that increasing the number of vortices \( N_v \) does not change the values of \( |a_m|^2 \) for \( m \ll N_v \). Secondly, since it holds that \( \sum_{m=0}^{\infty} |a_m|^2 = 1 \), it also follows that the \( a_m \) will be small for high values of \( m \). Combination of these two consequences leads to the claim that the wave function is largely independent of \( N_v \) and thus that the limit \( N_v \to \infty \) is a good one to take. This is consistent with the observation from Fig. 4.5(b) where \( E' \) was observed to be independent of \( N_v \).

We have the following physical picture in mind. Without the first order term in Eq. (4.13) the optimal density distribution is an uniform one. However, because this term in Eq. (4.13) is proportional to the angular momentum, its inclusion leads to the density being concentrated near the origin, i.e. to increase the optimal value of \( x \). Adding vortices far away from the
Fig. 4.5: The rescaled energy $E'$ as a function of $x$ for several values of $\epsilon\beta$ (a). The minimum of the rescaled energy $E'$ as a function of the vortex number $N_v$ for several values of $\epsilon\beta$ (b).

Fig. 4.6: The values of $|a_m|^2$ for two values of $m$ versus the number of vortices $N_v$. In (a) the square lattice for $m = 5, 9$ and in (b) the triangular lattice for $m = 1, 7$.

origin has a very small effect, since the density is very low there. To conclude, we state the result of this analysis. It is appropriate to study regular vortex lattices in the limit $N_v \to \infty$ if the density is peaked near the origin and falls of to 0 for large $r$. 
5. SINGLE COMPONENT VORTEX LATTICES

5.1 rewriting the LLL wave function

In this chapter we use an approach from Ref. [Ho01] to calculate the energy of regular infinite vortex lattices in condensates with one atomic species. We will denote these lattices single component vortex lattices. We consider arbitrary lattice configurations (i.e. arbitrary unit cell shapes), both in the absence and in the presence of an optical lattice potential. Above, we saw that in the LLL the wave function $\psi(x, y)$ is completely determined by the position of its vortices and that it is given by

$$
\psi(x, y) = C_0 \prod_{b=1}^{N_v} (z - \xi_b) e^{-|z|^2/2\ell^2},
$$

where $C_0$ is some normalization factor such that $\int \text{d}r |\psi|^2 = N$, the $\xi_b$ are the complex vortex positions, and $N_v$ is the number of vortices. Above we saw that it is reasonable to consider the limit $N_v \to \infty$ and we assume that the $\xi_b$ form a regular lattice:

$$
\{\xi_b \mid b \in \mathbb{N}\} = \{n_1 c_1 + n_2 c_2 \mid n_1, n_2 \in \mathbb{Z}\},
$$

where the $c_i$’s are the complex lattice vectors from Eq. (3.20). Using this equality, the amplitude of the wave function becomes

$$
|\psi(x, y)|^2 = C_0^2 \prod_{n_i \in \mathbb{Z}} |r - n_i c_i|^2 e^{-r^2/\ell^2}.
$$

(5.1)

We rewrite Eq. (5.1) as follows

$$
|\psi(x, y)|^2 \equiv C_0^2 e^{-\mathcal{H}}, \quad \text{where} \quad \mathcal{H} = r^2/\ell^2 - 2 \sum_{n_i \in \mathbb{Z}} \log |r - n_i c_i|.
$$
It holds that $\mathcal{H}$ obeys the differential equation

$$\left(\partial_x^2 + \partial_y^2\right) \mathcal{H} = 4\pi \left(\frac{1}{\pi \ell^2} - \sum_{n_i \in \mathbb{Z}} \delta(r - n_i c_i)\right), \quad (5.2)$$

and we note that Eq. (5.2) is precisely the two-dimensional Poisson equation for a collection of positive point charges of dimensionless strength $4\pi$ and at the positions $n_i c_i$ and a negative charged background of density $4/\ell^2$. Normalizability of the wave function requires that $\psi(r) \to 0$ when $r \to \infty$ and thus that $\mathcal{H} \to \infty$ when $r \to \infty$. Now, we use the Poisson resummation formula,

$$\sum_{n_i \in \mathbb{Z}} \delta(r - n_i c_i) = \frac{1}{\nu} \sum_{n_i \in \mathbb{Z}} e^{n_i K_i \cdot r},$$

where $\nu$ is the area of the unit cell and the $K_i$'s are the reciprocal lattice vectors defined in Eq. (3.21). From now on we write $\sum_v f(v)$ instead of $\sum_{n_i \in \mathbb{Z}} f(n_i v_i)$ for a summation of some function $f$ that depends on lattice vectors $v_i$. We use the Poisson resummation formula to rewrite Eq. (5.2) as

$$\left(\partial_x^2 + \partial_y^2\right) \mathcal{H} = \frac{4}{\sigma^2} - \frac{4\pi}{\nu} \sum_{K \neq 0} \cos(K \cdot r),$$

where we defined the effective radius $\sigma(\nu)$ as $1/\sigma^2(\nu) \equiv 1/\ell^2 - \pi/\nu$. From now on we will drop the explicit dependence of $\sigma$ on $\nu$, but it is important to keep in mind that $\sigma$ is completely determined by $\nu$ and does not depend on $p$ or $\theta$. We solve for $\mathcal{H}$ and we obtain for $|\psi(x, y)|^2$

$$|\psi(x, y)|^2 = C_0^2 e^{-r/\sigma^2} \prod_{K \neq 0} e^{-\xi_K \cos(K \cdot r)} \quad \text{with} \quad \xi_K = \frac{4\pi}{\nu K^2}. \quad (5.3)$$

In principle, $\mathcal{H}$ could also have a term linear in $x$ or $y$, but from symmetry considerations we assume they are not present. Following our discussion at the end of Section 3.3.2 we write $|\psi(x, y)|^2$ in terms of the real space lattice vectors

$$|\psi(x, y)|^2 = C_0^2 e^{-r/\sigma^2} \prod_{c \neq 0} e^{-\zeta_c \cos(2\pi c \cdot r'/\nu)} \quad \text{with} \quad \zeta_c = \frac{\nu}{\pi c^2}. \quad (5.4)$$

In Eq. (5.4) $r'$ is $r$ after an anti-clockwise of $\pi/2$ rotation around the origin. Since we will calculate terms like $\int dr g(r)|\psi(r)|^2$ for some function $g(r)$, we do not need to worry about this uniform rotation. In Section 5.7, where we consider an external optical lattice, which breaks the rotation invariance of
5. Single Component Vortex Lattices

In this section we calculate the energy functional Eq. (4.1) in terms of $|\psi|^2$. In the next section we will substitute the rewritten form of $|\psi|^2$ from Eq. (5.4). If
we ignore the constant contribution from \( h_z \), the single particle Hamiltonian in the \( z \)-direction, we obtain, after integrating out the \( z \)-direction, that the energy functional in Eq. (4.1) becomes

\[
\mathcal{K} = \int dx dy \psi^*(x, y) [h_\perp - \Omega L_z - \mu] \psi(x, y) + \frac{g}{2d_z} \int dx dy |\psi(x, y)|^4. 
\]

Since \( h_m = c_m z^m e^{-r^2/\ell^2} \), it holds that \( h_m^* L_z h_m = \hbar m |c_m|^2 (x^2 + y^2)^m e^{-r^2/\ell^2} = (\hbar/2) e^{-r^2/\ell^2} (x\partial_x + y\partial_y)(x^2 + y^2)^m \). Using this result, one can verify by partial integration that \( \int dx dy h_m^* L_z h_m = \hbar \int dx dy [(r/a)^2 - 1]|h_m|^2 \) and thus that in the LLL it holds that

\[
\int dx dy \psi^*(x, y) L_z \psi(x, y) = \hbar \int dx dy [(r/\ell)^2 - 1]|\psi(x, y)|^2. \quad (5.7)
\]

Furthermore, it follows from Eq. (4.3) that in the LLL it holds \( h_\perp = (L_z + \hbar)\omega \), thus for the energy functional \( \mathcal{K} \) we obtain

\[
\mathcal{K} = (-\mu + \hbar \omega)N + \frac{\hbar(\omega - \Omega)}{\ell^2} \langle r^2 |\psi(x, y)|^2 \rangle + \frac{g}{2d_z} \langle |\psi(x, y)|^4 \rangle, \quad (5.8)
\]

with \( \langle \ldots \rangle = \int dx dy \ldots \). Using Eq. (5.7) we can rewrite the first two terms of Eq. (5.8) in the following way

\[
(-\mu + \hbar \omega)N + \frac{\hbar(\omega - \Omega)}{\ell^2} \langle r^2 |\psi(x, y)|^2 \rangle = (-\mu + \hbar \omega)N + (\omega - \Omega) \langle L_z \rangle.
\]

We recall that in Chapter 4 we found the energy functional to be Eq. (4.12), where \( \epsilon = (\omega - \Omega)/\omega \), \( R = \langle L_z \rangle \), and \( I \) is the interaction energy. Thus, up to an unimportant constant, the energy functional Eq. (5.8) is the same as the one found in Chapter 4. Now, our goal is to minimize this energy functional using the lattice structure parameters \( (\nu, p, \theta) \), implicit in \( \psi(x, y) \), as variational parameters.

### 5.2.1 Averaged Vortex Approximation

To gain physical insight and as a first approximation, we only take the Gaussian factor of Eq. (5.4) into account, which is called the averaged vortex approximation. The normalized wave function is

\[
|\psi(x, y)|^2 = \frac{N}{\pi \sigma^2} e^{-(r/\sigma)^2}. \quad (5.9)
\]
Using Eq. (5.9) we find \( \langle r^2|\psi(x,y)|^2 \rangle = N\sigma^2 \) and \( \langle |\psi(x,y)|^4 \rangle = N^2/2\pi\sigma^2 \), and thus we obtain for \( \mathcal{K} \)

\[
\mathcal{K} = (-\mu + \hbar\Omega)N + \hbar(\omega - \Omega)N\sigma^2/\ell^2 + gN^2/4\pi\sigma^2d_z.
\]

We denote \( \sigma_0 \) the optimal value of the effective radius \( \sigma \) and \( \nu_0 \) the optimal size of the unit cell \( \nu \). By setting \( \partial\mathcal{K}/\partial\sigma = 0 \) we obtain for \( \sigma_0 \) and \( \nu_0 \)

\[
\sigma_0 = \left[ \frac{gN\ell^2}{4\pi\hbar(\omega - \Omega)d_z} \right]^{1/4} \quad \text{and} \quad \nu_0 = \frac{\nu^*}{1 - 2\ell\sqrt{\pi\hbar(\omega - \Omega)d_z/gN}}.
\]

Note that \( \sigma_0 \to \infty \) and \( \nu \to \nu^* \) when \( \Omega \to \omega \), which is consistent with the observation in Section 4.4 that when \( \Omega \to \omega \) and \( N_v \to \infty \), the optimal density configuration is a uniform one that spreads out to infinity. When \( \sigma_0 \to \infty \), it holds that \( \langle |\psi(x,y)|^4 \rangle \to 0 \), which is also consistent with Section 4.4: the interaction energy goes to 0 when \( \Omega \to \omega \) and \( N_v \to \infty \).

### 5.3 Rewriting the Structural Product

Since we want to consider the energy differences between vortex lattices having a different configuration, we need to go beyond the averaged vortex approximation and take the structural product over \( c \) in Eq. (5.4) into account.

We use of the Jacobi-Anger Expansion

\[
e^{-\alpha \cos \theta} = \sum_{n \in \mathbb{Z}} (-1)^n I_n(\alpha) e^{in\theta} = 2 \sum_{n=0}^{\infty} (-1)^n(2 - \delta_{n,0})I_n(\alpha) \cos(n\theta),
\]

with \( I_n(\alpha) \) the modified Bessel function of order \( n \), and write \( |\psi(x,y)|^2 \) as

\[
|\psi(x,y)|^2 = C_0^2 e^{-r^2/\sigma^2} \prod_{c \neq 0} \left[ \sum_{n_c} (-1)^n_c (2 - \delta_{n_c,0})I_{n_c}(\zeta_c) \cos(2\pi n_c c \cdot r'/\nu) \right],
\]

where for each \( c \neq 0 \) the summation over \( n_c \) goes from 0 to \( \infty \). Now, we define \( n \) to be the set of \( n_c \), where each integer \( n_c \) is associated to a particular lattice vector \( c = l_1c_1 + l_2c_2 \): \( n = \{ n_{l_1c_1 + l_2c_2} | (l_1, l_2) \in \mathbb{Z}^2/(0,0) \} \). Similarly, we define \( z = \{ \zeta_{l_1c_1 + l_2c_2} | (l_1, l_2) \in \mathbb{Z}^2/(0,0) \} \). Then, by switching the order of summation and product, we may rewrite the above expression as

\[
|\psi(x,y)|^2 = C_0^2 e^{-r^2/\sigma^2} \sum_{n} \Lambda[n, z] \cos(2\pi P[n] \cdot r'/\nu),
\]
where we defined
\[ \Lambda[n, z] = \prod_{c \neq 0} (-1)^{n_c (2 - \delta_{n_c, 0})} I_{n_c} (\zeta_c) \quad \text{and} \quad P[n] = \sum_c n_c c. \]

Normalizing to the number \( N \) of particles in the condensate, we find \( C_0^2 = N/\pi \sigma^2 Z_{\sigma^2} [z] \), which yields
\[ |\psi(x, y)|^2 = N e^{-r^2/\sigma^2} \frac{\sum_n \Lambda[n, z] \cos(2\pi P[n] \cdot r'/\nu)}{Z_{\sigma^2} [z]}, \quad (5.10) \]

where \( Z_{\sigma^2} [z] \) is the partition function defined by
\[ Z_{\sigma^2} [z] = \sum_n \Lambda[n, z] e^{-\pi^2 \sigma^2 P[n]^2/\nu^2}. \quad (5.11) \]

### 5.4 Evaluating the Energy Functional

Now, by using the expression for \( |\psi|^2 \) in Eq. (5.10), we can determine the various terms in the energy functional \( K \). We evaluate \( \langle r^2 |\psi(x, y)|^2 \rangle \):
\[ \int r^2 |\psi|^2 dr = \frac{N}{\pi \sigma^2 Z_{\sigma^2} [z]} \sum_n \Lambda[n, z] \int r^2 e^{-r^2/\sigma^2} \cos(2\pi P[n] \cdot r'/\nu) dr = \]
\[ \frac{N \sigma^2}{Z_{\sigma^2} [z]} \sum_n \Lambda[n, z] (1 - \pi^2 \sigma^2 P[n]^2/\nu^2) e^{-\pi^2 \sigma^2 P[n]^2/\nu^2}. \quad (5.12) \]

From the averaged vortex approximation, we know that in the LLL \( \sigma \to \infty \) and \( c_i \sim \sqrt{\nu} \). Hence, the definition of \( P[n] \) implies that in the LLL \( \sigma^2 P[n]^2 \gg \nu^2 \) if \( P[n] \neq 0 \). Thus, we only need to keep terms in Eq. (5.12) with \( P[n] = 0 \) and we obtain that \( \langle r^2 \rangle = N \sigma^2 \). This result is the same as we found in the averaged vortex approximation, and in particular, we find that \( \langle r^2 |\psi(x, y)|^2 \rangle \) only depends on the vortex density and not on the lattice structure. To calculate \( \langle |\psi(x, y)|^4 \rangle \) we use that
\[ |\psi(x, y)|^4 = N^2 \frac{e^{-r^2/(\sigma^2/2)}}{(\pi \sigma^2)^2} \sum_n \Lambda[n, 2z] \cos(2\pi P[n] \cdot r'/\nu). \]

The \( \Lambda[n, 2z] \) factor comes from the fact that
\[ \sum_{n_c} (-1)^{n_c} I_{n_c} (\zeta_c) e^{i n_c c \cdot r'/\nu} = e^{-2\zeta_c \cos(c \cdot r'/\nu)} = \sum_{n_c} (-1)^{n_c} I_{n_c} (2\zeta_c) e^{i n_c c \cdot r'/\nu}. \]

Using this result we find
\[ \int |\psi(x, y)|^4 dx = \frac{N^2}{(\pi \sigma^2)^2 Z_{\sigma^2} [z]} \sum_n \Lambda[n, 2z] \int e^{-r^2/(\sigma^2/2)} \cos(2\pi P[n] \cdot r'/\nu) dr = \]
Using the same argument as above, for the partition function defined in Eq. (5.11) we only need to take into account terms with \( P[n] = 0 \), and \( Z_{\sigma^2}[z] \) simplifies to

\[
Z_{\sigma^2}[z] = \sum_{n \in V_0} \prod_{c \neq 0} (-1)^{n_c} (2 - a_{n_c,0}) I_{n_c}(\zeta_c) \equiv \tilde{Z}[z],
\]

where \( V_0 \) is defined to be the set of all \( \infty \)-tuples \( n \) such that \( P[n] = 0 \). Note that \( \tilde{Z}[z] \) is independent of the vortex density and only depends on the lattice structure though the dependence of \( \zeta_c \) (and thus of \( z \)) on \( p \) and \( \theta \) in Eq. (5.6).

We define \( \alpha(p, \theta) \equiv \tilde{Z}[2z]/\tilde{Z}[z]^2 \) and obtain for the energy functional \( K \)

\[
K = (-\mu + \hbar \Omega) N + \hbar(\omega - \Omega) N \sigma^2(\nu) / \ell^2 + \frac{\alpha(p, \theta) g N^2}{4\pi \sigma^2(\nu) dz},
\]

where we explicitly indicated the dependence of \( \sigma \) on \( \nu \). To minimize \( K \) we first minimize \( \alpha(p, \theta) \) with \( p \) and \( \theta \) as variational parameters. This procedure yields the optimal values for the unit cell parameters \( \theta_0 \) and \( p_0 \). The optimal value of the unit cell \( \nu_0 \) and the optimal effective radius \( \sigma_0 \) are given by

\[
\nu_0 = \frac{\pi \ell^2}{1 - 2 \ell \sqrt{\frac{\pi \hbar (\omega - \Omega) dz}{\alpha(p_0, \theta_0) g N}}} \quad \text{and} \quad \sigma_0 = \sqrt{\frac{\alpha(p_0, \theta_0) g N \ell^2}{4\pi \hbar (\omega - \Omega) dz}}.
\]

Since, typically, we will find \( \alpha \) to be 0.5, the conclusions from the averaged vortex approximation remain valid. The LLL regime was experimentally realized [Cor01a] for a cloud of \( 1.9 \cdot 10^5 \) \(^{87}\)Rb atoms with trapping frequency \( 2\pi \cdot 8.3 \) Hz and \( \Omega = 0.993\omega \). The largest uncertainty is introduced by the crude step-function ansatz for the \( z \)-direction. We take \( dz = \ell \), which is motivated by the oblate shape the cloud has under high rotation speeds [Cor01a]. We find the following numerical values for \( \ell, \nu_0 \), and \( \sigma_0 \):

\[
\ell = 3.7 \mu m, \quad \sigma_0 = 12\ell, \quad \text{and} \quad \nu_0 = 1.0097\pi \ell^2.
\]

Recall that \( n_p \) is the density of particles in the condensate. Note that for the values stated \( gn_p / \hbar \omega \approx 2 \), and that the LLL criterion, \( gn_p \ll \hbar \omega \) is not satisfied. This inconsistency is caused by the crude step function ansatz for the \( z \)-direction and can be resolved by taking a Thomas-Fermi profile in the \( z \)-direction, as is done in [Ho01]. However, since we want to focus our attention on possible vortex lattice structures, we keep the simplifying ansatz for the \( z \)-direction.
5. Single Component Vortex Lattices

5.4.1 Determining $\tilde{Z}[z]$

To calculate $\tilde{Z}[z]$, we first rewrite it as $\tilde{Z}[z] = W[z]Y[z]$, with

$$W[z] = \prod_{c \neq 0} I_0(\zeta_c), \quad Y[z] = \sum_{n \in V_0} \prod_{c \neq 0} (-1)^{n_c} (2 - \delta_{n_c,0}) \tilde{I}_{n_c}(\zeta_c),$$

where $\tilde{I}_{n_c}(\zeta_c) = I_{n_c}(\zeta_c)/I_0(\zeta_c)$. Now, we perform an expansion in $\zeta_0$ by using that $I_n(\zeta) = \sum_{k=0}^\infty (\zeta/2)^{n+2k}/k!(n+k)!$. The expansion of $I_0(\zeta)$ up to third order is

$$I_0(\zeta) = 1 + \frac{\zeta^2}{8} + \frac{\zeta^4}{64}. \quad (5.14)$$

Using Eqs. (5.6) and (5.14), we find for $W[\zeta_c]$

$$W[\zeta_c] = \prod_{c \neq 0} \left(1 + \frac{\zeta^2}{4} + \frac{\zeta^4}{64}\right) = \prod_{l_i \in \mathbb{Z}} \left(1 + \frac{1}{4} h^2(l_1, l_2) \zeta_0^2 + \frac{1}{64} h^4(l_1, l_2) \zeta_0^4\right). \quad (5.15)$$

Now, we want to approximate this last expression up to third order in $\zeta_0$. Since $\zeta_0 \leq 1/\pi$, we expect this expression to be fast convergent in $\zeta_0$. Recall that $h(0,0) = 0$. By defining the lattice sum $S_n(p, \theta) = \sum_{l_1, l_2} h^n(l_1, l_2)$, it holds that up to third order in $\zeta_0$

$$W[z] = 1 + \frac{S_2(p, \theta)}{4} \zeta_0^2(p, \theta). \quad (5.15)$$

The next step is to determine

$$Y[z] = \sum_{n \in V_0} \prod_{c \neq 0} (-1)^{n_c}(2 - \delta_{n_c,0}) \tilde{I}_{n_c}(\zeta_c). \quad (5.16)$$

Using the series expansion for the modified Bessel function $\tilde{I}_n(\zeta_c)$, it holds that

$$\tilde{I}_n(\zeta_c) = \frac{\zeta_c^n}{2^n} \frac{1}{n!} + \frac{\zeta_c^2}{4(n+1)!} = \frac{\zeta_c^n}{2^n n!} \left(1 - \frac{n}{n+1} \frac{\zeta_c^2}{4}\right). \quad (5.17)$$

Inspection of Eq. (5.17) shows that for each $c$ there is a factor $\zeta_0^{n_c}$. Thus, to derive an expansion up to third order in $\zeta_0$, it must hold for most $c$’s that $n_c = 0$ and $\tilde{I}_{n_c}(\zeta_c) = 1$. For an expansion up to third order, we need to consider the second term in the brackets only if $\sum n_c = 1$. The $\infty$-tuples $n$
which yield terms of order three or lower are given in table 5.1 where $N_p$ is the number of $c$ with $n_c = p$.

We will refer to the contributions described by the $n$th row of the table as the $n$th possibility or $\#n$. Since in the determination of $Y[z]$ we need to sum over unordered $n$-tuples of $c$’s, combinatorial factors have to be included to avoid over-counting. These are shown in the last column of table 5.1. Finally, inspection of Eq. (5.16) shows that the contributions from possibilities 2, 5, 6, and 7 are negative, because for them $\sum n_c$ is odd. Now, we perform the expansion of $Y[z]$. Since it must hold that $P[n] = 0$, we can exclude possibilities 2, 4 and 7. For $\#3$, we must choose $n_{c_0} = n_{-c_0} = 1$ for some $c_0$ and all other $n_c$ equal to 0. Since $\zeta_c = \zeta_{-c}$ the contribution to $Y[n]$ from $\#3$ is equal to

\[
\frac{1}{2} \sum_c 2 \tilde{I}^2(\zeta_c) = 2 \sum_c \frac{\zeta_c^2}{4} = \frac{S_2(p, \theta)}{2} \zeta_0^2(p, \theta).
\]

For $\#5$ we need to sum over all distinct unordered triplets $(c_1, c_2, c_3)$, which have distinct elements and whose sum is equal to 0. Using Eq. (5.17), this calculation produces the term

\[
-\frac{1}{3!} \sum_{c_1 < c_2} \sum_{c_3 \neq c_1, c_2} \sum_{c_{c_1+c_2+c_3=0}} \zeta_{c_1} \zeta_{c_2} \zeta_{c_3} \delta_{c_1+c_2+c_3,0} =
\]

\[
= -\frac{\zeta_0^3(p, \theta)}{3!} \sum_{(l_1, l_2)} \sum_{(n_1, n_2) \neq (l_1, l_2)} h(l_1, l_2) h(n_1, n_2) h(l_1+n_1, l_2+n_2)
\]
Fig. 5.1: $\alpha(p, \theta)$ for $p = 1.00, 1.05, 1.10, 1.15$ for $\pi/3 \leq \theta \leq \pi/2$.

\[
(1 - \prod_i \delta_{n_i + l_i, -n_i})(1 - \prod_i \delta_{n_i + l_i, -l_i}) \equiv -A_3(p, \theta)\zeta_3^3(p, \theta).
\]

The Kronecker delta’s arise to ensure that $c_1 \neq c_3$ and $c_2 \neq c_3$. We don’t need to ensure separately that $c_3 \neq 0$ since $h(0, 0) = 0$ anyway. Lastly, we consider #6. We need to choose for one $c = c_0$ that $n_c = 2$, for $c = -2c_0$ that $n_c = 1$, and all other $n_c$’s equal to 0. Using Eq. (5.17) we then find the following contribution to $Y[z]$

\[
- \sum_{c \neq 0} \frac{4\zeta_c^2}{8} = -\frac{4\zeta_0^3}{4} \sum_{(l_1, l_2)} h^2(l_1, l_2)h(2l_1, 2l_2) \equiv -\frac{B_3(p, \theta)}{4} \zeta_0^3(p, \theta).
\]

Note that there is no combinatorial factor for this term. Combining these expressions, our expansion for $Y[z]$ becomes

\[
Y[z] = 1 + \frac{S_2(p, \theta)}{2}\zeta_0^2(p, \theta) - \frac{B_3(p, \theta)}{4}\zeta_0^3(p, \theta) - A_3(p, \theta)\zeta_0^3(p, \theta).
\]  

5.5 Results

Using the expansions for $W[z]$ and $Y[z]$ given by Eqs. (5.18) and (5.15), we can finally calculate $\langle |\psi(x, y)|^4 \rangle$
\[
\langle |\psi(x, y)|^4 \rangle = \frac{N^2 \tilde{Z}[2z]}{2\pi\sigma^2 \tilde{Z}[z]^2} \equiv \alpha(p, \theta) \frac{N^2}{2\pi\sigma^2} \approx \frac{N^2}{2\pi\sigma^2} \left(1 + \frac{3}{2} S_2(p, \theta) \zeta_0^2(p, \theta) - (6A_3(p, \theta) + 3B_3(p, \theta)/2)\zeta_0^3(p, \theta) - \frac{17}{16} S_2^2(p, \theta) \zeta_0^4(p, \theta)\right).
\]

Note that although Eq. (5.5) contains a fourth order term, the expansion for \(\alpha(p, \theta)\) is not a fourth, but a third order expansion. The fourth order term is kept, because the large magnitude of the coefficient \((17/16)S_2^2(p, \theta)\) renders this term to be important. Below, we will argue that a third order expansion of \(W[z]\) and \(Y[z]\) is sufficient for our purposes. In Fig. 5.1 we plot \(\alpha(p, \theta)\) for \(\pi/3 \leq \theta \leq \pi/2\) and \(p \in (1.00, 1.05, 1.10, 1.15)\). We see that the vortex lattice with a unit cell with \(p = 1\) and \(\theta = \pi/3\) is energetically favorable. This result is in agreement with well known theoretical predictions [Abr] and experimental observations. The values of \(\alpha(p, \theta)\) for a square ordering and a triangular ordering differ by approximately 5%.

5.5.1 Numerical Analysis

To obtain a better quantitative understanding of our result and to check the validity of the (third-order) approximation used in the calculation of \(Y[z]\), we now take a closer look at the magnitude of the various terms contributing to \(Y[z]\) and \(\alpha(p, \theta)\). For simplicity, we only consider \(p = 1\) and compare the values for \(\theta = \pi/3\) and \(\theta = \pi/2\). For the numerical evaluation of \(S_3(p, \theta)\) and \(B_3(p, \theta)\), a summation range was used of 100 and for \(A_3(p, \theta)\) a range of 16. The range for \(A_3(p, \theta)\) is much lower, since for it we need to perform a double summation over all lattice sites \(\sim \sum_{l_1,j_2} \sum_{m_1,m_2} \neq (l_1,j_2)\). This choice leads to a numerical uncertainty in \(S_2(p, \theta)\) of 0.0003, a negligible uncertainty in \(B_3(p, \theta)\), and an estimated uncertainty of 0.1 in \(A_3(p, \theta)\). In table 5.2 an overview is given of the numerical values of the various terms and factors contributing to \(Y[z]\) and \(\alpha(p, \theta)\). In the upper block, the values of \(\zeta_0(p, \theta)\), \(S_2(p, \theta)\), \(A_3(p, \theta)\), and \(B_3(p, \theta)\) are shown for \(p = 1\) and the two angles. In the middle block, the values of the terms in the expansion for \(\alpha(p, \theta)\) are shown, with \(T(S_2) = (3/2)S_2 \zeta_0^2\), \(T(A_3) = -6A_3 \zeta_0^3\), \(T(B_3) = -(3/2)B_3 \zeta_0^3\), and \(T(S_2^2) = -(17/16)S_2^2 \zeta_0^4\). In the lower block, the values of the terms in the expansion for \(Y[z]\) are shown, with \(R(S_2) = (1/2)S_2 \zeta_0^2\), \(R(A_3) = -A_3 \zeta_0^3\), and \(R(B_3) = -(1/4)B_3 \zeta_0^3\). The last line shows the value of \(W[\zeta]\) for the two
angles. In the last column, the differences between the values in the first two columns are shown. Note that the terms in the last column of the $R$-block sum up to the difference in $Y[z]$, but that the terms in the last column of the $T$-block do not sum up to $\alpha(p, \theta)$. This is caused by the fact that there are higher order terms with large coefficients present in the expansion, like $6S_2A_3\zeta_0^5$. However, closer inspection of the numerical values in the table shows that our third order expansion of $Y[z]$ is accurate. Indeed, for the difference between the two angles in both $Y[z]$ and $\alpha(p, \theta)$, we see that the terms with a factor $S_2(p, \theta)$ ($T(S_2)$, $R(S_2)$, and $T(S_2^2)$), which are produced by $\#3$ in table 5.1 (having $\sum n_c = 2$) dominate the terms with a factor $A_3(p, \theta)$ or $B_3(p, \theta)$ ($T(A_3)$, $T(B_3)$, $R(A_3)$, and $R(B_3)$), which are produced

\begin{table}[h]
\centering
\begin{tabular}{|l|ccc|}
\hline
 & $\theta = \pi/3$ & $\theta = \pi/2$ & $\Delta$
\hline
$\zeta_0(p, \theta)$ & 0.276 & 0.318 & \\
$S_2(p, \theta)$ & 7.71 & 6.03 & \\
$A_3(p, \theta)$ & 9.64 & 6.29 & \\
$B_3(p, \theta)$ & 1.59 & 1.16 & \\
$\alpha(p, \theta)$ & 0.504 & 0.530 & 0.027 & \\
$T(S_2)$ & 0.879 & 0.912 & 0.037 & \\
$T(A_3)$ & -1.21 & -1.22 & -0.006 & \\
$T(B_3)$ & -0.050 & -0.056 & -0.006 & \\
$T(S_2^2)$ & -0.36 & -0.40 & -0.031 & \\
$Y[z]$ & 1.083 & 1.093 & 0.010 & \\
$R(S_2)$ & 0.29 & 0.31 & 0.012 & \\
$R(A_3)$ & -0.202 & -0.203 & -0.001 & \\
$R(B_3)$ & -0.0083 & -0.0094 & -0.001 & \\
$W[z]$ & 1.146 & 1.153 & 0.0062 & \\
\hline
\end{tabular}
\caption{An overview of the numerical values of the terms and factors contributing to $Y[z]$ and $\alpha(p, \theta)$. $\Delta$ is the difference between the values of the second and first columns. The definitions of all quantities are given in the main text.}
\end{table}
by #5 and #6 in table 5.1 (having $\sum n_c = 3$). The former contributions are typically a factor 6 greater than the latter. We thus expect that the contribution of possibilities with $\sum n_c > 3$ in the expansion of $Y[z]$ is so small that we can safely neglect these terms.

### 5.6 Comparison with Ho

To check our analysis and calculations for errors, we now compare our results to the results obtained by Ho in Ref [Ho01], whose paper we followed. Ho calculates the energies of a square and triangular ordering for $p = 1$. He also finds that the triangular structure is energetically favorable, but quantitatively his results differ from ours. Typically, Ho finds that $\alpha \sim 1.4$, while we find $\alpha \sim 0.5$. This large difference is caused by his use of the identity

$$e^{-\alpha \cos \theta} = \sum_{n=0}^{\infty} (-1)^n I_n(\alpha)e^{in\theta} \quad \text{incorrect!!!},$$

which is not correct. The summation variable $n$ should go from $-\infty$ to $\infty$. To be able to compare our results to his, we will assume that the above identity holds and change our results accordingly. In practice, this means that the factors $(2 - \delta_{n,n_c})$ are not present in the summations in the previous sections. Below, we denote with a subscript $h$ the functions in the paper by Ho, corresponding to the ones we evaluated in the previous sections.

For the triangular case, Ho calculates lattice summations over the function $h_h(l_1, l_2) = (l_1^2 + l_2^2 + \sqrt{3}l_1l_2)^{-1}$. However, comparing this result to our form of $h(l_1, l_2)$, one sees that the right expression is $h_h(l_1, l_2) = (l_1^2 + l_2^2 + l_1l_2)^{-1}$. The difference is probably caused by the erroneous setting of $\cos(\pi/3) = \sqrt{3}/2$ instead of $\cos(\pi/3) = 1/2$. For the second order terms for the triangular lattice we obtain the same results as Ho, but for some unknown reason, Ho only takes triplets of vectors of equal length into account to calculate the contributions to $Y[z]$ with $\sum n_c = 3$, and leaves out triplets containing vectors of unequal length. This causes the magnitude of the third order terms to differ greatly.

For the square lattice, the second order terms agree with our results. However, Ho states that there are no third order terms, which, as shown by our analysis in Section 5.4, is not true.
5.7 Including an Optical Lattice Potential

5.7.1 Introduction

In this section we extend our model by adding a two-dimensional optical lattice potential. The motivation for this extension is the following. Above, we found that the vortex lattice with minimal energy has a triangular shape. For sufficient strength of the optical lattice, the vortices will be pinned at the potential maxima, because it is energetically favorable to lower the condensate density in an area of high potential. If we vary the strength of the optical lattice, we expect to find a transition between a state in which all vortices are pinned and a state in which no vortices are pinned. In the former state the vortex lattice has the same structure as the optical lattice, while in the latter it is in the triangular configuration. The transition between these two states is the so-called pinning-depinning transition and it is this transition we want to study. The latter was predicted theoretically by Reijnders and Duine [Du04,Du05] and observed experimentally in the Group of Eric Cornell in 2006 using a square optical lattice [Cor06]. In Fig. 5.2 the pinning-depinning transition from this experiment is shown. In Fig. 5.2(a) the triangular Abrikosov vortex lattice is shown in the absence of an optical lattice and in (d) one can clearly see the triangular structure in momentum space. Then, if the strength of the optical lattice is increased one observes a structural transition to a pinned phase with square structure, as shown in Figs. 5.2(c)
and (f).

The optical lattice potential has the form

\[ V(x, y) = V_0 \left[ \cos^2 \left( \frac{k_1 \cdot r}{2} \right) + \cos^2 \left( \frac{k_2 \cdot r}{2} \right) \right], \]

where \( V_0 \) determines the strength of the optical lattice and \( k_1 \) and \( k_2 \) are the reciprocal lattice vectors of the optical lattice. Our approach is the following. First, we determine which vortex lattice structure has minimal energy for fixed \( V_0 \), \( k_1 \), and \( k_2 \). With these results we will then construct a phase diagram in terms of the latter parameters, which specifies which vortex lattice has minimal energy for each point in parameter space. We assume that the optical lattice leaves the form of the LLL wave function (5.4) intact, and that it only alters the (regular) structure of the vortex lattice.

### 5.7.2 Parameterization of the optical lattice

We assume that \(|k_1| \leq |k_2|\). Let the pair of real-space lattice vectors \((b_1, b_2)\) be given by

\[ b_1 = \frac{\nu_{OL}}{2\pi} \hat{z} \times k_1 \quad \text{and} \quad b_2 = \frac{\nu_{OL}}{2\pi} \hat{z} \times k_2, \quad (5.20) \]

where \( \nu_{OL} \) is the area of the unit cell of the optical lattice. Then, the pair \((b_1, b_2)\) spans the optical lattice. We choose the smallest of those lattice vectors, \( b_1 \), to lie along the \( x \)-axis. Then, we can parameterize the \( b_i \)'s and the optical lattice by the area of the unit cell \( \nu_{OL} \), the ratio \( q \geq 1 \) between the lengths of \( b_2 \) and \( b_1 \), and by the (smallest) angle \( \phi \) between them: \( 0 \leq \phi \leq \pi/2 \),

\[ b_1 = \sqrt{\frac{\nu_{OL}}{\sin \phi}} (1, 0)^T \quad \text{and} \quad b_2 = \sqrt{\nu_{OL} \sin \phi (\cot \phi, 1)^T}. \quad (5.21) \]

If we fix the positions of the maxima of the optical lattice, we still have the freedom to choose the position of the minima. Thus, the optical lattice is not determined by the position of the maxima alone. This is caused by the fact that, e.g., it does not hold that \( \cos^2 \left( \frac{1}{2} k_1 \cdot r \right) + \cos^2 \left( \frac{1}{2} k_2 \cdot r \right) \neq \cos^2 \left( \frac{1}{2} (k_1 + k_2) \cdot r \right) + \cos^2 \left( \frac{1}{2} k_2 \cdot r \right) \) for all \( r \). As a consequence, we can not a priori restrict \( \phi \) as \( \pi/3 \leq \phi \leq \pi/2 \), as we did for the case of vortex lattices. However, for our purposes, it will be sufficient (and convenient) to impose this restriction ourselves, i.e., to only consider optical lattices which have \( \pi/3 \leq \phi \leq \pi/2 \). Furthermore, we only consider optical lattices with \( q = 1 \).
In the previous chapter, we calculated the energy of a vortex lattice in the absence of an optical lattice. In that case, the energy functional has rotation and reflection symmetries. However, by inclusion of the optical lattice these symmetries are broken and we have to extend the parameters defining the vortex lattice vectors by an angle $\kappa$ specifying a global rotation with respect to the optical lattice vectors and a parameter $n = 0, 1$ specifying whether or not we performed a reflection in the $x$-axis prior to this global rotation. In addition, we define the dimensionless parameter $r$ to be $\nu/\nu_{OL}$. In terms of these parameters, the real-space vortex lattice vectors are given by

$$c_1 = \sqrt{\frac{\nu_{OL}}{p \sin \theta}} R_\kappa (1, 0)^T \quad \text{and} \quad c_2 = \sqrt{pr \nu_{OL} \sin \theta} R_\kappa (\cot \theta, (-1)^n)^T,$$

where $R_\kappa$ is a matrix that rotates over an angle $\kappa$. Note that although we set $q = 1$, it can still be true that a vortex lattice structure with $p > 1$ has minimal energy.

### 5.8 Determining the Extended Energy Functional

In this section we determine the energy functional for the extended system. The energy functional we calculated before in Eq. (5.13) gets an extra term $E_{OL} = \langle V(x, y) | \psi \rangle^2$ after inclusion of the optical lattice. We assume that there is a vortex in the origin, which is also one of the maxima of the optical lattice. We rewrite the optical lattice potential as

$$V(x, y) = V_0 \left[ \cos^2 \left( \frac{k_1 \cdot r}{2} \right) + \cos^2 \left( \frac{k_2 \cdot r}{2} \right) \right] = V_0 \left[ \cos^2 \left( \frac{\pi \nu_{OL}}{b_1 \cdot r'} \right) + \cos^2 \left( \frac{\pi}{\nu_{OL}} b_2 \cdot r' \right) \right], \quad (5.22)$$

where again $r'$ is $r$ after an anti-clockwise rotation of $\pi/2$ around the origin. Then, we can determine $\langle V(x, y) | \psi \rangle^2$

$$\langle V(x, y) | \psi \rangle^2 = V_0 \int \sum_i \cos^2 \left( \frac{\pi}{\nu_{OL}} b_i \cdot r' \right) |\psi(x, y)|^2 \, dr$$

$$= \frac{V_0 N Z}{\pi \sigma^2 Z_{\sigma^2} |Z|} \sum_{n, i} \Lambda[n, z] \int e^{-r^2/\sigma^2} \cos \left( \frac{2\pi}{r \nu_{OL}} n \cdot r' \right) \cos^2 \left( \frac{\pi}{\nu_{OL}} b_i \cdot r' \right) \, dr.$$
\[
\frac{V_0 N}{2} \left( 1 + \frac{1}{Z_{\sigma^2}[z]} \sum_{n,i} \Lambda[n, z] e^{-\pi^2 \sigma^2 (P[n]/r - b_i)^2 / \nu \sigma^2} \right),
\]

where we used the expressions for the wave function and \(Z_{\sigma^2}[z]\) in Eq. (5.10) and Eq. (5.11). As before, only the terms with \(P[n] = r b_i\) survive, leading to
\[
\langle V(x, y) \mid \psi \mid \rangle^2 = \frac{V_0 N}{2} \left( 1 + \frac{1}{Z[z]} \sum_{i, n \in V_{r, b}} \Lambda[n, z] \right),
\]

where \(V_{r, b}\) is defined as the set of all \(n\) such that \(P[n] = r b\). From now on we will drop the constant term \(V_0 N/2\), since it does not depend on the particular vortex lattice structure. In analogy to \(\tilde{Z}[z] = W[z]Y[z]\), we write
\[
\sum_{n \in V_{r, b}} \Lambda[n, z] = W[z] \sum_{n \in V_{r, b}, c \neq 0} (-1)^n (2 - \delta_{0,n}) \tilde{I}_{nc}(\zeta_c) \equiv W[z]V_b[z],
\]

and we arrive at the following expression for \(\langle V(x, y) \mid \psi \mid \rangle^2\):
\[
\langle V(x, y) \mid \psi \mid \rangle^2 = \frac{V_0 N}{2Z[z]} W[z] \sum_i V_{b_i}[z] = \frac{V_0 N}{2Y[z]} \sum_i V_{b_i}[z].
\]

**Determining \(V_b[z]\)**

In this section we will determine an expression for \(V_b[z]\). To calculate \(V_b[z]\), we need to sum over all ordered pairs of integers \((l_1, l_2)\) that are such that \(l_1 c_1 + l_2 c_2 = r b\). There can be either none or one of such pairs. In the former case the summation is empty and \(V_b[z] = 0\), whereas in the latter case \(V_b[z]\) has a non-zero contribution which we now calculate. We perform an expansion up to third order in \(\zeta_0\) using the series expansion for the normalized modified Bessel function \(\tilde{I}_n(\zeta_c)\) given by Eq. (5.17). Our approach will be similar to the one used in the determination of \(Y[z]\): we specify the contributions to \(V_b[z]\) for each possibility in Table 5.1.

It is clear that we can exclude #1. The contribution from #2 is found by setting \(n_{-b} = 1\) and all other \(n_c\) equal to zero. We thus find
\[
-2 \tilde{I}_1(\zeta_b) = -\zeta_b \left( 1 - \frac{\zeta_b^2}{8} \right) = -h(l_1, l_2) \zeta_0(p, \theta) + \frac{h^3(l_1, l_2)}{8} \zeta_0^3(p, \theta).
\]
The contribution from #3 is found by summing over all unordered distinct duo’s \((c_1, c_2)\) with \(c_1 + c_2 = -b\) and \(c_1 \neq c_2\). This procedure leads to the contribution

\[
\frac{1}{2} \sum_{c_1} \sum_{c_2 \neq c_1} 4 \tilde{I}_1(\zeta_{c_1}) \tilde{I}_1(\zeta_{c_2}) \delta_{c_1 + c_2, -b} =
\]

\[
\frac{\zeta_0^2}{2} \sum_{(n_1, n_2)} h(n_1, n_2) h(l_1 + n_1, l_2 + n_2) (1 - \delta_{2n_1, -l_1} \delta_{2n_2, -l_2}) \equiv D(l_1, l_2, p, \theta) \zeta_0^2(p, \theta).
\]

Now we consider #4. This contribution is only present if there is a \(c\) such that \(c = b/2\), i.e., if \(l_1\) and \(l_2\) are even. In that case we choose \(n_c = 2\) for \(c_0 = -b/2\), leading to the term

\[
2 \tilde{I}_2(\zeta_{c_0}) = \frac{\zeta_0^2}{4} = \frac{1}{4} \zeta_0^2 h^2(l_1/2, l_2/2),
\]

where we define \(h(a, b)\) to be 0 if either \(a\) or \(b\) is not an integer. We find the contribution #5 by summing over all unordered 3-tuples with distinct elements \((c_1, c_2, c_3)\), whose sum is equal to \(-b\). This calculation leads to the term

\[
-\frac{1}{3!} \sum_{c_1} \sum_{c_2 \neq c_1} \sum_{c_3 \neq \{c_1, c_2\}} \zeta_{c_1} \zeta_{c_2} \zeta_{c_3} \delta_{c_1 + c_2 + c_3, -b} =
\]

\[
= -\frac{\zeta_0^3(p, \theta)}{3!} \sum_{(n_1, n_2)} \sum_{(m_1, m_2) \neq (n_1, n_2)} h(n_1, n_2) h(m_1, m_2) h(l_1 + n_1 + m_1, l_2 + n_2 + m_2)
\]

\[
(1 - \prod_{i=1,2} \delta_{l_i + m_i + n_i, -n_i}) (1 - \prod_{i=1,2} \delta_{l_i + m_i + n_i, -n_i}) \equiv -E(l_1, l_2, p, \theta) \zeta_0^3(p, \theta),
\]

where again the Kronecker-\(\delta\)’s arise to ensure that \(c_3 \neq c_1, c_2\). We consider the contribution of #6: summing over distinct unordered duo’s \(c_1, c_2\) with \(2c_1 + c_2 = -b\), leads to the term

\[
- \sum_{c_1 \neq c_2} 4 \frac{\zeta_1^2}{8} \frac{\zeta_2}{2} \delta_{2c_1 + c_2, -b} =
\]

\[
- \frac{\zeta_0^3(p, \theta)}{4} \sum_{(n_1, n_2)} h^2(n_1, n_2) h(2n_1 + l_1, 2n_2 + l_2) (1 - \prod_{i=1,2} \delta_{l_i + 2n_i, -n_i}) \equiv
\]

\[
- \frac{F(l_1, l_2, p, \theta)}{4} \zeta_0^3(p, \theta).
\]
Finally, for #7, we only find a contribution if there is a \( c \) such that \( c = b/3 \), i.e., if \( l_1 \) and \( l_2 \) are multiples of 3. In that case we choose \( n_c = 3 \) for \( c_0 = -b/3 \), leading to the term

\[
-2\tilde{I}_3(\zeta_{c_0}) = 2\frac{\zeta_{c_0}^2}{8 \cdot 3!} = -\frac{1}{24}c_0^3\hbar^3(l_1/3, l_2/3)
\]

We define \( \beta(l_1, l_2, p, \theta) \) as the sum of all previous terms divided by \( Y[z] \)

\[
\beta(l_1, l_2, p, \theta) \equiv \frac{1}{Y[z]} \left[ D(l_1, l_2, p, \theta)\zeta_0^2(p, \theta) - E(l_1, l_2, p, \theta)\zeta_0^3(p, \theta) \right]
\]

\[
-\frac{F(l_1, l_2, p, \theta)}{4}\zeta_0^3(p, \theta) - \hbar(l_1, l_2)\zeta_0(p, \theta) + \frac{h^3(l_1, l_2)}{8}\zeta_0^3(p, \theta)
\]

\[
+ \frac{1}{4}\zeta_0^2\hbar^2(l_1/2, l_2/2) - \frac{1}{24}c_0^3\hbar^3(l_1/3, l_2/3)
\]

Then, \( V_b[z]/Y[z] \) is given by

\[
\frac{V_b[z]}{Y[z]} = \sum_{S(c_1, c_2; b, r)} \beta(l_1, l_2, p, \theta),
\]

where we defined \( S(c_1, c_2; b, r) \) to be the set of all pairs of integers \( (l_1, l_2) \) such that \( l_1c_1 + l_2c_2 = rb \). It is important to note that the function \( \beta \) does not depend on the area of the unit cell of the vortex lattice \( \nu \) or on the parameters \( q \) (which we set to 1), \( \phi \), and \( \nu_{OL} \) that parameterize the optical lattice.

Furthermore, from the definition of \( h(l_1, l_2) \) in Eq. (5.6), it can be seen that the following identities hold

\[
\beta(l_1, l_2, p, \theta) = \beta(-l_1, -l_2, p, \theta),
\]

\[
\beta(l_1, l_2, 1, \theta) = \beta(l_2, l_1, 1, \theta),
\]

\[
\beta(l_1, l_2, p, \pi/2) = \beta(|l_1|, |l_2|, p, \pi/2).
\]

These identities reduce the amount of numerical calculations we have to do.

We drop the constant contribution from the energy functional Eq. (5.13) and obtain for \( \mathcal{K} \)

\[
\mathcal{K}(c_1, c_2) = \hbar(\omega - \Omega)N\frac{\sigma^2(\nu)}{\ell^2} + \frac{\alpha(p, \theta)gN^2}{4\pi\sigma^2(\nu)d_z} + \frac{V_0N}{2} \sum_i \sum_{S(c_1, c_2; b_i, r)} \beta(l_1, l_2, p, \theta).
\]

Note that we indicated the dependence of \( \mathcal{K} \) on the vortex lattice vectors \( c_i \) and of \( \sigma \) on \( \nu \) explicitly. We emphasize that for given \( c_1, c_2, \) and \( b_1 \), the set \( S(c_1, c_2; b_1, r) \) contains 0 or 1 pair of integers \( (l_1, l_2) \).
5. Single Component Vortex Lattices

5.8.1 Possible Lattice Structures

An important question is what the identity $P[n] = r b_1$ means physically. We will now answer this question. Assume that $P[n] = r b_1$, then there is a pair of integers $(l_1, l_2)$ such that $l_1 c_1 + l_2 c_2 = r b_1$. Recall that $r$ is not necessarily an integer. Since $c_1$ and $c_2$ are independent, there is a pair of (necessarily integer) numbers $(k_1, k_2)$ such that $k_1 c_1 + k_2 c_2 = b_2$. Taking the outer product of both identities leads to $|l_1 k_2 - l_2 k_1| \nu = r \nu_{OL}$ and hence $|l_1 k_2 - l_2 k_1| = 1$. Now, solving for the $c_i$’s leads to

$$\pm c_1 = l_2 b_2 - r k_2 b_1 \quad \text{and} \quad \pm c_2 = -l_1 b_2 + r k_1 b_1,$$

and to the conclusion that for both $c_i$’s the coefficient of $b_2$ is an integer. In Fig. 5.3(a) we show for a square lattice the lattice vectors $b_i$ and the distribution of the minima and maxima of the optical lattice potential. If for both $c_i$’s the coefficient of $b_2$ is an integer, all vortices will lie on the dashed lines in Fig. 5.3(b), where the potential varies between the equilibrium value and the maxima, instead of between the minima and the maxima. The vortices are pinned on the lines of maximal potential and hence the optical lattice potential energy is lowered. Now, there are three possible cases, depending on whether there are 0, 1 or 2 integer pairs $(l_1, l_2)$ such that $l_1 c_1 + l_2 c_2 = r b_1$ or $r b_2$.

1. Unpinned Situation

If there are no integer pairs $(l_1, l_2)$ such that $l_1 c_1 + l_2 c_2 = r b_1$ or $r b_2$, 

Fig. 5.3: The distribution of the minima and maxima of the optical lattice potential for the square optical lattice. (a) The pinning lines (dashed). (b)
the vortices are not pinned on the lines spanned by the optical lattice vectors and we denote this situation as the unpinned situation. There are no terms in the summation in Eq. (5.25) and we find that \( \langle V(x, y)|\psi|^2 \rangle = 0 \). The optical lattice potential yields a constant (zero) contribution to the energy of the system, because the incommensurability of the vortex and optical lattices causes the optical lattice potential energy to average to zero. The vortex lattice will order in a triangular structure with \( p = 1 \) and \( \theta = \pi/3 \). Because this situation is unpinned, the energy of the lattice has complete translation and rotation symmetries. By this we mean that if we rotate or translate the vortex lattice with respect to the optical lattice, the energy of the system stays the same. The area of the unit cell is given by \( \nu_0 \), as we found in Section 5.5 in the absence of an optical lattice. Note that in particular \( \nu_0 \) is independent of \( \nu_{OL} \). The energy of the system is equal to

\[
\mathcal{K}_0 = \sqrt{\frac{\alpha(1, \pi/3)N^3g\hbar(\omega - \Omega)}{\pi \ell^2 d_z}},
\]

which we obtained by substituting \( \sigma_0 \) in the expression for \( \mathcal{K} \).

2. Half Pinned

If there are \((l_1, l_2)\) such that \( l_1c_1 + l_2c_2 = b_1 \) but no \((n_1, n_2)\) such that \( n_1c_1 + n_2c_2 = b_2 \) (or vice versa, with \( b_1 \leftrightarrow b_2 \)) all vortices are pinned at the lines of maximal potential, a situation that we denote as half pinned. For a particular vortex lattice unit cell geometry, the energy of this situation has complete translational symmetry along the pinning lines, but along the other optical lattice vector the translational symmetry of the energy functional is broken to a discrete symmetry. We will consider two kinds of half-pinned structures. The first one has an Abrikosov lattice structure with \( p = 1, \theta = \pi/3 \) and \( r \neq 1 \) and is shown in Fig. 5.4(a), where the pinning sites are indicated by empty circles, the vortices by crosses. The second has \( r = 1 \) but a deformed unit cell and is shown in Fig. 5.4(b).

Considering the first situation, it holds that \( p = 1, \theta = \pi/3 \), and that the area of the unit cell \( \nu \) depends on the geometry of the optical lattice. We will now calculate \( \nu \). Consider an optical lattice spanned by the vectors \( b_1 \) and \( b_2 \) given in Eq. (5.20) that have length \( \sqrt{\nu_{OL}/\sin \phi} \) and relative angle \( \phi \). Assume all vortices are pinned on the lines spanned
by \(\mathbf{b}_1\). The minimal distance between the pinning lines is given by the \(y\)-coordinate of \(\mathbf{b}_2\), \(\sqrt{\nu_{OL}\sin\phi}\). The length of the vortex lattice vectors is given by \(|\mathbf{c}_1| = \sqrt{\nu_{OL}\sin\phi/\sin(\pi/3)} = 2\sqrt{\nu_{OL}\sin\phi}/3\) and the area of the unit cell by \(\nu = |\mathbf{c}_1|^2\sin(\pi/3) = (2/\sqrt{3})\nu_{OL}\sin\phi\). Hence, \(r\) is given by \(r = (2/\sqrt{3})\sin\phi\) and it holds that \(\mathbf{c}_1 = r\mathbf{b}_1\). The energy functional \(K\) from Eq. (5.25) for this situation is given by

\[
K = \hbar(\omega - \Omega)N\frac{\sigma((2/\sqrt{3})\nu_{OL}\sin\phi)^2}{\ell^2} + \frac{\alpha(1, \pi/3)gN^2}{4\pi\sigma((2/\sqrt{3})\nu_{OL}\sin\phi)^2}dz + \frac{V_0N}{2}\beta(1, 0, 1, \pi/3). \tag{5.27}
\]

In the second situation it holds that \(\nu = \nu_{OL}\) and the vortex lattice vectors are given by \(\mathbf{c}_1 = \mathbf{b}_1\) and \(\mathbf{c}_2 = \mathbf{b}_1/2 + (\hat{y} \cdot \mathbf{b}_2)\hat{y} = \sqrt{\nu_{OL}\sin\phi}(1/(2\sin\phi), 1)\). The value of \(p\) is given by \(p = (1/2)\sqrt{1 + 4\sin^2\phi}\) and \(\theta\) is given by \(\theta = \cos^{-1}[1/\sqrt{1 + 4\sin^2\phi}]\). These expressions correspond to \((p, \theta) = (\sqrt{5}/2, \cos^{-1}[1/\sqrt{5}])\) for \(\phi = \pi/2\) and \((p, \theta) = (1, \pi/3)\) for \(\phi = \pi/3\). The energy functional \(K\) from Eq. (5.25) for this situation is given by

\[
K = \hbar(\omega - \Omega)N\frac{\sigma^2(\nu_{OL})}{\ell^2} + \frac{gN^2}{4\pi\sigma^2(\nu_{OL})}dz\alpha\left(\frac{1}{2}\sqrt{1 + 4\sin^2\phi}, \cos^{-1}\left[\frac{1}{\sqrt{1 + 4\sin^2\phi}}\right]\right) + \frac{V_0N}{2}\beta\left(1, 0, \sqrt{1 + 4\sin^2\phi}, \cos^{-1}\left[\frac{1}{\sqrt{1 + 4\sin^2\phi}}\right]\right). \tag{5.28}
\]

Note that for \(\nu_{OL} = \nu_0\), the two half pinned structures considered are the two limiting structures of a competition between an lattice with optimal unit cell area, and a lattice with optimal geometry (i.e. with \(p = 1\) and \(\theta = \pi/3\)). We also remark that other half-pinned lattice structures with higher values of \(r\) (e.g. \(r = 2\)) are possible, but we do not consider them in this thesis. We will, however, consider fully pinned structures with \(r = 2\).
Fig. 5.4: The two possibilities for half pinned configurations for the case of a square optical lattice. The Abrikosov lattice with an enlarged unit cell is shown in (a), and the deformed lattice with $r = 1$ in (b). The pinning sites are indicated by empty circles, the vortices by crosses.

3. Fully Pinned

If there are integer pairs $(l_1, l_2)$ and $(k_1, k_2)$ such that both $l_1 c_1 + l_2 c_2 = b_1$ and $k_1 c_1 + k_2 c_2 = b_2$, the vortices will be pinned on both the horizontal and the vertical dashed lines in Fig. 5.3(b), i.e. they will be pinned at the potential maxima. The translational symmetry of the energy functional is broken in both directions and only discrete lattice symmetries remain. By taking outer products between the two equalities above we obtain $l_1 k_2 - l_2 k_1 = \pm r$ and we reach the conclusion that $r$ must be an integer. For arbitrary angle of the optical lattice $\phi$ we will consider only the case $r = 1$. Here, it holds that $p = 1$, $\theta = \phi$, $\nu = \nu_0$, $c_1 = b_1$, and $c_2 = b_2$. For a square optical lattice, this fully pinned situation is shown in Fig. 5.5(a). The energy functional is given by

$$\mathcal{K} = \hbar(\omega - \Omega) N \frac{\sigma^2(\nu_{OL})}{\ell^2} + \frac{\alpha(1, \phi) g N^2}{4\pi \sigma^2(\nu_{OL}) d_z} + V_0 N \beta(1, 0, 1, \phi). \quad (5.29)$$

For a square optical lattice we will consider two other configurations with $r = 2$. The first one has $p = 2$, $\theta = \pi/2$, $\nu = 2\nu_0$, $2c_1 = 2b_1$ and $c_2 = 2b_2$, and is shown in Fig. 5.5(b). Its energy is given by
Fig. 5.5: Possible realizations of the fully pinned situation for (a) \( r = 1 \) and (b),(c) \( r = 2 \). The empty circles are the pinning centers, the crosses the vortices.

\[
\mathcal{K} = \hbar(\omega - \Omega)N \frac{\sigma^2(2\nu_{OL})}{\ell^2} + \frac{\alpha(2, \pi/2)gN^2}{4\pi \sigma^2(2\nu_{OL})d_z} + \frac{V_0N}{2} [\beta(2, 0, 2, \pi/2) + \beta(1, 0, 2, \pi/2)]. \tag{5.30}
\]

The other possibility with \( r = 2 \) has \( p = 1, \theta = \pi/2, \nu = 2\nu_0, c_1 + c_2 = 2b_1 \) and \( c_1 - c_2 = 2b_2 \), which is shown in Fig. 5.5 (c). Its energy is given by

\[
\mathcal{K} = \hbar(\omega - \Omega)N \frac{\sigma^2(2\nu_{OL})}{\ell^2} + \frac{\alpha(1, \pi/2)gN^2}{4\pi \sigma^2(2\nu_{OL})d_z} + V_0N\beta(1, 1, 1, \pi/2). \tag{5.31}
\]

5.9 Results

After obtaining the expressions for the energy functional \( \mathcal{K} \) for the different lattice structures, we are ready to determine which lattice structure is the ground state for each point in parameter space. However, our parameter space is 5-dimensional and has the following parameters: the optical lattice unit cell area \( \nu_{OL} \), the unit cell angle \( \phi \), the optical lattice strength \( V_0 \), the interaction strength \( g \), and the difference between the trapping frequency \( \omega \) and rotation frequency \( \Omega \). For each point in parameter space, there are several possible fully pinned and half-pinned structures and one unpinned structure. For the parameters \( g \) and \( \omega - \Omega \) we will use the values from
the experimental paper Ref. [Cor04a] and furthermore we will set the optical lattice unit cell area $\nu_{OL}$ equal to $\nu_0$, the unit cell area of the unpinned vortex lattice. Since $\nu_{OL} = \nu_0$, it is reasonable to consider only fully pinned and half-pinned vortex lattices with $r = 1$, i.e. those shown in Fig. 5.4(b) and Fig. 5.5(a).

In Fig. 5.6 we show the phase diagram for a one-component vortex lattice in an optical lattice. On the horizontal axis, we plot the angle of the optical lattice $\phi$, and on the vertical axis, the strength of the optical lattice $V_0$ (in units of $E_0/N \approx 7 \cdot 10^{-14}$ eV, where $E_0$ is the energy of the system in the unpinned situation and $N$ is the number of particles). The unpinned structure is denoted by UP. The fully pinned structure from Fig. 5.5(a) is denoted by FP and the half-pinned structure from Fig. 5.4(b) by HP. If we start in the unpinned phase for a square optical lattice and slowly increase the strength of the optical lattice $V_0$, there is a structural transition to the half-pinned phase around $V_0 = 0.06$. Increasing $V_0$ even further, we find a second structural transition from the half-pinned to the fully pinned phase at $V_0 = 0.12$. This fully pinned phase at $\phi = \pi/2$ is the same one as shown in Fig. 5.2(c) and (f). Considering optical lattice angles $\phi < \pi/2$ one observes that a smaller optical lattice strength $V_0$ is sufficient to achieve the structural transitions from the unpinned to the half-pinned and from the half-pinned to the fully pinned structures. The extreme case of this effect is seen at optical lattice angle $\phi = \pi/3$ where it takes only an infinitesimal $V_0$ to achieve the structural transition to the fully pinned phase. This effect can be explained by the observation that for lower optical lattice angles $\phi$, the fully pinned and half pinned structures coincide with the triangular Abrikosov lattice structure.

The typical energy that the optical lattice yields to an atom in the condensate is the optical lattice strength $V_0$. The value of the latter, which is needed to achieve a structural transition is typically $V_0^t = 7 \cdot 10^{-15}$ eV. Now, since $2\hbar\omega \approx 7 \cdot 10^{-14}$, it holds that $V_0^t \ll 2\hbar\omega$ and we reach the conclusion the the optical lattice energy per particle is much smaller than the gap of $2\hbar\omega$ between the Landau levels. Hence, the optical lattice strength needed to achieve the pinning-depinning transition does not induce transitions to higher Landau levels, thus supporting the LLL assumption used in this work.
Fig. 5.6: Phase diagram for a one-component vortex lattice in an optical lattice. On the horizontal axis we show the angle $\phi$ of the optical lattice, whereas on the vertical axis the strength of the optical lattice $V_0$ is plotted in units of $E_0/N \approx 7 \cdot 10^{-14}$ eV, where $E_0$ is the energy of the system in the unpinned situation and $N$ is the number of particles.
6. TWO-COMPONENT VORTEX LATTICES

6.1 Introduction

The next step in this thesis is to study BEC’s consisting of two types of particles. These can be, e.g., two different atomic species or two different spin states of the same atom. At the mean field level, such a two-component condensate can be described by two macroscopic wave functions, $\Psi_1(\mathbf{r})$ and $\Psi_2(\mathbf{r})$, characterizing species 1 and 2, respectively. Hence, as we saw in Chapter 3, the condensate supports angular momentum through vortices, and vortices belong either to species 1 or 2. If we increase the angular momentum in the system, a vortex lattice forms, that consists of two types of vortices. In 2002, Mueller and Ho predicted that in the LLL, among other structures, this vortex lattice can have an interlaced square structure [Ho02]. In this structure, the vortices of both species separately form a square lattice, and these two lattices have the same unit cell area and orientation. However, they do not lie on top of each other, but are displaced in such a way that the vortices of type 1 lie in the middle of the vortex lattice unit cells of the vortex lattice of type 2. In 2004, the group of Eric Cornell succeeded in creating this interlaced square vortex lattice experimentally [Cor04b]. Loosely speaking, they started by creating a vortex lattice in a one-component condensate and then they added a second component. In the absence of the second component, the vortex lattice has the triangular Abrikosov structure, as shown in Fig. 6.1(a). Then, by

Fig. 6.1: When the second component is added, a structural transition occurs from the Abrikosov lattice structure to an interlaced square vortex lattice. Picture taken from [Cor04b].
adding the second component, a structural transition occurs to the interlaced square lattice, as shown in Fig. 6.1(b), where due to the observational technique used, only the vortex lattice of the first component is shown. From the experiment, it follows that the intercomponent interaction inside the vortex cores is important in determining what the ground state of the system is. The interlaced square vortex lattice is the structure that minimizes the interaction energy by making the density distribution as smooth as possible. Furthermore, we remark that the rotation frequency in the experiment described above was $\Omega \approx 0.75\omega$, i.e., outside the LLL. Thus, the interlaced square structure was predicted by a calculation valid only in the LLL regime, but the structure was found experimentally outside this regime. This fact is a suggestion that the results and phase diagrams we obtain in the LLL regime are qualitatively correct also outside this regime. In the next section we will reproduce and discuss the results from Ref. [Ho02] and after that we will consider two-component condensates in the presence of an optical lattice.

### 6.2 Rewriting the Wave Functions

As mentioned above, a two-component condensate can be described by two wave functions $\Psi_1(r)$ and $\Psi_2(r)$, characterizing species 1 and 2. We assume again a step function for the wave function in the $z$-direction, $\Psi_i(r) = \psi_i(x, y)\theta(d_z/2 - z)/\sqrt{d_z}$. After integrating out the trivial $z$-direction, we obtain the following energy functional $K$ in the absence of an optical lattice

$$K = \sum_{i=1,2} \left[ \int \! dx \, dy \, \psi_i^*(x, y) \left( h_{\perp} - \Omega L_z - \mu_i \right) \psi_i(x, y) \right] + \frac{1}{d_z} \int \! dx \, dy \left( \frac{g_1}{2} |\psi_1(x, y)|^4 + \frac{g_2}{2} |\psi_2(x, y)|^4 + g_{12} |\psi_1(x, y)|^2 |\psi_2(x, y)|^2 \right),$$

where the intracomponent interaction strengths $g_i$ are given by $g_i = 4\pi\hbar^2 a_i/M$, with $a_i$ the intracomponent $s$-wave scattering length, and where the intercomponent interaction strength $g_{12}$ is given by $g_{12} = 2\pi\hbar^2 a_{12}/M_{12}$, with $a_{12}$ the intercomponent $s$-wave scattering length and $M_{12}$ the reduced mass.

We showed in Chapter 5 that if we assume that the zeros of $\psi_i$ form a regular lattice, it holds in the LLL that the wave functions $\psi_i$ are given by the product of a Gaussian and a function with lattice periodicity: $|\psi_i(x, y)|^2 = e^{-r^2/\sigma^2} f_i(x, y)$, where $\sigma$ is the effective radius of the cloud, and $f_i(r) = f_i(r + R)$,
where $\mathbf{R}$ is a lattice vector. We set $N_1 = N_2 = N$ and assume that this leads to $\sigma_1 = \sigma_2$, i.e. for each component the condensate cloud has the same size. Furthermore, we assume that $f_1(\mathbf{r}) = f_2(\mathbf{r} + \mathbf{r}_0) \equiv f(\mathbf{r})$, i.e., that the two vortex lattices have the same geometry and only differ by a relative displacement $\mathbf{r}_0$. Thus, it holds for the unnormalized component wave functions

$$|\psi_1(\mathbf{r})|^2 = e^{-r^2/\sigma^2} f(\mathbf{r}) \quad \text{and} \quad |\psi_2(\mathbf{r})|^2 = e^{-r^2/\sigma^2} f(\mathbf{r} - \mathbf{r}_0).$$

Going to reciprocal space, we write $f(\mathbf{r}) = (1/\nu) \sum_\mathbf{K} \hat{f}_\mathbf{K} e^{i\mathbf{K} \cdot \mathbf{r}}$ for some Fourier coefficients $\hat{f}_\mathbf{K}$, where the $\mathbf{K}$ are the reciprocal lattice vectors, and $\nu$ is the area of the unit cell of the vortex lattice. Normalizing the $\psi_i$ to $N$, we obtain

$$|\psi_1(\mathbf{r})|^2 = \frac{N}{\pi \sigma^2} \sum_\mathbf{K} \hat{f}_\mathbf{K} e^{i\mathbf{K} \cdot \mathbf{r}} e^{-r^2/\sigma^2} \quad \text{and} \quad |\psi_2(\mathbf{r})|^2 = \frac{N}{\pi \sigma^2} \sum_\mathbf{K} \hat{f}_\mathbf{K} e^{i\mathbf{K} \cdot (\mathbf{r} - \mathbf{r}_0)} e^{-r^2/\sigma^2},$$

where $\hat{f}_\mathbf{K} = f(\mathbf{K})/(\sum_{\mathbf{K}'} f_{\mathbf{K}'} \nu e^{-\sigma^2 K'^2/4})$ and $\hat{f}_\mathbf{K} = f(\mathbf{K})/\nu (\sum_{\mathbf{K}'} f_{\mathbf{K}'} e^{-i\mathbf{K}' \cdot \mathbf{r}_0} e^{-\sigma^2 K'^2/4})$.

Now, using the expressions for the reciprocal lattice vectors $\mathbf{K}_i$ from Eq. (3.21), we obtain for the length of an arbitrary reciprocal lattice vector $\mathbf{K} = m_1 \mathbf{K}_1 + m_2 \mathbf{K}_2$

$$K^2 = \frac{4\pi^2}{\nu \sin \theta} \left( m_1^2 + p^2 m_2^2 - 2p m_1 m_2 \cos \theta \right). \quad (6.2)$$

Again, we restrict the unit cell angle $\theta$ to $\pi/3 \leq \theta \leq \pi/2$ and consider the fast-rotation limit where $\sigma^2/\nu \gg 1$. Then, all terms with $K \neq 0$ drop out in the expressions for $\hat{f}_\mathbf{K}$ and $\hat{f}_\mathbf{K}$ and we obtain $\hat{f}_\mathbf{K} = \hat{f}_0$. It is possible to derive an explicit expression for the $\hat{f}_\mathbf{K}$’s by performing an analysis using the Jacobi-Theta function. We will not do this derivation here, but instead refer the interested reader to [Ho02]. The result is

$$f_\mathbf{K} = (-1)^{m_1 + m_2 + m_1 m_2} e^{-i\mathbf{K}^2/8\pi \nu /2}, \quad (6.3)$$

where the $m_i$’s are defined by the expansion of $\mathbf{K}$ in terms of the reciprocal basis vectors $\mathbf{K}_i$, $\mathbf{K} = m_1 \mathbf{K}_1 + m_2 \mathbf{K}_2$. The above result for $f_\mathbf{K}$ seems to depend on the particular choice of basis vectors, since it depends on the $m_1$’s and $m_2$’s. However, it is easy to see that this is not the case. It holds that $m_1 + m_2 + m_1 m_2$ is always odd, unless both $m_1$ and $m_2$ are even. In that case also $\mathbf{K}/2$ is a reciprocal lattice vector. Thus, we see that for all reciprocal lattice vectors $\mathbf{K}$ for which $\mathbf{K}/2$ is a reciprocal lattice vector, the quantity $m_1 + m_2 + m_1 m_2$ is even, and for all other $\mathbf{K}$’s the quantity is odd. Thus, $f_\mathbf{K}$ does not depend on the choice of basis vectors.
6.3 Determining the Energy Functional

Using the same arguments as in Section 5.2 we rewrite the single particle part (the first line) of $K$ as

$$\sum_{i=1,2} \left[ (\mu_i - \hbar \Omega) N_i + \frac{\hbar(\omega - \Omega)}{\ell^2} \langle r^2 | \psi_i |^2 \rangle \right].$$

By performing the gaussian integration, we obtain

$$\langle r^2 | \psi_i |^2 \rangle = \frac{N}{\pi \sigma^2} \sum_{\mathbf{K}} \left[ \frac{\pi \sigma^4}{4} (4 + \mathbf{K}^2 \sigma^2) e^{-\sigma^2 \mathbf{K}^2 / 4} \right] = N \sigma^2,$$

where we again used that $\sigma^2 \mathbf{K}^2 \gg 1$ for $\mathbf{K} \neq 0$. Thus, we obtain the result that $\langle r^2 | \psi_i |^2 \rangle$ does not depend on the vortex lattice structure, as it happened in Chapter 5. This follows from the fact that $\langle r^2 | \psi_i |^2 \rangle$ does not depend on the function $f(\mathbf{r})$.

The next step is to calculate the interaction terms, which we will do explicitly. It holds that

$$\int d\mathbf{x} d\mathbf{y} |\psi_1(\mathbf{x}, \mathbf{y})|^4 = \frac{N^2}{\pi^2 \sigma^4} \sum_{\mathbf{K}, \mathbf{K}'} \frac{f_{\mathbf{K}} f_{\mathbf{K}'}}{f_0^2} \int d\mathbf{x} d\mathbf{y} e^{i(\mathbf{K} + \mathbf{K}') \cdot \mathbf{r}} e^{-2r^2/\sigma^2} =$$

$$\frac{N^2}{2\pi \sigma^2} \sum_{\mathbf{K}, \mathbf{K}'} \frac{f_{\mathbf{K}} f_{\mathbf{K}'}}{f_0^2} e^{-\sigma^2 |\mathbf{K} + \mathbf{K}'|^2 / 8} \equiv \frac{N^2}{2\pi \sigma^2} I_1.$$

$$\int d\mathbf{x} d\mathbf{y} |\psi_2(\mathbf{x}, \mathbf{y})|^4 = \frac{N^2}{\pi^2 \sigma^4} \sum_{\mathbf{K}, \mathbf{K}'} \frac{f_{\mathbf{K}} f_{\mathbf{K}'}}{f_0^2} \int d\mathbf{x} d\mathbf{y} e^{i(\mathbf{K} + \mathbf{K}') \cdot (\mathbf{r} - \mathbf{r}_0)} e^{-2r^2/\sigma^2}$$

$$\frac{N^2}{2\pi \sigma^2} \sum_{\mathbf{K}, \mathbf{K}'} \frac{f_{\mathbf{K}} f_{\mathbf{K}'}}{f_0^2} e^{-i(\mathbf{K} + \mathbf{K}') \cdot \mathbf{r}_0} e^{-\sigma^2 |\mathbf{K} + \mathbf{K}'|^2 / 8} \equiv \frac{N^2}{2\pi \sigma^2} I_2.$$

$$\int d\mathbf{x} d\mathbf{y} |\psi_1(\mathbf{x}, \mathbf{y})|^4 |\psi_2(\mathbf{x}, \mathbf{y})|^4 = \frac{N^2}{\pi^2 \sigma^4} \sum_{\mathbf{K}, \mathbf{K}'} \frac{f_{\mathbf{K}} f_{\mathbf{K}'}}{f_0^2} \int d\mathbf{x} d\mathbf{y} e^{i(\mathbf{K} + \mathbf{K}') \cdot (\mathbf{r} - \mathbf{r}_0)} e^{-2r^2/\sigma^2}$$

$$\frac{N^2}{2\pi \sigma^2} \sum_{\mathbf{K}, \mathbf{K}'} \frac{f_{\mathbf{K}} f_{\mathbf{K}'}}{f_0^2} e^{-i\mathbf{K}' \cdot \mathbf{r}_0} e^{-\sigma^2 |\mathbf{K} + \mathbf{K}'|^2 / 8} \equiv \frac{N^2}{2\pi \sigma^2} I_{12}.$$
If we again use that \( \sigma^2 K^2 \gg 1 \) for \( K \neq 0 \), the only terms which survive are the ones for which \( K = -K' \). Using that \( f_K^* = f_{-K} \), this leads to

\[
I = I_1 = I_2 = \sum_K \left| \frac{f_K}{f_0} \right|^2 \quad \text{and} \quad I_{12} = \sum_K \left| \frac{f_K}{f_0} \right|^2 \cos(K \cdot r_0). \tag{6.4}
\]

With these results and definitions, the energy functional \( \mathcal{K} \) becomes

\[
\mathcal{K} = \sum_{i=1,2} \left[ (-\mu_i + \hbar \Omega) + \hbar (\omega - \Omega) \frac{\sigma^2}{\ell^2} \right] N + \frac{N^2}{2\pi \sigma^2 d_z} \left( \frac{g_1}{2} I_1 + \frac{g_2}{2} I_2 + g_{12} I_{12} \right). \tag{6.5}
\]

For simplicity, we set the two intracomponent interaction strengths equal: \( g \equiv g_1 = g_2 \). Furthermore we define \( \alpha = g_{12}/g \). Since \( \sigma \) only depends on the area of the unit cell \( \nu \) and not on the unit cell angle \( \theta \) or on the ratio \( p \), the optimal vortex lattice geometry, i.e. the optimal values of \( p \) and \( \theta \), can be found by minimizing the interaction energy \( I + \alpha I_{12} \). This task will be performed in the next section.

### 6.4 Results

In this section we determine the phase diagram of a two component vortex lattice in the absence of an optical lattice. By using Eqs. (6.2), (6.3), and (6.4), we minimize the interaction energy \( I + \alpha I_{12} \), keeping the angle \( \theta \), the ratio \( p \), and the displacement vector \( r_0 \) as variational parameters. The result of this procedure is shown in Figs. 6.2 and 6.3. In Fig. 6.2 we show the parameters determining the geometry of the ground state vortex lattice as a function of \( \alpha \). These parameters are the ratio between the lengths of the vortex lattice vectors \( p \), the length \( r_0 \) of the displacement vector, \( r_0 = r_0(c_1 + c_2) \), and the vortex lattice angle \( \theta \). Furthermore, snapshots of the vortex lattices at the positions (1), (2), (3), and (4) are shown in Fig. 6.3 where the white circles correspond to vortices of species 1, and the black circles to vortices of species 2. We will now discuss the phases and structural transitions shown in the figures.

1. At low values of \( \alpha \), the vortex lattices of species 1 and 2 almost ignore each other and each one forms a triangular Abrikosov lattice structure with \( p = 1 \) and \( \theta = \pi/3 \). In order to minimize the inter-component interaction, the lattices position themselves with respect to each other
in such a way that the vortices of species 1 are as far away as possible from the vortices of species 2. The optimal value of $r_0$ is $1/3$.

(2) If we increase $\alpha$ to a value higher than 0.17, the intercomponent interaction energy becomes more important and a structural transition occurs. The vortex lattices are deformed by the intercomponent interaction and jump from an Abrikosov lattice structure to a structure with $\theta > \pi/3$ and $r_0 = 1/2$. After the transition, the value of $\theta$ increases continuously to $\theta = \pi/2$ at $\alpha = 0.37$.

(3) For $0.37 < \alpha < 0.93$, the ground state is the interlaced square lattice structure from Fig. 6.1. The intercomponent interaction deforms the vortex lattices to the configuration where the intra-component interaction is maximal (given that $p = 1$). The large range of $\alpha$ for which this structure is the ground state suggests that this structure is very stable.

(4) Finally, for $\alpha > 0.93$, the intercomponent interaction starts to dominate and pushes the vortices of like species toward each other and of unlike species away from each other. At the special point $\alpha = 1$, it holds that $p = \sqrt{3}$: there is no distinction between the two types of vortices and the system has the optimal Abrikosov lattice structure.

We can summarize these results as follows: Increasing the intercomponent interaction pushes the two vortex lattices away from the optimal Abrikosov lattice towards a structure where the distance between unlike vortices is maximized. Note that Figs. 6.2 and 6.3 contain result that we obtained by using an approach from [Ho02], and that similar figures can also be found in that paper.
Fig. 6.2: The optimal values of $p$, $r_0$, and $\theta$ as a function of $\alpha$. Note that this figure was obtained using an approach from [Ho02], and that a similar figure can also be found in [Ho02].
Fig. 6.3: Snapshots of the vortex lattices at the positions (1), (2), (3), and (4). The white circles correspond to vortices of species 1, the black circles to vortices of species 2. Note that this figure was obtained using an approach from [Ho02], and that a similar figure can also be found in [Ho02].
6.5 Including an Optical Lattice

The final topic of this thesis is a two-component condensate in an optical lattice potential. As before, the optical lattice is given by

\[ V(x, y) = V_0 \left[ \cos^2 \left( \frac{k_1 \cdot r}{2} \right) + \cos^2 \left( \frac{k_2 \cdot r}{2} \right) \right], \]

and it leads to the following term in the energy functional \( K \)

\[ \langle V_{OL} \rangle = \int dx dy (|\psi_1(x, y)|^2 + |\psi_2(x, y)|^2) V(x, y), \]

i.e., the product of the value of the potential at a point times the total particle density at that point, integrated over all space. Note that the optical lattice is the same for species 1 and 2. In this thesis we will restrict ourselves to optical lattices with a square geometry. Furthermore, we only consider filling factors of two vortices per unit cell of the optical lattice, in order to able to compare our results to the one-component case. Now, we rewrite the cosine in terms of complex exponentials and use Eq. (6.1) to calculate

\[ \langle V_{OL} \rangle \]

\[ = \frac{V_0 N}{4\pi r^2} \sum_k \frac{f_k}{f_0} (1 + e^{-iK \cdot r_0}) \int dx dy e^{iK \cdot r} e^{-r^2/\sigma^2} \left( 4 + \sum_{k=\pm k_1, k_2} e^{ik \cdot r} \right) \]

\[ = \frac{V_0 N}{4} \sum_k \frac{f_k}{f_0} (1 + e^{-iK \cdot r_0}) \left[ 4e^{-\sigma^2 K^2/4} + \sum_{k=\pm k_1, k_2} e^{-\sigma^2 (K+k)^2/4} \right]. \]  

(6.6)

(6.7)

Again, we only take the exponential terms into account whose argument is 0. Let us define a function \( d(k) \), which is equal to 1 if \( k \) is part of the reciprocal vortex lattice, and equal to 0 if it is not. Then, we obtain

\[ \langle V_{OL} \rangle \]

\[ = \frac{V_0 N}{4} \left[ 8 + \sum_{k=\pm k_1, k_2} \frac{f_{-k}}{f_0} d(-k) \left( 1 + e^{iK \cdot r_0} \right) \right]. \]  

(6.8)

\[ = \frac{V_0 N}{2} \left[ 4 + \sum_{k=k_1, k_2} \frac{f_k}{f_0} d(k) \left( 1 + \cos(k \cdot r_0) \right) \right]. \]  

(6.9)

\[ = V_0 N \left[ 2 + \sum_{k=k_1, k_2} \frac{f_k}{f_0} d(k) \cos^2 \left( \frac{k \cdot r_0}{2} \right) \right]. \]  

(6.10)
6. Two-Component Vortex Lattices

Dropping the constant term, we define the function $v(p, \theta, r_0)$ as

$$\langle V_{OL} \rangle = V_0 N \sum_{k=k_1, k_2} \frac{f_k}{f_0} d(k) \cos^2 \left( \frac{k \cdot r_0}{2} \right) \equiv V_0 N v(p, \theta, r_0).$$

The relevant terms in the energy functional $\mathcal{K}$ are the interaction and pinning energies,

$$\mathcal{K} = \frac{gN^2}{2\pi \sigma^2} [I(p, \theta) + \alpha I_{12}(p, \theta, r_0)] + V_0 N v(p, \theta, r_0),$$

where we explicitly indicated the dependence on the minimization parameters $p$, $\theta$, and $r_0$. The minimization procedure is the following: for each $(p, \theta, d(k_1), d(k_2))$ the energy functional $\mathcal{K}$ is minimized with respect to $r_0$. In this way, we obtain a function $r_0(p, \theta, d(k_1), d(k_2))$, which gives for all values of its variables the optimal value of $r_0$. We can then substitute this function in $\mathcal{K}$ and minimize the latter with respect to the variables $(p, \theta, d(k_1), d(k_2))$.

### 6.6 Phase Diagram

By carrying out the minimization procedure described above, we obtain the phase diagram shown in Fig. 6.4. Horizontally, we show the value of $\alpha = g_{12}/g$, whereas, vertically, we show the value of the optical lattice strength $V_0$ (in units of $E_0/N \approx 7 \cdot 10^{-14}$ eV, where $E_0$ is the energy of the one-component system in the unpinned situation and $N$ is the number of particles). The white circles correspond to vortices of species 1, the black circles to vortices of species 2. Note that the phase diagram only specifies the phases for positive values of $\alpha$ and $V_0$.

- **Unpinned Structures**: For small values of $V_0$, we recognize the 4 unpinned structures described above for the situation of a two-component condensate in the absence of an optical lattice (see Figs. 6.2 and 6.3). These energies of these structures have rotation symmetry and continuous translation symmetry in both directions. The vortex lattices in these structures completely ignores the optical lattice.

- **Fully Pinned Structure**: The large area above the (approximately) straight line $V_0 = (3/2)\alpha$ corresponds to a fully pinned structure where both types of vortices are pinned on top of each other at the pinning
centers. The pinning centers are not displayed but their positions are at the same positions as the black dots. Note that although the vortices of species 1 and 2 repel each other, the optical lattice pushes them on top of each other.

- **Half-Pinned Structures**: Around the line $V_0 = (3/2)\alpha$ until $\alpha \approx 1.2$ there are two half pinned structures, pinned on the horizontal lines of maximal potential. We denote the left one as the triangular structure, and the right one as the square structure.

In the triangular structure the vortex lattices of both species form the one-component half-pinned structure shown in Fig. 5.4(b). The two vortex lattices are displaced with half a lattice vector along the pinning lines to minimize the intercomponent interaction energy.

When we increase the value of $\alpha$, there can be a structural transition to the square phase. Here, both vortex lattices have a square structure and are displaced with half a lattice vector along the pinning lines. The transition can be understood by noting that in the square structure the distance between vortices of unlike type has increased in comparison with the triangular structure. In this way, the intercomponent interaction energy is lowered. Because the vortices are restricted to lie on the pinning lines, it is not possible to increase the distance between vortices of unlike type in a half-pinned phase further. This is the reason why the half-pinned phases disappear from the phase diagram for $\alpha > 1.2$.

We note that for low values of $\alpha$, the vortex lattices of the two types of particles should ignore each other and our results should reproduce the results for the one-component case in an optical lattice. Comparing Fig. 6.4 and Fig. 5.6 we see that this is indeed the case. From this comparison one also deduces that the typical optical lattice strength to achieve a structural transition for the two-component case is a factor 10 higher than in the one-component case. Hence, it holds that $V_0 \sim 2\hbar \omega$, i.e., the typical energy that the optical lattice yields to an atom is approximately equal to the LLL gap. Thus, the assumption of being in the LLL regime is not a valid one for these optical lattice strengths. However, the main reason for considering the LLL was that here we are able to obtain analytical results. Furthermore, we noted that phases predicted by doing a calculation valid only in the LLL were found experimentally outside the LLL regime. This fact leads us to expect
that although the assumption of being in the LLL is strictly not valid, the results and phase diagrams we obtain are, at least qualitatively, correct.
Fig. 6.4: Phase diagram is shown for a two-component vortex lattice in an optical lattice. We plot on the horizontal axis the (scaled) intercomponent interaction strength $\alpha$, and on the vertical axis the strength of the optical lattice in units of $E_0/N \approx 7 \cdot 10^{-14}$ eV, where $E_0$ is the energy of the one-component system in the unpinned situation and $N$ is the number of particles. The white circles correspond to vortices of species 1, the black circles to vortices of species 2. The optical lattice has a square structure.
7. CONCLUSIONS AND OUTLOOK

In this thesis we determined the vortex lattice phase diagrams of rotating Bose-Einstein condensates (BEC’s). We considered the situations of rotating one- or two-component BEC’s in the absence or presence of a square optical lattice potential. The vortex phase diagrams we obtained for these situations are shown in Figs. 5.1, 5.6, 6.2, and 6.4, respectively. Our results are consistent with previous experimental and theoretical results (where available), that were obtained in different parameter regimes and/or using different methods. For the one-component case, we find that in the absence of an optical lattice the well-known triangular Abrikosov lattice is the groundstate. In the presence of a strong optical lattice, instead, the vortex lattice acquires the square structure of the optical lattice and we find the same fully pinned phase as was found experimentally in Ref. [Cor06]. For two-component condensates in the absence of an optical lattice, we reproduced the results from Ref. [Ho02]. Our new result, i.e., the phase diagram for the two-component case in the presence of an optical lattice, exhibits new phases where all or half of the two types of vortices are pinned at pinning centers of the optical lattice.

We performed our calculations by extending approaches from Refs. [Ho01] and [Ho02], which assume that the rotation frequency $\Omega$ is close to the frequency $\omega$ of the magnetic trapping potential. Within this assumption, the system resides, under certain conditions, in the so-called lowest Landau level regime. In this regime, the macroscopic condensate wave function is completely determined by the positions of the vortices, a fact that makes analytical results feasible. Furthermore, we assume that the collection of vortex positions is given by an infinite regular lattice with arbitrary geometry. In Chapter 4, we show that the limit in which we send the number of vortices to infinity is appropriate and well-controlled.

One motivation for this work is that previous theoretical approaches concerning vortex lattices in two-component BEC’s in the presence of an optical lattice [Du04] are not suitable to treat all vortex lattices in two-component
condensates, because they do not correctly take into account the intercomponent interaction inside the vortex cores. Our approach does not have this problem and therefore is suitable for treating all vortex-lattice-structure-transitions in rotating two-component condensates in an optical lattice. Furthermore, the treatment of the effect of the optical lattice potential on a condensate inside the LLL regime is new. In the near future we expect to publish our results.

We envisage the following suggestions for further research. Firstly, we used a step-function for the $z$-dependence of the macroscopic wave function $\Psi(r)$. This was done to simplify the calculations and because we wanted to concentrate our attention on the two-dimensional ordering of the vortices. To improve the accuracy of the results, it is possible to use a more realistic dependence on the $z$-coordinate, as was done in Ref. [Ho01], using a Thomas-Fermi profile. In this approach, the energy of the system will depend on the profile in the $z$-direction, and it will be interesting to study whether or not this extra freedom is relevant in determining the phase diagram. Furthermore, one can consider optical lattice unit cell sizes that are not equal to the unpinned Abrikosov lattice unit cell. Especially the question what physically happens at strong pinning when the optical lattice unit cell size is smaller than the critical vortex lattice unit cell size $\pi \ell^2$ is interesting, since then the fully pinned vortex lattice with filling factor equal to 1 is not normalizable.

We hope and expect that our theoretical results will be confronted with experiments in the near future. Furthermore, we are convinced that the approach outlined in this thesis will provide a suitable starting point, even if the experiments are in a different regime of parameters than considered here.
8. ACKNOWLEDGEMENTS

I would like to thank Cristiane de Morais Smith and Rembert Duine for the supervision of my thesis work and interesting discussions. Also, I thank my parents for their continuing support.
9. REFERENCES


NIST Image Gallery National Institute of Standards and Technology.