UNIVERSITY
OF OSLO

Master's thesis

A Phase Field Crystal Model for Dislocations in Square Crystal Lattices

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Physics: Theoretical Physics
60 ECTS study points

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Autumn 2022

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Abstract

The phase field model is a powerful model used to describe crystals and their mechanical properties based on symmetries and topological conservation. In this thesis, we provide an introduction to phase field crystal modelling of crystals with defects and how to compute their dynamics, as well as how stress is defined and computed. We exemplify the general analytical expressions for stress and dislocation dynamics for a hexagonal lattice based on the one mode expansion. We then attempt to extend the earlier work done on the hexagonal lattice to two-mode expansion representative for a square lattice to derive the stress-strain relation and the dislocation mobility of the Peach-Koehler law to the square lattice using the same kind of approach. Surprisingly, we find that in the two-mode expansion, the expression for the Peach-Koehler force cannot be directly related to the stress acting on a dislocation, henceforth it is challenging to derive a closed expression for the mobility within this present formulation. Hence the Peach-Koehler force and the dislocation mobility in the square lattice warrant further analytical investigation, and we suggest a few such avenues.

Acknowledgements

I would like to thank my supervisors Luiza and Vidar for their continued support and patience. Your guidance has been invaluable to this project.

Also thanks to the staff and students of the theory section for good and lively discussions. Especially to my office mate Andrea for sticking with me this final year and for your help creating such beautiful figures.

Finally, thanks to those who have climbed with me the last couple of years. Life would have been worse without you.

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Chapter 1

Introduction

Imagine you have a perfect sphere. No matter how you twist and turn it, it will always look the same. Or consider a cube. Cubes are invariant under specific discrete rotations about their center but not necessarily under any rotation. The sphere is more symmetric than the cube because a bigger set of transformations leaves it invariant. By symmetry, we mean a transformation on some mathematical object that leaves it invariant. Symmetry also appears in many physical systems. Consider a liquid, for instance, water, in some box. If you consider microscopically what the water looks like at any particular point in the box and then compare it to what it looks like at any other point in the box, you will not notice any difference. This is because the liquid exhibits complete translational symmetry. Similarly, if you study the water at any point and then rotate your frame of reference by some angle, you will also not notice any difference because the water has complete rotational symmetry, similar to the sphere we mentioned earlier. Now the temperature of the water is reduced to below its freezing point such that the liquid becomes a crystal. In this phase, the water will have some specific, discrete symmetries both rotationally and translationally. Still, most of the symmetry we had in the liquid phase will no longer be there. We say the crystal phase exhibits broken symmetries because the water lost symmetry by undergoing a phase transition.

In this thesis, we will study the mechanical properties of such a system. In addition, we will explore the mechanical deformation of crystal lattices. Mainly, we will focus on square lattices. Square lattices occur in many kinds of systems, like in photonic crystals [5] and magnets [3]. We present a theoretical analysis of dislocations in crystals with square lattice symmetry. Chapter 1 introduces basic concepts from algebraic topology and continuum mechanics used to describe such systems. In Chapter 2, we will introduce the phase field crystal model, using the hexagonal lattice as an example to illustrate some of the theory's core concepts, like how the crystal is modeled through an appropriate phase field and defects are represented in this theoretical approach. We proceed by deriving analytical expressions for the dislocation velocity and the stress for the hexagonal lattice. In Chapter 3, we turn to the square lattice and derive the matching results for this crystal symmetry. We check that by coarse-graining the microscopic stress determined by phase field distortions, we obtain stress fields consistent with elasticity theory.

Furthermore, we solve numerically for the stress field profile induced by dislocations dipoles in the square lattice. We also seek to derive an analytical expression for the mobility of the Peach-Koehler force for a square geometry in the same way as others have done for the hexagonal lattice. Concluding remarks and a summary is discussed in the last chapter.

Chapter 2

Crystals and dislocations

This chapter will review fundamental concepts used to describe crystals and their mechanical properties. We start by introducing some of the core concepts in elasticity theory. Then, we introduce crystal lattices and their defects, known as dislocations, from the point of view of symmetry-breaking states and associated topological defects. We also discuss how dislocations and their motion are conventionally described in the theory of elasticity.

2.1 Basics of Elasticity Theory

2.1.1 Stress and Strain

The theory of elasticity describes how a continuous body will deform when exposed to forces. A deformation field describes the deformation $\mathbf{u}(\mathbf{r}) = \mathbf{r}' - \mathbf{r}$ which is a vector field describing how each point $\mathbf{r}$ in the solid is displaced relative to some reference point $\mathbf{r}'$. It is clear that if the relative position between all points in the body is changed in the same way, the body has not been deformed but has just been moved from one place to another. Therefore we are interested in a measure of how differently the body is deformed at each point in space. This can be achieved by considering the gradient of the deformation field $\mathbf{W} = \nabla \mathbf{u}$ or in index notation

$$W_{ij} = \partial_i u_j. \tag{2.1}$$

The symmetric part of W_{ij} is called the strain of the body and is given by

$$e_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i). \tag{2.2}$$

We are typically only interested in the symmetric part of W_{ij} because this is the part of W_{ij} related to volume changes and shearing of the body. In contrast, the anti-symmetric part is only associated with rotations of the body. Rotations do not cause forces to arise in the body, and we do not consider this part of the gradient. If the body is only

deformed infinitesimally, the deformation field is well approximated by its first-order Taylor expansion, which gives us

$$u_i \approx u_i(\mathbf{r}') + (r_j - r'_j)\partial_i u_j. \tag{2.3}$$

Choosing the coordinate system such that $u_i(\mathbf{r}') = 0$ we get

$$u_i = r_j W_{ij}. \tag{2.4}$$

Under the assumption that the body is not rotated so that the anti-symmetric part of $\mathbf{W}$ is zero, we get the equation

$$u_i = r_j e_{ij} \tag{2.5}$$

relating the deformation field to the strain tensor. When a body is deformed, it is no longer in its equilibrium state. This means that there will arise forces in the body that will cause the body to return to its equilibrium state if left alone. Consider two infinitesimal areas inside the body $d\boldsymbol{\Sigma}_1$ and $d\boldsymbol{\Sigma}_2$ which are contiguous. Then the first area will exert a force $d\boldsymbol{F}_1$ on the second area, and the second will exert a force $d\boldsymbol{F}_2$ on the first. By Newtons third law $d\boldsymbol{F}_1 = -d\boldsymbol{F}_2$. Consider now some infinitesimal volume V inside the body. The total force $\boldsymbol{F}$ of this area will be given by the integral

$$\boldsymbol{F} = \int_\Omega \boldsymbol{f}\, dV \tag{2.6}$$

where $\boldsymbol{f}$ is the force per unit volume and Ω is some volume element in the body. Since the forces of every slice of an area that makes up the volume must cancel each other, the net force in the volume Ω must be equal to the force acting on it from the surface, which is continuous on the boundary of the volume. Hence we can write the total force as an integral over a surface. Using Gauss theorem, we get

$$F_i = \int_\Omega f_i\, dV = \int_\Omega \frac{\partial \sigma_{ik}}{\partial x_k}\, dV = \oint_{\partial\Omega} \sigma_{ik}\, dS_k \tag{2.7}$$

where S_k is some infinitesimal boundary area. The tensor $\boldsymbol{\sigma}$ is called the stress tensor. As defined above, the first index of the stress tensor gives the force per area component in that particular direction, and the second index is the orientation of the surface element on which the force is exerted.

2.1.2 The Stress-Strain Relationship

The force acting on a body attached to a massless spring can often be modeled as experiencing a force proportional to the displacement away from the spring's equilibrium. Mathematically this is expressed by Hooke's law

$$\mathbf{F} = k\mathbf{x} \tag{2.8}$$

where $\mathbf{F}$ is the force acting on the body, k is the spring constant and x is the displacement away from equilibrium. The same kind of phenomenon takes place in elastically deformed

bodies. To describe what happens in continuous bodies, we must write Hooke's law in a more general form

$$\sigma_{ij} = C_{ijkl} u_{kl}, \tag{2.9}$$

where σ_{ij} and e_{kl} is the stress and strain tensors defined in the previous subsection, and C_{ijkl} is called the elastic modulus tensor. The elastic modulus tensor describes how the stress in the body depends on deformations and depends on the kind of material we are studying. In fact, the material is often characterized by the form of the elastic modulus tensor. We talk of materials being isotropic and anisotropic. The material is said to be isotropic if the elastic modulus tensor can be written

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{jk}\delta_{il}). \tag{2.10}$$

where λ and μ are constants determined by the material. Inserting this form of the elastic modulus tensor into Eq. 2.9 we get

$$\sigma_{ij} = 2\mu u_{ij} + \lambda \delta_{ij} u_{kk} \tag{2.11}$$

as the stress-strain relationship. Materials with such a stress-strain relationship have no sense of direction and so respond in the same manner no matter which direction they are deformed in. Otherwise, the material has anisotropic properties. This is, for instance, the case with an elastic medium with an underlying square lattice, which will be discussed in detail in the latter chapters.

2.2 Crystals as ordered systems

At the atomic level, solids are collections of atoms with some ordered structure, repeating themselves in a pattern. This repeating pattern gives rise to a lattice structure. Lattices can be described by unit cells, which consist of the smallest repeating pattern of atoms. We can describe the unit cell using a set of vectors that describe the position of the atoms relative to each other, called lattice vectors. We can then describe any point in the lattice as a sum of integer multiples of these lattice vectors. Important examples of lattices in this thesis will be the square lattice and the hexagonal lattice. The crystal phase exhibits broken rotational and translational symmetries. For instance, if we have a square lattice, the geometry is invariant under rotations of $\pi/2$ and by translations of a_0 in the x and y directions. An example of a square lattice can be seen in figure 2.1. Such symmetries are called broken because, in the liquid phase, the system has continuous rotational and translational symmetry, which disappear when the system goes through the liquid-to-solid phase transition. The presence of crystal lattices with discrete rotational and translation symmetries allows the system also to form lattice defects, such as dislocations. Dislocations appear when an extra half-plane of atoms ends at the dislocation position. They come in two flavors, edge dislocations, and screw dislocations, depending on the shear or toque forces that generate this extra half-plane of atoms. If you count the three atoms horizontally towards the right around the dislocation line, then three atoms vertically upwards, three towards the left, and three downwards,

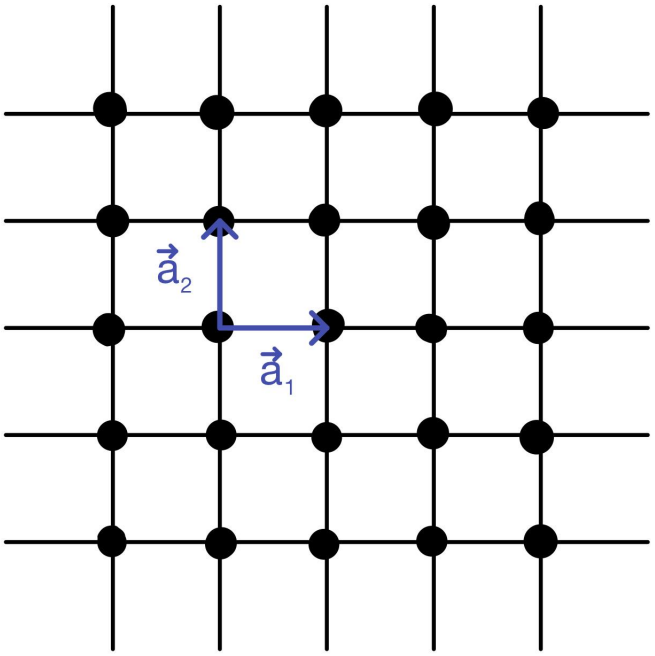

Figure 2.1: Drawing of a square lattice with no defects. The vectors $\vec{a}_1$ and $\vec{a}_2$ defines a unit cell.

you will not end up where you started. The lattice jump from the beginning to the end of this circuit surrounding a dislocation position defines a vector called the Burgers vector **b**, which has the magnitude determined by the lattice spacing and orientation determined by the line tangent and direction of motion of the dislocation.

2.3 Dislocations and the Peach-Koehler Force

Dislocations in elasticity theory are characterized by the Burgers vector, **b**. We define the Burgers vector of a dislocation in a continuous body as the line integral of the deformation field along a closed path L enclosing the dislocation point P once

$$\oint_L du_i = \oint_L \frac{\partial u_i}{\partial x_k} dx_k = -b_i. \tag{2.12}$$

Consider a defect in a crystal, characterized by some Burgers vector **b**, exposed to some external stress field $\boldsymbol{\sigma}$. The deformation field across the defect will vary by **b**. If the defect moves, it will cause the deformation field of the crystal to change. The change in deformation will be larger close to the defect, and smaller further away, so the crystal will be strained by the dislocation movement. The change in strain will cause the elastic energy of the system to change, so the stress field is doing work on the defect. The work

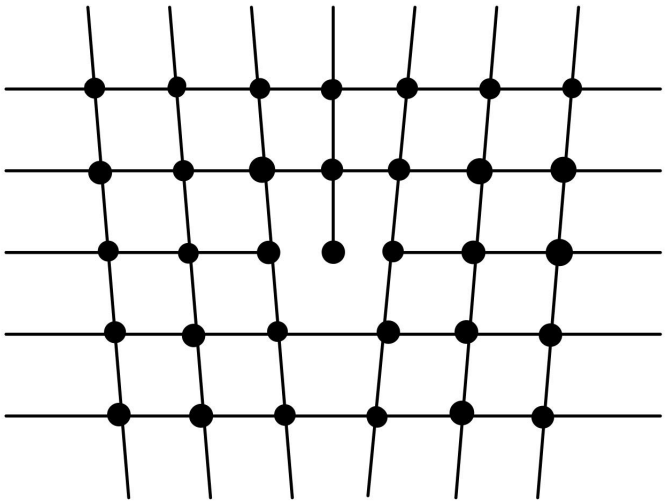

Figure 2.2: A drawing showing the square lattice with a point defect.

is given by the integral

$$\int \sigma_{ik} \delta e_{ik} dV. \tag{2.13}$$

From this, it can be shown [4] that the effective force doing work on the dislocation is given by

$$F_i = \epsilon_{ilm} t_l \sigma_{mk} b_k \tag{2.14}$$

where t_l is the tangent vector to the dislocation line, σ_{mk} is the stress tensor and b_k is the Burgers vector of the dislocation. In the case of a two-dimensional system, the tangent vector in the z-direction contracts the l index of the Levi-Civita tensor, such that the Peach-Koehler force reduces to

$$F_i = \epsilon_{im} \sigma_{mk} b_k \tag{2.15}$$

This force determines the overdamped motion of the dislocation where the dislocation velocity is proportional with **F**

$$v_i = M F_i \tag{2.16}$$

where M is the dislocation mobility.

2.4 Order parameters

In condensed matter physics, the systems we study have too many components that it's inconvenient or unfeasible to track the state of every particle in the system. Even if we could track every particle, the microstate of the system does not necessarily tell us what we are interested in knowing, which are often emergent, macroscopic features of the system. A significant problem to solve when studying emergent physical systems is to determine the system's interesting features. We call this property of the system an order

parameter. For instance, when studying magnets, we care about the local magnetization of the material. In contrast, we usually care about how deformed the crystal is when we study crystals, i.e., the deformation field.

In this thesis, the most critical order parameter will be a dimensionless density field ψ that is used to describe to describe crystal lattices, which will be introduced in the next chapter. What the real space is and what the order parameter space is depends on the system at hand. For an n-dimensional material, the real space will typically be $\mathbb{R}^n$. For example, suppose the system is a magnet. In that case, the system at hand might have an order parameter space $\mathbb{S}^2$ because the spins generating the magnetic field are typically considered to have unit length.

2.5 Symmetry and topology

In this section, we will introduce the idea of the fundamental group of a space as a way to characterize defects. This is done through the xy-model. The xy model consists of a lattice with spins at each lattice site.The spin vector $\mathbf{s}$ given by

$$\mathbf{s} = s(\sin(\theta(\mathbf{x})), \cos(\theta(\mathbf{x}))) \tag{2.17}$$

where s is the magnitude of the spin, θ is the spatial orientation of the spin, and $\mathbf{x}$ is the position inside the lattice, which describes the direction of the spin at the site. Furthermore there is an interaction Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j \tag{2.18}$$

where J is a constant characterizing the strength of the interaction. We will only consider the two-dimensional case. Then the lattice is two-dimensional and the spins can point in any direction in the plane. The angle of the spins θ is the order parameter of the system. Clearly, $\mathbf{s}(\mathbf{x})$ is a continuous function since both sine and cosine are continuous functions. However, if we require $\theta(\mathbf{x})$ to be single-valued then it is not a continuous function, as it makes a discontinuous jump of $-2\pi n$, $\forall n \in \mathbb{N}$ whenever it crosses the positive x-axis going counterclockwise. Furthermore, $\nabla\theta = \frac{1}{r}$ is not well defined at $r = 0$. The singularity at the origin can be removed by removing the point from the space, such that we operate with $\mathbb{R}^2 - \{0\}$ as the domain instead of $\mathbb{R}^2$, or we can require the spin to go to zero within some radius of the origin such that the gradient of the angle is not well defined because the spin value is zero. The point in the space where the angle is not well defined is what we call a topological defect, so-called because it is a defect in the spin direction that cannot be made to disappear by any continuous transformation of the function θ. In two dimensions, this visually means that if you have two spin configurations and cannot deform one configuration into the other by gradually changing the direction of the spins, then the systems are topologically distinct. Some spins might have to be changed discontinuously in order to deform one system into the other. Because such discrete flips require large discontinuous jumps in the systems' free

energy they are unlikely to happen. Hence states of matter with topological defects are often semi-stable as they minimize the free energy locally. We can define an integral in the parameter space

$$I = \oint_L \theta(\mathbf{x}) dx. \tag{2.19}$$

where L is some close curved. Each time the line encloses the origin, the integral will pick up an additional $\pm 2\pi n$. We call n the winding number of the defect, or the topological charge of the defect.

We can generalize the above discussion by introducing the notion of an order parameter space $\mathbb{M}$, a coordinate space domain $\mathbb{D}$, and a map

$$f : \mathbb{D} \to \mathbb{M}. \tag{2.20}$$

In the xy-model, the coordinate space is $\mathbb{R}^2$, and the order parameter space is $\mathbb{S}^1$. The spin configuration determines the map f. Paths in $\mathbb{D}$ can then be mapped into $\mathbb{M}$, which will give rise to paths in $\mathbb{M}$. Say we have two paths in $\mathbb{M}$, f_1 and f_2. If there exists a continuous function

$$H(x,t) : \mathbb{M} \times I \to \mathbb{M} \tag{2.21}$$

such that $H(x,0) = f_1(x)$ and $H(x,1) = f_2(x)$ $\forall x \in \mathbb{M}$ we say that $H(x,t)$ is a homotopy and that f_1 and f_2 are homotopic paths. The function H corresponds to the intuitive idea of continuously deforming one state into another. We can define an equivalence relation of paths by saying that $f_1 \sim f_2$ if they are homotopic. We denote the equivalence class of f by $[f]$. Furthermore, it is possible to define a product of paths $h = f * g$ by the equation

$$h = \begin{cases} f(2s) & \text{for s} \in [0, \frac{1}{2}] \\ g(2s-1) & \text{for s} \in [\frac{1}{2}, 1] \end{cases}. \tag{2.22}$$

This product of paths also induces a product of equivalence classes of paths

$$[f] * [g] = [f * g]. \tag{2.23}$$

Note that the product between two paths f and g is only well defined if $f(1) = g(0)$. The point $f(0) = x_0$ is called the base point of the path f. The set of equilva loops with base point x_0 equipped with the binary operation $*$ is called the fundamental group of the space $\mathbb{M}$ and is denoted $\pi_1(\mathbb{M}, x_0)$. For $\mathbb{M} = \mathbb{S}^1$, the fundamental group is $\pi_1(\mathbb{S}^1, x_0) = \mathbb{Z}$, which makes sense in light of the earlier discussion of the xy-model where we found that taking the integral along a loop that encompassed a defect will give us some integer multiple of 2π. These concepts will be relevant in the next chapter when studying crystals with defects. The dislocations introduced earlier are topological defects and the Burgers vector will give us the topological charge of the defects.

Chapter 3

Phase Field Modelling of Crystals

This section will introduce a phase field crystal density representing the underlying crystal lattice. The equation of motion that governs the time evolution of the field will be presented together with its free energy. We will relate dislocations with topological defects in the phase field and derive expressions for the stress in terms of distortions in the phase field. The discussion will be as general as possible. Still, where it is necessary to introduce a specific phase field crystal model to illustrate some part of the theory, we will use that corresponding to the hexagonal lattice. In particular, we will consider hexagonal lattices to present the general formalism that allows us to identify the dislocations as topological singularities in the lattice and track their motion [10].

3.1 The Phase Field

In phase field modeling, the crystal is represented by a dimensionless density field ψ [2]. The field ψ is an order parameter of the crystal lattice's underlying rotational and broken translational symmetries. At equilibrium, this phase field is a minimizer of an appropriate free energy

$$F = \int_{\Omega} d^2 r f \tag{3.1}$$

where f is the free energy density of the system and Ω is some volume. The form of F is constructed to favor the geometry of the field's underlying lattice at equilibrium. When the lattice is out of equilibrium, it follows a diffusive relation to equilibrium by obeying the equation of motion

$$\partial_t \psi = \nabla^2 \mu \tag{3.2}$$

where

$$\mu = \frac{\delta F}{\delta \psi} \tag{3.3}$$

is the chemical potential of the phase field. The periodicity of the ψ field is determined by the geometry of the crystal the field is modeling. In its equilibrium state, we can

expand the phase field as a Fourier series

$$\psi(\mathbf{r}) = \psi_0 + \sum_{n=1}^{N} \eta_n e^{i\mathbf{r}\cdot\mathbf{q}^{(n)}} \tag{3.4}$$

where $\mathbf{q}^{(n)}$ is the reciprocal lattice vectors and η_n are the mode amplitudes that are constant for a perfect lattice.

We will now discuss what happens to the phase field and its mode amplitudes when the lattice is distorted. Consider two neighboring atoms on the crystal lattice. If the distortion field is such that the distance between them has changed, you have to move a distance $\mathbf{u}(\mathbf{r})$ extra to make up for the distortion. Hence the exponents in the Fourier expansion become

$$\psi(\mathbf{r}) = \psi_0 + \sum_{n=1}^{N} \eta_n e^{i(\mathbf{r}-\mathbf{u})\cdot\mathbf{q}^{(n)}}. \tag{3.5}$$

Writing the amplitudes as complex fields $\eta_n = \rho_n e^{i\theta_0^{(n)}}$ we can absorb the additional $-i\mathbf{u}\cdot\mathbf{q}^{(n)}$ into the argument of the amplitude so that

$$\theta_n = -\mathbf{u}\cdot\mathbf{q}^{(n)}. \tag{3.6}$$

The expression for the phase field becomes

$$\psi(\mathbf{r}) = \psi_0 + \sum_{n=1}^{N} \eta_n(\mathbf{r}) e^{i\mathbf{r}\cdot\mathbf{q}^{(n)}} \tag{3.7}$$

where the amplitude now has become a complex field, and the amplitude phase contains information about the deformation field of the lattice.

3.1.1 Deformation Field of the Hexagonal Lattice

A concrete set of reciprocal lattice vectors is needed to obtain an explicit expression for the deformation field of a crystal from a phase field description. The simplest geometry to work with is the hexagonal lattice. The phase field of the hexagonal lattice is well approximated by the one-mode Fourier expansion [10] and can therefore be written

$$\psi(\mathbf{r}) = \psi_0 + \sum_{n=1}^{N} \eta_n e^{i(\mathbf{r}-\mathbf{u})\cdot\mathbf{q}^{(n)}} \tag{3.8}$$

where $\mathbf{q}^{(n)}$'s are now the reciprocal lattice vectors of the hexagonal lattice. Multiplying both sides of Eq. 3.6 with the reciprocal lattice vector q_j^n and summing over n gives us the equation

$$\sum_{n=1}^{N} \theta_n q_j^{(n)} = -\sum_{n=1}^{N} q_j^{(n)} q_i^{(n)} u_i(\mathbf{r}). \tag{3.9}$$

Using the dyadic product identity [9]

$$\sum_{n=1}^{N} q_i^{(n)} q_j^{(n)} = \frac{N q_0^2}{2} \delta_{ij} \tag{3.10}$$

which holds for the hexagonal lattice, we can solve for the displacement field

$$\mathbf{u}(\mathbf{r}) = -\frac{2}{N q_0^2} \sum_{n=1}^{N} \mathbf{q}^{(n)} \theta_n(\mathbf{r}) \tag{3.11}$$

where $q_0 = \sqrt{\mathbf{q}^2}$. This expression allows us to relate the mechanical deformation of the crystal lattice with phase deformations of the discrete Fourier modes of the ψ-field.

3.2 Dislocations in a Crystal Density Field

In this section, we will consider how dislocations are represented in the phase field description of crystals and how we can study their dynamics. As in continuum mechanics, defects are characterized by a Burgers vector $\mathbf{b}$ which is determined by an integral around the dislocation point

$$\mathbf{b} = \int_L d\mathbf{u} = \mathbf{u}^+ - \mathbf{u}^-,$$

where L is some curve in the plane enclosing the dislocation and $\mathbf{u}^+$ and $\mathbf{u}^-$ are the values of the deformation field at each side of the branch cut. The dislocation density vector $\boldsymbol{\alpha}$ for a single dislocation is defined as

$$\boldsymbol{\alpha} = \boldsymbol{b}\, \delta(\boldsymbol{r} - \boldsymbol{r}') \tag{3.12}$$

where $\mathbf{r}'$ is the position of a dislocation. Using Eq. 3.6 we can relate the Burgers vector to the phase of the amplitude

$$\oint_L \theta_n = -\oint_L \mathbf{q}^{(n)} \cdot d\mathbf{u}. \tag{3.13}$$

The reciprocal vectors $\mathbf{q}^{(n)}$ are constant and can be pulled out of the integral, leaving only an integral over $d\mathbf{u}$, which we know is just the Burgers vector. The integral over the phase will be an integer multiple of 2π signaling the presence of a vortex in the complex amplitude η_n. Hence the equation

$$2\pi s_n = \mathbf{q}^{(n)} \cdot \mathbf{b}. \tag{3.14}$$

Inspired by this equation we define a vortex charge density associated to a given periodic mode with amplitude η_n,

$$\rho_n = s_n \delta(\mathbf{r} - \mathbf{r}'). \tag{3.15}$$

Next, we show that the superposition of these vortices in the Fourier amplitudes provides a complete description of dislocations and their motion in the periodic crystal lattice.

3.2.1 Dynamics of dislocations

To find the time evolution of the defect, we differentiate Eq. 3.12 with respect to time, thus

$$\partial_t \alpha_i = b_i \partial_t \delta(\mathbf{r} - \mathbf{r}'(t)). \tag{3.16}$$

Using the chain rule, we express the right-hand side as

$$= b_i \frac{dr'_k}{dt} \frac{\partial}{\partial r'_k} \delta(\mathbf{r} - \mathbf{r}'). \tag{3.17}$$

We define the dislocation velocity as

$$V_{k'} = \frac{dr'_k}{dt}. \tag{3.18}$$

Furthermore

$$\frac{\partial}{\partial r_{k'}} \delta(\boldsymbol{r} - \boldsymbol{r}') = -\frac{\partial}{\partial r_k} \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{3.19}$$

Hence we can write

$$\begin{aligned} -b_i V_{k'} \frac{\partial}{\partial r_k} \delta(\mathbf{r} - \mathbf{r}') &= -\partial_k(\alpha_i V_k) \\ &= -\partial_k(\alpha_i \delta_{kl} V_l) \\ &= -\epsilon_{kp} \partial_k(\alpha_i \epsilon_{lp} V_l) \\ &= -\epsilon_{kp} \partial_k \mathcal{J}^{(\alpha)}_{ip}, \end{aligned} \tag{3.20}$$

where we have used the identity $\delta_{kl} = \epsilon_{kp}\epsilon_{lp}$ and defined the topological current

$$\mathcal{J}^{\alpha}_{ip} = \epsilon_{lp} \alpha_i V_l. \tag{3.21}$$

From this calculation, we then deduce that the dislocation density follows a conservation law, namely

$$\partial_t \alpha_i + \epsilon_{kp} \partial_k \mathcal{J}^{(\alpha)}_{ip} = 0. \tag{3.22}$$

The next step is to find an explicit expression for the dislocation density vector, compute the corresponding current for this representation of the vector and equate the two expressions. To do this we need to consider a specific system, so we turn to the hexagonal lattice.

Dynamics of Defects in the Hexagonal Lattice

The complex amplitude field $\eta_n(\mathbf{r})$ is isomorphic to the real two-dimensional vector field

$$\boldsymbol{\Psi}(\mathbf{r}) = (\Psi_1(\mathbf{r}), \Psi_2(\mathbf{r})) = (\Re(\eta_n(\mathbf{r})), \Im(\eta_n(\mathbf{r}))). \tag{3.23}$$

The field $\mathbf{\Psi}$ is zero whenever η is zero and we know η_n is zero at the point of the defect. Hence we can express the dislocation density in terms of the field $\mathbf{\Psi}$ by a change of variables

$$s_n \delta^{(2)}(\vec{r} - \vec{r}') = s_n |D(\mathbf{r})| \delta^{(2)}(\mathbf{\Psi}(\mathbf{r})) \tag{3.24}$$

where $D(\mathbf{r}) = \epsilon_{ij}(\partial_i \Psi_1(\mathbf{r}))(\partial_j \Psi_2(\mathbf{r}))$ is the determinant field. Because s_n will be -1 in the case of a negatively charged defect and $+1$ in the case of a positively charged defect, and the determinant differs by a sign difference for these two cases, the determinant can absorb s_n if we remove the absolute value and obtain

$$s_n \delta^{(2)}(\mathbf{r} - \mathbf{r}') = D(\mathbf{r}) \delta^{(2)}(\mathbf{\Psi}(\mathbf{r})). \tag{3.25}$$

Contracting both sides of Eq. 3.12 by $q_i^{(n)}$ gives

$$\frac{1}{2\pi} \alpha_i q_i^{(n)} = s_n \delta^{(2)}(\mathbf{r} - \mathbf{r}'). \tag{3.26}$$

Using Eq. 3.25, we get the equation

$$\frac{1}{2\pi} \alpha_i q_i^{(n)} = D^{(n)} \delta^{(2)}(\mathbf{\Psi}). \tag{3.27}$$

Because η_n and $\mathbf{\Psi}$ is zero at the same points in space we can express this in terms of the complex field η_n instead

$$\frac{1}{2\pi} \alpha_i q_i^{(n)} = D^{(n)} \delta(\eta_n) \tag{3.28}$$

where $D^{(n)} = \epsilon_{ij}(\partial_i \Re(\eta_n))(\partial_j \Im(\eta_n))$ and $\delta(\eta_n) = \delta(\Re(\eta))\delta(\Im(\eta))$. Multiplying both sides of the equation above by $q_j^{(n)}$ and summing over n, and using the diadic product we used earlier, we find a general expression that relates the dislocation density with a superposition of vortices in the complex amplitudes represented as zeros of the amplitudes

$$\frac{1}{2\pi} \frac{N}{2} q_0^2 \alpha_j = \sum_{n=1}^{N} q_j^{(n)} D^{(n)} \delta^{(2)}(\eta_n). \tag{3.29}$$

Solving for α_j we find a new expression for the dislocation density vector

$$\alpha_j = \frac{4\pi}{N q_0^2} \sum_{n=1}^{N} q_j^{(n)} D^{(n)} \delta^{(2)}(\eta_n). \tag{3.30}$$

Taking the time derivative of Eq. (3.30), we obtain

$$\partial_t \alpha_i = \frac{4\pi}{N q_0^2} \sum_{n=1}^{N} q_i^{(n)} (\partial_t D^{(n)}) \delta^{(2)}(\eta_n) + \frac{4\pi}{N q_0^2} \sum_{n=1}^{N} q_i^{(n)} D^{(n)} \partial_t (\delta^{(2)}(\eta_n)). \tag{3.31}$$

We need to evaluate $\partial_t D^{(n)}$ and $\partial_t \delta(\eta_n)$. Starting with the D-field, we do this by finding a current for $D^{(n)}$, i.e. by finding a $J^{(n)}$ such that $\partial_t D + \epsilon_{ij} \partial_j J_l = 0$. We can start by considering the time derivative of the D-field

$$\begin{aligned}
\frac{\partial D^{(n)}}{\partial t} &= \frac{\partial}{\partial t}\left(\frac{1}{2i}\epsilon_{ij}(\partial_i\eta_n)(\partial_j\bar{\eta}_n)\right) \\
&= \frac{1}{2i}\epsilon_{ij}\Big(\big(\partial_t\partial_i\eta_n\big)\big(\partial_j\bar{\eta}_n\big) + \big(\partial_i\eta_n\big)\big(\partial_t\partial_j\bar{\eta}_n\big)\Big) \\
&= \frac{1}{2i}\epsilon_{ij}\Big(\big(\partial_t\partial_i\eta_n\big)\big(\partial_j\bar{\eta}_n\big) - \big(\partial_j\eta_n\big)\big(\partial_t\partial_i\bar{\eta}_n\big)\Big) \\
&= \frac{1}{2i}\epsilon_{ij}\Big(\big(\partial_t\partial_i\eta_n\big)\big(\partial_j\bar{\eta}_n\big) - c.c.\Big) \\
&= \epsilon_{ij}\Im\Big((\partial_t\partial_i\eta_n)(\partial_j\bar{\eta}_n)\Big) \\
&= \epsilon_{ij}\partial_i\Im\Big(\big(\partial_t\eta_n\big)\big(\partial_j\bar{\eta}_n\big)\Big) \qquad (3.32)
\end{aligned}$$

where $\Im(...)$ denotes taking the imaginary part of the expression. Hence

$$\partial_t D^{(n)} + \epsilon_{ij}\partial_i J_j^{(n)} = 0 \qquad (3.33)$$

where $J_j = \Im\big((\partial_t\eta_n)(\partial_j\eta_n)\big)$. Next we have to evaluate $D^{(n)}\partial_t\delta(\eta_n))$. The details of this calculation can be found in appendix A and gives us

$$D^{(n)}\partial_t\delta(\eta_n) = -\epsilon_{kl}\partial_k J_l^{(n)}\delta(\eta_n). \qquad (3.34)$$

Putting this together we get an equation of motion of the dislocation density in terms of vortex current densities in the amplitudes

$$\partial_t\alpha_i = \frac{4\pi}{Nq_0^2}\sum_{n=1}^{N} q_i^{(n)}(-\epsilon_{kl}\partial_k J_l^{(n)})\delta^{(2)}(\eta_n) + \frac{4\pi}{Nq_0^2}\sum_{n=1}^{N} q_i^{(n)}(-\epsilon_{kl}J_l^{(n)})\partial_k\delta^{(2)}(\eta_n) \qquad (3.35)$$

so

$$\partial_t\alpha_i = -\epsilon_{kl}\partial_k\left(\frac{4\pi}{Nq_0^2}\sum_{n=1}^{N} q_i^{(n)}J_l^{(n)}\delta^{(2)}(\eta_n)\right) = -\epsilon_{kl}\partial_k\mathcal{J}_{il} \qquad (3.36)$$

where we have defined the singular dislocation density current as a superposition of the singular vortex density currents

$$\mathcal{J}_{il} = \frac{4\pi}{Nq_0^2}\sum_{n=1}^{N} q_i^{(n)}J_l^{(n)}\delta^{(2)}(\eta_n). \qquad (3.37)$$

We now equate the expressions for $\mathcal{J}_{il}^{(\alpha)}$ and $\mathcal{J}_{il}$. Note that we have not shown that these two expressions are necessarily equal, we have only shown that their derivatives are. Therefore there could be some surface term that must be added to achieve equality. In this thesis, we will assume that any such surface term is zero. This gives

$$\frac{4\pi}{Nq_0^2}\sum_{n=1}^{N} q_i^{(n)}J_l^{(n)}\delta^{(2)}(\eta_n) = \epsilon_{pl}\alpha_i V_p. \qquad (3.38)$$

In order to proceed we an explicit expression for $\delta(\eta_n)$. Using Eq. (3.26), we obtain

$$\frac{2}{Nq_0^2}\sum_{n=1}^{N} q_i^{(n)} J_l^{(n)} \frac{\alpha_j q_j^{(n)}}{D^{(n)}} = \epsilon_{pl}\alpha_i V_p. \tag{3.39}$$

At the point of the defect $\alpha_i = b_i\delta^{(2)}(\mathbf{r}-\mathbf{r}')$ so we get

$$\frac{2}{Nq_0^2}\sum_{n=1}^{N} q_i^{(n)} J_l^{(n)} \frac{b_j\delta^{(2)}(\mathbf{r}-\mathbf{r}')q_j^{(n)}}{D^{(n)}} = \epsilon_{pl}b_i\delta^{(2)}(\mathbf{r}-\mathbf{r}')V_p. \tag{3.40}$$

The delta functions can be removed by integrating both sides of the equation over some area containing the defect. Furthermore, we can contract both sides of the equation by the vector b_i. Using Eq. 3.14 twice we then obtain

$$\frac{2}{Nq_0^2}\sum_{n=1}^{N} (2\pi s_n)^2 J_l^{(n)} \frac{1}{D^{(n)}} = b^2\epsilon_{pl}V_p. \tag{3.41}$$

Simplifying we obtain an expression for the dislocation velocity in a hexagonal lattice

$$V_i = \frac{8\pi^2}{Nb^2q_0^2}\epsilon_{li}\sum_{n=1}^{N} s_n^2 \frac{J_l^{(n)}}{D^{(n)}}. \tag{3.42}$$

In the next section, we will derive analytical expressions of the stress field induced by distortions of the ψ field and how that, in the long wavelength limit, we recover the elasticity theory of continuum media.

3.3 Stress in a Phase Field Crystal

We can derive a microscopic stress in a crystal by taking the variational of the free energy as [7, 9]

$$\delta F = -\int_\Omega d^D r \partial_i \tilde{\sigma}_{ij}\delta x_j + \int_{\partial\Omega} \tilde{\sigma}_{ij}\delta x_j \tag{3.43}$$

where Ω is some volume element in the field, $\partial\Omega$ is its surface, δx_j is the variation of some displacement and $\tilde{\sigma}_{ij}$ is the stress tensor of the crystal [9]. If we wish to find the stress of a system we must vary the free energy and write it in the form of Eq. 3.43. The stress tensor $\tilde{\sigma}_{ij}$ can be decomposed in the following way

$$\tilde{\sigma}_{ij} = (f - \mu\psi)\delta_{ij} + \tilde{h}_{ij}. \tag{3.44}$$

Only the latter term in this equation is related to stress caused by deformation. In this thesis we are only interested in studying this kind of stress, and therefore we will henceforth refer to $\tilde{h}_{ij}$ as the microstress of the system. Furthermore it can be shown [9] that the microstress is given by the equation

$$\tilde{h}_{ij} = \sum_{\alpha=1}^{\infty} M_{ij}^{(\alpha)} \tag{3.45}$$

where

$$M_{ij} = \sum_{\beta=1}^{\alpha} (-1)^{\beta} (\partial_{m_1 \ldots m_{\beta-1}} f'_{m_1 \ldots m_{\alpha-1} i}) \partial_{j m_\beta \ldots m_{\alpha-1}} \psi \tag{3.46}$$

and

$$f'_{m_1 \ldots m_\alpha} = N(\{m_i\}_{i=1}^{\alpha}) \frac{\partial f}{\partial(\partial_{m_1 \ldots m_\alpha} \psi)}. \tag{3.47}$$

$N(\{m_i\}_{i=1}^{\alpha})$ here is given by the equation

$$N(\{m_i\}_{i=1}^{\alpha}) = \frac{N_x! N_y! N_z!}{\alpha!} \tag{3.48}$$

where N_x, N_y and N_z are the number of elements in $\{m_i\}_{i=1}^{\alpha}$ that correspond to x, y and z respectively.

3.3.1 Continuum stress: From a crystal lattice to a continuum

The phase field contains information about the microscopic, atomic structure of the lattice. The same holds for any field that is computed directly from the phase field, such as the microstress field we defined above. Often we are not only interested in the microscopic quantities but also in macroscopic quantities can be hard to detect when you have all information about the system at hand. For instance it is often interesting to check the results of the phase field model against classical results from elasticity theory. Elasticity theory is a macroscopic longer wavelength theory than the phase field model. In order to compare the two we must eliminate higher spatial frequencies from the fields computed from the phase field. This is done by coarse graining the fields. Mathematically, this is done by computing the convolution of the field we are considering with a Gaussian distribution. The convolution integral which we use to coarse grain is

$$\langle f(\mathbf{r}) \rangle = \int d^2 r' \frac{f(\mathbf{r}')}{2\pi a_0^2} \exp\left\{ -\frac{(\mathbf{r} - \mathbf{r}')^2}{2a_0^2} \right\} \tag{3.49}$$

where a_0 is the distance between neighboring molecules if the lattice is in its relaxed state and f is whichever field we are coarse graining.

3.3.2 Stress-strain relation of a hexagonal lattice

We can illustrate how to obtain the continuum stress of a crystal by considering the hexagonal lattice. First we need the free energy density, which for the hexagonal lattice is given by, e.g. [2]

$$f = \frac{1}{2}\mathcal{L}_1 \psi^2 + \frac{r}{2}\psi^2 + \frac{1}{4}\psi^4 \tag{3.50}$$

where $\mathcal{L}_1 = (1 + \nabla^2)$. We can now proceed to compute the stress for the hexagonal lattice. Starting with $M_{ij}^{(1)}$ we immediately see that

$$M_{ij}^{(1)} = (-1) f'_i \partial_j \psi = 0 \tag{3.51}$$

because the free energy for the hexagonal lattice does not contain any single derivatives, which gives $f_i' = 0$. Continuing we have

$$M_{ij}^{(2)} = (-1)f'_{m_1 i}\partial_{m_1 j}\psi + (-1)^2(\partial_{m_1}f'_{m_1 i})\partial_j\psi). \tag{3.52}$$

which requires us to evaluate

$$f'_{m_1 i} = \frac{1}{2}\frac{\partial}{\partial(\partial_{m_1 i}\psi)}(\mathcal{L}_1\psi)^2. \tag{3.53}$$

Using the chain rule and the identity

$$\frac{\partial(\partial_{kk}\psi)}{\partial(\partial_{m_1 i}\psi)} = \delta_{m_1 i} \tag{3.54}$$

we get

$$f'_{m_1 i} = \mathcal{L}_1\psi\delta_{m_1 i}. \tag{3.55}$$

Hence

$$\tilde{h}_{ij} = -\mathcal{L}_1\psi\partial_{ij}\psi + \partial_i(\mathcal{L}_1\psi)\partial_j\psi \tag{3.56}$$

Using the chain rule we find that

$$\tilde{h}_{ij} = -2\mathcal{L}_1\psi\partial_{ij}\psi + \partial_i(\mathcal{L}_1\psi\partial_j\psi). \tag{3.57}$$

The coarse-grained stress is straightforward to compute from this expression. It can be shown [9] that surface terms disappear under coarse graining. Hence we are left with the coarse-grained stress of the hexagonal lattice, given by

$$h_{ij} = -2\langle(\mathcal{L}_1\psi)\partial_i\partial_j\psi\rangle. \tag{3.58}$$

For small lattice distortions, we can show that this expression reduces to the stress-strain relation from linear elasticity. Inserting the one-mode Fourier expansion for ψ into this expression we obtain

$$h_{ij} = 4A^2\partial_k u_l \sum q_{ni}q_{nj}q_{nk}q_{nl}. \tag{3.59}$$

The sum can be rewritten [9]

$$\sum q_i^{(n)}q_j^{(n)}q_k^{(n)}q_l^{(n)} = \frac{3}{4}(\delta_{ij}\delta_{kl} + 2\delta_{ki}\delta_{jl} + 2\delta_{kj}\delta_{il}). \tag{3.60}$$

Inserting this into the equation for the stress we obtain

$$h_{ij} = 3A^2(\delta_{ij}\delta_{kl} + 2\delta_{ki}\delta_{jl} + 2\delta_{kj}\delta_{il})\partial_k u_l \tag{3.61}$$

which is the stress-strain relationship for an isotropic medium. Hence, the underlying hexagonal lattice has an isotropic elastic response in the continuum limit determined by two elastic constants, i.e. the bulk and shear moduli. Furthermore, from the above expression, we see that the elastic constants are determined by the equilibrium lattice properties, in this case the equilibrium amplitude A.

Chapter 4

Results on dislocations in square lattices

In Refs. [7, 8], it was shown that for the 2D hexagonal lattice and the 3D bcc lattice, respectively, the dislocations are driven by the Peach-Koehler force, with an explicit expression for the mobility. In this chapter, we will see what happens when these calculations are generalized for the 2D square lattice. We first need to derive an expression for the dislocation velocity in a square lattice, which requires explicit expressions for the deformation field and the dislocation density vector. In order to evaluate the dislocation velocity in the long wavelength approximation analytically, an expression for the time evolution of amplitudes is needed. This can be obtained by demodulating the equation of motion of the phase field. In order to connect the dislocation velocity to the stress tensor we will also need to compute the stress of the square lattice. Where the derivation of the results for the square lattice is similar to the hexagonal lattice we will make use of the derivations in the previous chapter and only highlight the differences. For the square lattice, the phase field is well approximated by the one-mode Fourier expansion[9]

$$\Psi(\mathbf{r}) = \Psi_0 + \sum_{\mathbf{p}^{(n)}} A_n e^{i\mathbf{r}\cdot\mathbf{p}^{(n)}} + \sum_{\mathbf{k}^{(n)}} B_n e^{i\mathbf{r}\cdot\mathbf{k}^{(n)}} \tag{4.1}$$

where $\mathbf{p^{(n)}}$ denotes the first harmonics of lowest unit length $|\mathbf{p}_0| = p_0 = 1$ and $\mathbf{k^{(n)}}$ denotes the second harmonics of lowest length $|\mathbf{k}_0| = k_0 = \sqrt{2}$. We will adopt the notation of using A_n and $\mathbf{p}^{(n)}$ to refer to amplitudes and reciprocal lattice vectors associated with the first harmonic, B_n and $\mathbf{k}^{(n)}$ to refer to amplitudes and reciprocal lattice vectors associated with the second harmonic and η_n and $\mathbf{q}^{(n)}$ when referring to an arbitrary amplitude and arbitrary reciprocal lattice vector.

4.1 Deformation Field for the Square Lattice

We start by deriving the deformation field of the square lattice. This derivation is identical to that of the hexagonal lattice up until equation 3.9. From this point, the

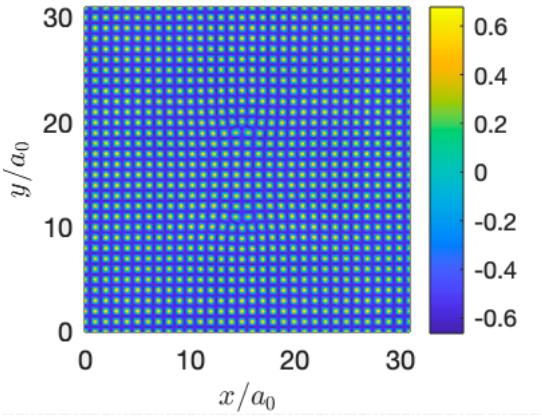

Figure 4.1: Snapshot of a phase field representing a square lattice with two dislocations in different slip planes.

derivation is similar, but not completely identical. We still multiply by q_j, except now q_j can now be equal to either p_j or k_j. Hence greater care must be taken when making use of the dyadic product identity. Because we have two different modes $\mathbf{p}^{(n)}$ and $\mathbf{k}^{(n)}$ we must separate the two kinds of vector because we can make use of the identity. Hence the analogy of equation 3.9 for the relation between amplitude phases and lattice deformation for the square lattice is

$$\sum_{n=1}^{N/2} \theta_n p_j^{(n)} + \sum_{n=1}^{N/2} \theta_{n+N/2} k_j^{(n)} = -\sum_{n=1}^{N/2} p_i^{(n)} p_j^{(n)} u_i - \sum_{n=1}^{N/2} k_i^{(n)} k_j^{(n)} u_i. \tag{4.2}$$

The dyadic product identity can be applied to both the terms on the right-hand side of the equation separately. This gives the equation

$$\sum_{n=1}^{N/2} \theta_n p_j^{(n)} + \sum_{n=1}^{N/2} \theta_{n+N/2} k_j^{(n)} = -\frac{N}{4}(p_0^2 + k_0^2)\delta_{ij} u_i \tag{4.3}$$

which can be solved the deformation field

$$u_j(\mathbf{r}) = -\frac{4}{N(p_0^2 + k_0^2)} \sum_{n=1}^{N} \theta_n q_j^{(n)}. \tag{4.4}$$

4.2 Dislocations in the Square Lattice

In this section, we will derive the dislocation density vector for the square lattice. We will then derive the dislocation velocity for a defect in a square lattice, in a similar way to what was done for the hexagonal lattice in Chapter 3. A plot of the phase field of a square lattice with two dislocations located in different slip planes is shown in figure 4.1.

4.2.1 The Dislocation Density Vector and its Dynamics

The derivation of the dislocation velocity is the same as for any lattice up until equation 3.28. From this point the strategy for the square lattice is similar to what was done for the hexagonal lattice, except for the square lattice we have to distinguish between the two sets of reciprocal lattice vectors of different length. Thus, when we multiply by $q_j^{(n)}$ and sum over n such as

$$\frac{1}{2\pi}\alpha_i \sum_{n=1}^{N} q_i^{(n)} q_j^{(n)} = \sum_{n=1}^{N} D^{(n)} q_j^{(n)}, \tag{4.5}$$

we split the sum on the left hand side into two sums and get

$$\frac{1}{2\pi}\alpha_i \left(\sum_{n=1}^{N/2} p_i^{(n)} p_j^{(n)} + \sum_{n=1}^{N/2} k_i^{(n)} k_j^{(n)} \right) = \sum_{n=1}^{N} D^{(n)} q_j^{(n)}. \tag{4.6}$$

Again we apply the dyadic product identity to each of the terms on the left-hand side and solve for α_j to obtain

$$\alpha_j = \frac{4}{N(p_0^2 + k_0^2)} \sum_{n=1}^{N} D^{(n)} q_j^{(n)}. \tag{4.7}$$

From this point the derivation of the defect velocity in a square lattice is algebraically identical to that of the hexagonal lattice, the only difference being the prefactor in front of the sum in the expression for α_j. Hence we can immediately conclude that

$$\partial_t \alpha_i = -\epsilon_{kl}\partial_k \left(\frac{8\pi}{N(p_0^2 + k_0^2)} \sum_{n=1}^{N} q_i^{(n)} J_l^{(n)} \delta^{(2)}(\eta_n) \right) = -\epsilon_{kl}\mathcal{J}_{il} \tag{4.8}$$

where

$$\mathcal{J}_{il} = \frac{8\pi}{N(p_0^2 + k_0^2)} \sum_{n=1}^{N} q_i^{(n)} J_l^{(n)} \delta^{(2)}(\eta_n). \tag{4.9}$$

The topological current $\mathcal{J}_{il}^{\alpha}$ is the same for any lattice. Proceeding in the same way as for the hexagonal lattice, we find that the dislocation velocity in the square lattice is given by

$$V_i = \frac{16\pi^2}{Nb^2(p_0^2 + k_0^2)} \epsilon_{li} \sum_{n=1}^{N} \frac{J_l^{(n)}}{D^{(n)}}. \tag{4.10}$$

To obtain a closed expression for the dislocation velocity we need to evaluate the vortex density currents from the evolution of the amplitudes.

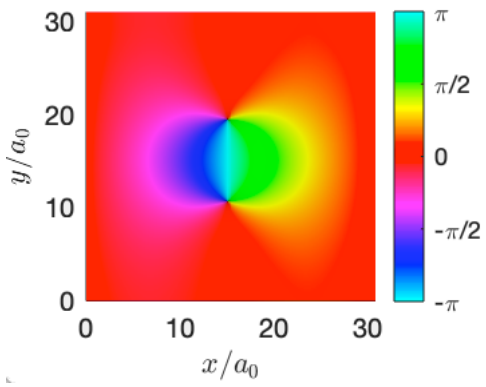

Figure 4.2: A snapshot of the argument of A_1 corresponding to a configuration with two dislocations with opposite Burgers vectors.

4.3 Evolution of Amplitudes Near Defects

In the previous section, we found an expression for the defect velocity in a square lattice. The expression is made up of two quantities we must determine, $J_l^{(n)}$ and $D^{(n)}$. The determinant is straightforward to evaluate if we have an expression for the amplitudes. However, in $J_l^{(n)}$ there is a time derivative of the amplitudes that we have not yet seen how to determine. Hence we now turn to the question of the time evolution of amplitudes close to defects. We will then consider an explicit expression for the amplitude and compute the time evolution for such amplitudes. A snapshot of an amplitude field is shown in figure 4.2.

4.3.1 Generic amplitude evolution: near defect core approximation

We start by considering the time evolution of the phase field. The equation of motion is given by Eq. 3.2. First, we determine the chemical potential of the square lattice. We start from the free energy of the square lattice given by [9]

$$F = \int_\Omega d^2\mathbf{r}\left(\frac{1}{2}(\mathcal{L}_1\mathcal{L}_2\psi)^2 + \frac{1}{2}r\psi^2 + \frac{1}{4}\psi^4\right). \tag{4.11}$$

where $\mathcal{L}_X = (X + \nabla^2)$. By a variational of this free energy with respect to the ψ field, we obtain

$$\delta F = \int_\Omega d^2\mathbf{r}\left(\mathcal{L}_1\mathcal{L}_2\psi\delta(\mathcal{L}_1\mathcal{L}_2\psi) + r\psi\delta\psi + \psi^3\delta\psi\right). \tag{4.12}$$

Differential operators commute with the variation so this can be rewritten

$$= \int_\Omega d^2\mathbf{r}\left(\mathcal{L}_1\mathcal{L}_2\psi\mathcal{L}_1\mathcal{L}_2\delta\psi + (r\psi + \psi^3)\delta\psi\right). \tag{4.13}$$

The variation in ψ can be isolated through integration by parts

$$= \int_\Omega d^2\mathbf{r}(\mathcal{L}_1^2\mathcal{L}_2^2\psi + r\psi + \psi^3)\delta\psi \tag{4.14}$$

such that the chemical potential as the conjugate of the ψ field is given by

$$\frac{\delta F}{\delta \psi} = \mathcal{L}_1^2\mathcal{L}_2^2\psi + r\psi + \psi^3 \tag{4.15}$$

and determines the diffusive evolution of the ψ field

$$\partial_t\psi = \nabla^2\left[\mathcal{L}_1^2\mathcal{L}_2^2\psi + r\psi + \psi^3\right] \tag{4.16}$$

which encodes the evolution of the distortions in the square lattice including the dynamics of dislocations. However, we are interested in finding the time evolution of the amplitudes rather than of the entire phase field. It is straight forward to isolate the amplitudes by demodulation using the method reviewed in Ref. [6]. We start by considering the left-hand side of Eq. 4.16

$$\int_{u.c.} \frac{d\mathbf{r}}{V}\left(\frac{\partial}{\partial t}\psi\right)e^{-i\mathbf{q}^{(n)}\cdot\mathbf{r}} \tag{4.17}$$

where $u.c.$ denotes a unit cell and V is its volume. Because there is no time dependence in the exponential we can move the time derivative out in front of the integral and obtain

$$\frac{\partial}{\partial t}\int_{u.c.}\frac{d\mathbf{r}}{V}\left[\left(\psi_0 + \sum_m \eta_m e^{i\mathbf{q}^{(m)}\cdot\mathbf{r}}\right)e^{-i\mathbf{q}^{(n)}\cdot\mathbf{r}}\right] = \frac{\partial\eta_n}{\partial t}. \tag{4.18}$$

Next, we turn to the right-hand side of the diffusion equation. By successive integration by parts, we can move the Laplace operator onto the Fourier mode, such as

$$\begin{aligned}\partial_t\eta_n &= \int_{u.c.}\frac{d\mathbf{r}}{V}e^{-i\mathbf{q}^{(n)}\cdot\mathbf{r}}\nabla^2\left[\mathcal{L}_1^2\mathcal{L}_2^2\psi + r\psi + \psi^3\right] \\ &= -q_0^2\int_{u.c.}\frac{d\mathbf{r}}{V}e^{-i\mathbf{q}^{(n)}\cdot\mathbf{r}}\left[\mathcal{L}_1^2\mathcal{L}_2^2\psi + r\psi + \psi^3\right].\end{aligned} \tag{4.19}$$

We are interested in the evolution of the η_n amplitude near the defect core. We start by demodulating the linear $r\psi$ term

$$\int_{u.c.}\frac{d\mathbf{r}}{V}r\psi e^{-i\mathbf{q}^{(n)}\cdot\mathbf{r}} \tag{4.20}$$

$$= r\int_{u.c.}\frac{d\mathbf{r}}{V}[\psi_0 + \sum_m \eta_m e^{i\mathbf{q}^{(m)}\cdot\mathbf{r}}]e^{-i\mathbf{q}^{(n)}\cdot\mathbf{r}} = r\eta_n. \tag{4.21}$$

Because η_n goes to zero at the point of the defect we then know that the contribution to the time evolution is zero. Next we turn to the ψ^3 term. In order to simplify the algebra we start by rewriting the Fourier expansion slightly

$$\sum_n \eta_n e^{i\mathbf{q}^{(n)}\cdot\mathbf{r}} \tag{4.22}$$

where we have defined $\eta_0 = \psi_0$ and $\mathbf{q}^{(0)} = 0$. Demodulating the ψ^3 term gives us

$$\int_{u.c.} \frac{d\mathbf{r}}{V} \sum_{mlo} \eta_m \eta_l \eta_o e^{i\mathbf{q}^{(m)}\cdot\mathbf{r}} e^{i\mathbf{q}^{(l)}\cdot\mathbf{r}} e^{i\mathbf{q}^{(o)}\cdot\mathbf{r}} e^{-i\mathbf{q}^{(n)}\cdot\mathbf{r}}. \tag{4.23}$$

The only terms in the sum that contribute to the integral are those for which

$$\mathbf{q}^{(m)} + \mathbf{q}^{(l)} + \mathbf{q}^{(o)} = \mathbf{q}^{(n)}. \tag{4.24}$$

Dotting both sides with the Burgers vector of the defect $\mathbf{b}$ we obtain

$$s_m + s_l + s_o = s_n. \tag{4.25}$$

Because there is a defect present we know that $s_n \neq 0$. Hence at least one of s_m, s_l or s_o must also be non-zero. But then the amplitude corresponding to this winding number must go to zero, and so every term in the sum that contributes to the integral is zero. Thus, the local (algebraic) part of the free energy density does not contribute to the evolution of the amplitude zeros, aka vortices.

Lastly, we turn to the non-local terms containing differential operators. Because we are looking for an equation of motion for the amplitudes, we would like to rewrite how ∇^2 acts on the ψ field in terms of how a corresponding differential operator $\nabla^2_{\mathbf{q}^{(n)}}$ acts on the η_n amplitude. In other words, we would like to find $\nabla^2_{\mathbf{q}^{(n)}}$ so that

$$\nabla^2\psi = \nabla^2\psi_0 + \nabla^2 \sum_n \eta_n e^{i\mathbf{q}^{(n)}\cdot\mathbf{r}} \equiv \nabla^2\psi_0 + \sum_n e^{i\mathbf{q}^{(n)}\cdot\mathbf{r}} \nabla^2_{\mathbf{q}^{(n)}} \eta_n. \tag{4.26}$$

We find this operator by considering how the Laplace operator acts on the amplitude demodulation

$$\begin{aligned}
\nabla^2\psi &= \nabla^2\psi_0 + \sum_n \nabla^2(\eta_n e^{i\mathbf{q}^{(n)}\cdot\mathbf{r}}) \\
&= \nabla^2\psi_0 + \sum_n \partial_j\partial_j(\eta_n e^{i\mathbf{q}^{(n)}\cdot\mathbf{r}}) \\
&= \nabla^2\psi_0 + \sum_n \partial_j\left[(\partial_j\eta_n)e^{i\mathbf{q}^{(n)}\cdot\mathbf{r}} + \eta_n (p^{(n)})_i(\partial_j r_i)e^{i\mathbf{q}_n\cdot\mathbf{r}}\right] \\
&= \nabla^2\psi_0 + \sum_n e^{i\mathbf{q}^{(n)}\cdot\mathbf{r}}\left[(\partial_j\partial_j\eta_n) + 2(\partial_j\eta_n)i(q^{(n)})_i(\partial_j r_i) - \eta_n q_0^2\right] \\
&= \nabla^2\psi_0 + \sum_n e^{i\mathbf{q}_n\cdot\mathbf{r}}\left[\nabla^2 + 2i\mathbf{q}^{(n)}\cdot\nabla - q_0^2\right]\eta_n \\
&= \nabla^2\psi_0 + \sum_n e^{i\mathbf{q}^{(n)}\cdot\mathbf{r}} \nabla^2_{\mathbf{q}^{(n)}}\eta_n
\end{aligned} \tag{4.27}$$

where $\nabla^2_{\mathbf{q}^{(n)}} = \nabla^2 + 2i\mathbf{q}^{(n)}\cdot\nabla - q_0^2$. We introduce a new differential operator that acts on η_n

$$\mathcal{L}_{\mathbf{q}^{(n)}} = (1 + \nabla^2_{\mathbf{q}^{(n)}})(2 + \nabla^2_{\mathbf{q}^{(n)}}). \tag{4.28}$$

Rewriting $\mathcal{L}^2\psi$ in terms this new operator $\mathcal{L}_{\mathbf{q}^{(n)}}$ acting on amplitudes and demodulating both sides of the equation of motion of the ψ-field, we can deduce the equation of motion for the η_n amplitude as

$$\partial_t \eta_n = -q_0^2 \mathcal{L}^2_{\mathbf{q}^{(n)}} \eta_n. \tag{4.29}$$

This equation is restricted only to the vicinity of a zero of η_n where the additional algebraic terms do not matter. This we call this the evolution of zeros of the amplitudes.

4.3.2 Evolution of Amplitude Zeros due to an External Perturbation

Having found an equation of motion for the amplitudes of the square lattice we now need an expression for the amplitudes themselves. We start by assuming that the amplitudes are linear close to the defect. Then they can be written

$$\eta_n^{(0)} = x + s_n i y = |\mathbf{r}| e^{i s_n \arctan(y/x)}. \tag{4.30}$$

When evaluating the time evolution we must consider the case of $\mathbf{q}^{(n)} = \mathbf{p}^{(n)}$ and $\mathbf{q}^{(n)} = \mathbf{k}^{(n)}$ separately, as they correspond to different equations of motion. We first consider the case $\mathbf{q}^{(n)} = \mathbf{p}^{(n)}$. Then the differential operator is given by

$$\mathcal{L}^2_{\mathbf{p}_n} = (\nabla^2 + 2i\mathbf{p}_n \cdot \nabla)^2 (\nabla^2 + 2i\mathbf{p}_n \cdot \nabla + 1)^2. \tag{4.31}$$

Because

$$\nabla \cdot \nabla (x + isy) = \nabla \cdot (\mathbf{e}_x + is\mathbf{e}_y) = 0 \tag{4.32}$$

any term containing more than two derivatives must be zero. But every term contains more than two derivatives so

$$\mathcal{L}^2_{\mathbf{p}^{(n)}} \eta_n^{(0)} = 0 \tag{4.33}$$

so $\eta_n^{(0)}$ is a stationary solution for the equation of motion corresponding to the first harmonic. For the case $\mathbf{q}^{(n)} = \mathbf{k}^{(n)}$ the differential operator is given by

$$\mathcal{L}^2_{\mathbf{k}^{(n)}} = (\nabla^2 + 2i\mathbf{k}^{(n)} \cdot \nabla - 1)^2 (\nabla^2 + 2i\mathbf{k}^{(n)} \cdot \nabla)^2. \tag{4.34}$$

By the same argument as before any term containing more than two derivatives will vanish when $\mathcal{L}^2_{\mathbf{k}^{(n)}}$ acts on $\eta_n^{(0)}$. But every term contains more than two derivatives so

$$\mathcal{L}^2_{\mathbf{k}^{(n)}} \eta_n^{(0)} = 0 \tag{4.35}$$

as well and $\eta_n^{(0)}$ is a steady state solution for all values of n. Next we perturb the stationary amplitude by some small external deformation field. Mathematically we do this by multiplying the stationary solution with a factor $e^{-i\mathbf{q}^{(n)} \cdot \mathbf{u}}$ where $|\nabla \mathbf{u}| \ll 1$. The amplitude will then be of the form

$$\eta_n = \eta_n^{(0)} e^{-i\mathbf{q}^{(n)} \cdot \mathbf{u}} \tag{4.36}$$

In order to find the time evolution, we must consider how $\mathcal{L}^2_{\mathbf{q}_n}$ acts on amplitudes of this form, i.e.

$$\mathcal{L}^2_{\mathbf{q}^{(n)}}\eta_n = (\nabla^2 + 2i\mathbf{q}^{(n)}\cdot\nabla + (1-q_0^2))^2(\nabla^2 + 2i\mathbf{q}^{(n)}\cdot\nabla + (2-q_0^2))^2\eta_n. \tag{4.37}$$

We define

$$\Gamma = -i\mathbf{q}^{(n)}\cdot\mathbf{u} \tag{4.38}$$

to simplify the algebra. We start by considering three derivatives acting on such an amplitude and use the small-distortion limit and that $\eta_n^{(0)}$ is linear and , thus

$$\begin{aligned}\partial_i\partial_j\partial_k\eta_n &= \partial_i\partial_j\partial_k(\eta_n^{(0)}e^{\Gamma}) \\ &= \partial_i\partial_j\big[(\partial_k\eta_n^{(0)})e^{\Gamma} + \eta_n^{(0)}(\partial_k\Gamma)e^{\Gamma}\big] \\ &= \partial_i\big[(\partial_j\eta_n^{(0)})(\partial_k\Gamma)e^{\Gamma} + (\partial_k\eta_n^{(0)})(\partial_j\Gamma)e^{\Gamma}\big] = 0.\end{aligned} \tag{4.39}$$

We see from the calculation above that any terms in $\mathcal{L}^2_{\mathbf{q}_n}$ containing more than two derivatives will yield zero when acting on η_n and as such they can be neglected. Consider $\mathbf{q}^{(n)} = \mathbf{p}^{(n)}$. Then

$$\mathcal{L}^2_{\mathbf{p}^{(n)}} = (\nabla^2 + 2i\mathbf{p}^{(n)}\cdot\nabla)^2(\nabla^2 + 2i\mathbf{p}^{(n)}\cdot\nabla + 1)^2 \tag{4.40}$$

Neglecting terms with three or more derivatives we are left with

$$\mathcal{L}^2_{\mathbf{p}^{(n)}}A_n = -4(\mathbf{p}^{(n)}\cdot\nabla)^2A_n. \tag{4.41}$$

Writing this out we get

$$\begin{aligned}&-4(\mathbf{p}^{(n)}\cdot\nabla)p_i^{(n)}\partial_i(\eta_n^{(0)}e^{\Gamma}) = -4(\mathbf{p}^{(n)}\cdot\nabla)p_i^{(n)}\big[(\partial_i\eta_n^{(0)})e^{\Gamma} + \eta_n^{(0)}(\partial_i\Gamma)e^{\Gamma}\big] \\ = \;& -4p_j^{(n)}p_i^{(n)}\big[(\partial_i\eta_n^{(0)})(\partial_j\Gamma)e^{\Gamma} + (\partial_j\eta_n^{(0)})(\partial_i\Gamma)e^{\Gamma}\big].\end{aligned} \tag{4.42}$$

Next we consider the case $\mathbf{q}^{(n)} = \mathbf{k}^{(n)}$. Then

$$\mathcal{L}^2_{\mathbf{k}^{(n)}} = (\nabla^2 + 2i\mathbf{k}^{(n)}\cdot\nabla - 1)^2(\nabla^2 + 2i\mathbf{k}^{(n)}\cdot\nabla)^2 \tag{4.43}$$

Like before we can neglect terms containing more than two derivatives when the operator acts on η_n. Then the only term from the expression above that we cannot neglect will be

$$(-1)^2(2i\mathbf{k}^{(n)}\cdot\nabla)^2 = -4(\mathbf{k}^{(n)}\cdot\nabla)^2 \tag{4.44}$$

Hence

$$\mathcal{L}^2_{\mathbf{k}^{(n)}}B_n = -4k_i^{(n)}k_j^{(n)}\partial_i\partial_j(\eta_n^{(0)}e^{\Gamma}) \tag{4.45}$$

$$= -4k_j^{(n)}k_i^{(n)}\big[(\partial_i\eta_n^{(0)})(\partial_j\Gamma)e^{\Gamma} + (\partial_j\eta_n^{(0)})(\partial_i\Gamma)e^{\Gamma}\big] \tag{4.46}$$

which is the same expression as for the case $\mathbf{q}^{(n)} = \mathbf{p}^{(n)}$. Note that contrary to for the steady state solution, this time the time evolution will be different between the two kinds of amplitude. Using the generic evolution of the amplitude zeros from Eq. 4.29 for $\mathbf{q}^{(n)} = \mathbf{p}^{(n)}$ we get

$$\begin{aligned} \partial_t A_n &= 4p_0^2 p_i^{(n)} p_j^{(n)} \left[(\partial_i \eta_n^{(0)})(\partial_j \Gamma) + (\partial_j \eta_n^{(0)})(\partial_i \Gamma) \right] e^{\Gamma} \\ &= 8p_0^2 p_i^{(n)} p_j^{(n)} (\partial_i \eta_n^{(0)})(\partial_j \Gamma) e^{\Gamma} \end{aligned} \tag{4.47}$$

where we used the expression is symmetric with respect to i and j indices. Similarly, for the case $\mathbf{q}^{(n)} = \mathbf{k}^{(n)}$ we get

$$\begin{aligned} \partial_t B_n &= 4k_0^2 k_j^{(n)} k_i^{(n)} \left[(\partial_i \eta_n^{(0)})(\partial_j \Gamma) + (\partial_j \eta_n^{(0)})(\partial_i \Gamma) \right] e^{\Gamma} \\ &= 8k_0^2 k_j^{(n)} k_i^{(n)} (\partial_i \eta_n^{(0)})(\partial_j \Gamma) e^{\Gamma} \end{aligned} \tag{4.48}$$

as the equations of motion of amplitudes zeros in the square lattice. We will use these expressions to determine an expression for the dislocation velocity due to an external lattice distortion or stress. First, we will determine the corresponding expression for the stress in the square lattice.

4.4 Stress-Stress Relation for Square Lattices

In this section we will consider the stress of the square lattice. The stress is interesting in its own right and allows us to compare the stress in the phase field model with the stress known from continuum mechanics. It is a necessary ingredient when deriving the mobility of the Peach-Koehler law that we must have before we can proceed. Like discussed before we distinguish between the microscopic stress $\tilde{h}_{ij}$ and stress h_{ij}. For our purposes we only need the stress h_{ij}, which is given by [9].

For the square lattice the stress is given by [9]

$$h_{ij} = -2\langle (\mathcal{L}_1 \mathcal{L}_2 \psi)(\mathcal{L}_1 + \mathcal{L}_2) \partial_i \partial_j \psi \rangle. \tag{4.49}$$

In order to investigate whether the stress in the phase field model reduces to the stress we know from elasticity theory we insert the two mode expansion into the expression above and assume that the deformation field is slowly-varying in space. This assumption captures that we want the field to vary on a macroscopic scale and not be sensitive to lattice periodicity. Mathematically, this means that we only retain terms that are first order in spatial derivatives. The deformed phase field of the square lattice is expanded in the two-mode approximation as

$$\psi = \psi_0 + A \sum_{n=1}^{N/2} e^{i\mathbf{p}^{(n)} \cdot (\mathbf{r} - \mathbf{u})} + B \sum_{n=1}^{N/2} e^{i\mathbf{k}^{(n)} \cdot (\mathbf{r} - \mathbf{u})} \tag{4.50}$$

where A and B is the amplitudes of the square lattice at equilibrium. Inserting this into Eq. 4.49, and using the orthogonality conditions we get

$$\begin{aligned} h_{ij} &= -2\langle(\mathcal{L}_1\mathcal{L}_2\psi_0)(\mathcal{L}_1+\mathcal{L}_2)\partial_i\partial_j\psi_0\rangle \\ &\quad -2\langle(\mathcal{L}_1\mathcal{L}_2 A\sum_n e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})(\mathcal{L}_1+\mathcal{L}_2)\partial_i\partial_j(A\sum_n e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})\rangle \\ &\quad -2\langle(\mathcal{L}_1\mathcal{L}_2 B\sum_n e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})(\mathcal{L}_1+\mathcal{L}_2)\partial_i\partial_j(B\sum_n e^{i\mathbf{k}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})\rangle. \end{aligned} \tag{4.51}$$

The first term is simply zero because the coarse graining of a constant is zero. The second term is evaluated in detail in Appendix A and gives

$$\begin{aligned} &-2\langle(\mathcal{L}_1\mathcal{L}_2 A\sum_n e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})(\mathcal{L}_1+\mathcal{L}_2)\partial_i\partial_j(A\sum_n e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})\rangle \\ &= 4A^2\partial_a u_c\sum_n p_a^{(n)}p_c^{(n)}p_i^{(n)}p_j^{(n)}. \end{aligned} \tag{4.52}$$

The third term can be evaluated in a manner similar to the second and gives us [9]

$$\begin{aligned} &-2\langle(\mathcal{L}_1\mathcal{L}_2 B\sum_n e^{i\mathbf{k}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})(\mathcal{L}_1+\mathcal{L}_2)\partial_i\partial_j(B\sum_n e^{i\mathbf{k}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})\rangle \\ &= 4B^2\partial_a u_c\sum_n k_a^{(n)}k_c^{(n)}k_i^{(n)}k_j^{(n)}. \end{aligned} \tag{4.53}$$

Hence, the stress-strain relation in the continuum limit is given by

$$h_{ij} = 4\partial_k u_l\left(A^2\sum_n p_i^{(n)}p_j^{(n)}p_k^{(n)}p_l^{(n)} + B^2\sum_n k_i^{(n)}k_j^{(n)}k_k^{(n)}k_l^{(n)}\right) \tag{4.54}$$

Using the dyadic sum relations for the reciprocal vectors [9]

$$\sum_n p_i^{(n)}p_j^{(n)}p_l^{(n)}p_k^{(n)} = 2\delta_{ijkl} \tag{4.55}$$

and

$$\sum_n k_i^{(n)}k_j^{(n)}k_l^{(n)}k_k^{(n)} = 4(\delta_{ij}\delta_{kl}+2\delta_{ki}\delta_{jl}+2\delta_{kj}\delta_{il}-2\delta_{ijkl}) \tag{4.56}$$

we get the equation

$$h_{ij} = 8\partial_k u_l\left[(A^2-4B^2)\delta_{ijkl}+2B^2(\delta_{ij}\delta_{kl}+2\delta_{ki}\delta_{jl}+2\delta_{kj}\delta_{il})\right] \tag{4.57}$$

for the stress in the hexagonal lattice, which shows that the stress in the square lattice is anisotropic, i.e. the elastic constants C_{ijkl} corresponding to the equation above are not isotropic due to the extra δ_{ijkl} factor. We see that isotropic limit is a special case when $A = 4B^2$ as discussed in details in Ref. [9]. We can see the difference in the stress profile between h_{xx} and h_{xy} in figure 4.3.

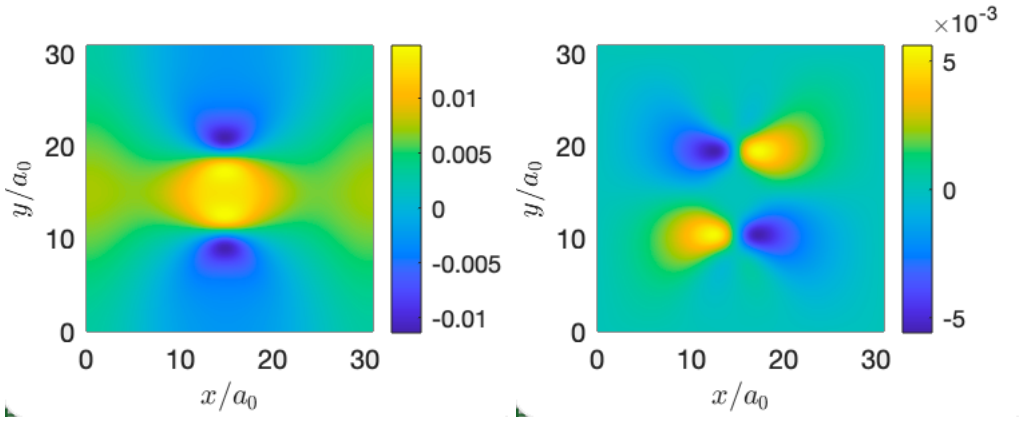

Figure 4.3: On the left is a snapshot of h_{xx} and on the right is a snapshot of h_{xy} for a for a dipole of dislocations located in different slip planes.

4.5 Peach-Kohler Force in a Square Lattice

Having collected all the necessary ingredients we now attempt to derive the mobility in the Peach-Koehler law for the square lattice. This will serve as a test for whether the phase field model in the long wavelength approximation can reproduce the results of elasticity theory. In order to evaluate the dislocation velocity we need to compute $D^{(n)}$ and $J_l^{(n)}$. We will use the amplitude given stated in Eq. 4.36. Starting with the determinant we have

$$\begin{aligned}
D^{(n)} &= \frac{\epsilon_{ij}}{2i}\Big[\big[(\partial_i\eta_n^{(0)})e^{\Gamma}+\eta_n^{(0)}(\partial_i\Gamma)e^{\Gamma}\big]\big[(\partial_j\bar{\eta}_n^{(0)})e^{\bar{\Gamma}}+\bar{\eta}_n^{(0)}(\partial_j\bar{\Gamma})e^{\bar{\Gamma}}\big]\Big] \\
&= \frac{\epsilon_{ij}}{2i}\Big[(\partial_i\eta_n^{(0)})(\partial_j\eta_n^{(0)})+(\partial_i\eta_n^{(0)})\bar{\eta}_n^{(0)}(\partial_j\bar{\Gamma})+\eta_n^{(0)}(\partial_i\Gamma)(\partial_j\bar{\eta}_n^{(0)})+|\eta_n^{(0)}|^2(\partial_i\Gamma)(\partial_j\bar{\Gamma})\Big] \\
&= \frac{\epsilon_{ij}}{2i}\Big[(\partial_i\eta_n^{(0)})(\partial_j\eta_n^{(0)})+(\partial_i\eta_n^{(0)})\bar{\eta}_n^{(0)}(\partial_j\bar{\Gamma})-\eta_n^{(0)}(\partial_i\Gamma)(\partial_j\bar{\eta}_n^{(0)})+|\eta_n^{(0)}|^2(\partial_i\Gamma)(\partial_j\bar{\Gamma})\Big] \\
&= \frac{\epsilon_{ij}}{2i}\Big[(\partial_i\eta_n^{(0)})(\partial_j\bar{\eta}_n^{(0)})+|\eta_n^{(0)}|^2(\partial_i\Gamma)(\partial_j\bar{\Gamma})+2i\Im\big[(\partial_i\eta_n^{(0)})\bar{\eta}_n^{(0)}\partial_j\bar{\Gamma}\big]\Big]. \quad (4.58)
\end{aligned}$$

Because $\Gamma = -\bar{\Gamma}$ the second term is a symmetric tensor, which will vanish when we contract with the Levi-Civita symbol. The first term can be evaluated explicitly. This gives us

$$(\partial_x(x+isy))(\partial_y(x-isy))-(\partial_y(x+isy)(\partial_x(x-isy))=-2si. \quad (4.59)$$

Hence we get

$$D_n=\epsilon_{ij}\Im\Big[(\partial_i\eta_n^{(0)})\bar{\eta}_n^{(0)}\partial_j\bar{\Gamma}\Big]-s_n. \quad (4.60)$$

We now turn to the vortex density current

$$J_l^{(n)} = \Im\big[(\partial_t \eta_n)(\partial_l \bar{\eta}_n)\big]. \tag{4.61}$$

We have previously found that the evolution of amplitude zeros reduces to

$$\partial_t \eta_n = -8iq_0^2 q_j^{(n)} q_i^{(n)} q_k^{(n)} \partial_i \eta_n^{(0)} \partial_j u_k e^{\Gamma} \tag{4.62}$$

Evaluating the derivative of the amplitude we get that the current $J_l^{(n)}$ is

$$\partial_l \bar{\eta}_n = (\partial_l \bar{\eta}_n^{(0)} + \bar{\eta}_n^{(0)} \partial_l \bar{\Gamma}) e^{\bar{\Gamma}} = (\partial_l \bar{\eta}_n^{(0)} + i q_k^{(n)} \bar{\eta}_n^{(0)} \partial_l u_k) e^{\bar{\Gamma}}. \tag{4.63}$$

Putting this together we get

$$\Im\big[(\partial_t \eta_n)(\partial_l \bar{\eta}_n)\big] \tag{4.64}$$

$$= -8q_0^2 q_i^{(n)} q_j^{(n)} q_k^{(n)} \partial_j u_k \Im\left[i\partial_i \eta_n^{(0)} \left(\partial_l \bar{\eta}_n^{(0)} + \bar{\eta}_n^{(0)} \partial_l \bar{\Gamma}\right)\right]. \tag{4.65}$$

In the small-distortion limit this simplifies to

$$\Im\big[(\partial_t \eta_n)(\partial_l \bar{\eta}_n)\big]$$

$$= -8q_0^2 q_i^{(n)} q_j^{(n)} q_k^{(n)} \partial_j u_k \Im\left[i\partial_i \eta_n^{(0)} \partial_l \bar{\eta}_n^{(0)}\right]. \tag{4.66}$$

The expression inside $\Im[...]$ can be evaluated to yield

$$\begin{aligned}
&\Im\big[i(\partial_i \eta_n^{(0)}) \partial_l \bar{\eta}_n^{(0)}\big] \\
&= \Im\big[i(\delta_{ix} + is\delta_{iy})(\delta_{lx} - is\delta_{ly})\big] \\
&= \Im\big[i(\delta_{ix}\delta_{lx} - is\delta_{ix}\delta_{ly} + is\delta_{iy}\delta_{lx} + s^2\delta_{iy}\delta_{l}y)\big] \\
&= \delta_{ix}\delta_{lx} + s_n^2 \delta_{iy}\delta_{ly}.
\end{aligned} \tag{4.67}$$

s_n will either be -1, 1 or 0 depending on the amplitude under consideration. Amplitudes for which s_n is zero are constant and do not contribute to the defect velocity. Hence we can assume that $s_n = \pm 1$ and the above expression can be taken to be

$$\delta_{ix}\delta_{lx} + \delta_{iy}\delta_{ly}. \tag{4.68}$$

We can determining which tensor this is by considering its action on an arbitrary rank 2 tensor

$$(\delta_{ix}\delta_{lx} + \delta_{iy}\delta_{ly}) A_{il} = A_{xx} + A_{yy} = \delta_{il} A_{il}. \tag{4.69}$$

Hence

$$\Im\big[i(\partial_i \eta_n^{(0)}) \partial_l \bar{\eta}_n^{(0)}\big] = \delta_{il} \tag{4.70}$$

and we get that the current is

$$J_l^{(n)} = -8q_0^2 q_l^{(n)} q_j^{(n)} q_k^{(n)} \partial_j u_k. \tag{4.71}$$

Inserting these into the general expression for the velocity in a square lattice given in 4.10 we get the expression

$$V_i = \frac{8\pi^2}{N(p_0^2+k_0^2)b^2}\epsilon_{li}\sum_n s_n^2 \frac{-8q_0^2 q_l^{(n)} q_j^{(n)} q_k^{(n)} \partial_j u_k}{\epsilon_{ij}\Im\left[(\partial_i \eta_n^{(0)})\bar{\eta}_n^{(0)}\partial_j \bar{\Gamma}\right] - s_n}. \tag{4.72}$$

Because Γ is very small compared to $-s$ we get that this is approximately equal to

$$\approx \frac{8\pi^2}{N(p_0^2+k_0^2)b^2}\epsilon_{li}\sum_n s_n^2 \left[\frac{-8q_0^2 q_l^{(n)} q_j^{(n)} q_k^{(n)} \partial_j u_k}{-s_n}\right]. \tag{4.73}$$

We can rearrange Eq. 3.14 to give the identity

$$\frac{b_m q_m^{(n)}}{2\pi s_n} = 1 \tag{4.74}$$

which we can insert into Eq. 4.73 to obtain Using this identity we can manipulate the expression for the dislocation velocity to yield

$$= \frac{32\pi}{N(p_0^2+k_0^2)b^2}\epsilon_{li} b_m \partial_j u_k \sum_{n=1}^{N} q_0^2 q_m^{(n)} q_l^{(n)} q_j^{(n)} q_k^{(n)}. \tag{4.75}$$

We are then left with the expression

$$= \frac{32\pi}{N(p_0^2+k_0^2)b^2}\epsilon_{li} b_m \partial_j u_k \sum_{n=1}^{N} q_0^2 q_m^{(n)} q_l^{(n)} q_j^{(n)} q_k^{(n)}, \tag{4.76}$$

which we can split into two parts to obtain

$$= \frac{32\pi}{N(p_0^2+k_0^2)b^2}\epsilon_{li} b_m \partial_j u_k \left(p_0^2 \sum_{n=1}^{N/2} p_m^{(n)} p_l^{(n)} p_j^{(n)} p_k^{(n)} + k_0^2 \sum_{n=1}^{N/2} k_m^{(n)} k_l^{(n)} k_j^{(n)} k_k^{(n)} \right). \tag{4.77}$$

This is a valid expression for the velocity of the dislocations, expressed in terms of the local added distortion and dyadic products of reciprocal lattice vectors. The challenge, however, is to try to connect this to the expression of the stress tensor in equation (4.54), which we reprint here for convenience

$$h_{ij} = 4\partial_k u_l \left(A^2 \sum_n p_i^{(n)} p_j^{(n)} p_k^{(n)} p_l^{(n)} + B^2 \sum_n k_i^{(n)} k_j^{(n)} k_k^{(n)} k_l^{(n)} \right). \tag{4.54}$$

As we see, while the form of the two expressions is similar, the difference is that the weight of the fourth order dyadic products are different, in the former weighted by p_0^2 and k_0^2 and in the latter by the equilibrium amplitudes. Thus, equation (4.77) cannot be immediately used to obtain the mobility of the Peach-Koehler force in a square lattice, because there is no way to introduce the equilibrium amplitudes A and B we need in order to insert the expression for the stress.

Chapter 5

Discussion and Conclusion

In this thesis, we have studied the properties of a square lattice with dislocations using the phase field crystal model. By using the methods proposed in Refs. [7, 8], we have derived expressions of the dislocation velocity for the case of the 2D square lattice. By coarse-graining the results from the phase field, we have compared these results to those of classical elasticity theory. The stress of the square lattice is anisotropic, which we can see from the analytical expression of Eq. (4.54). We have also attempted to derive the dislocation mobility from the Peach-Koehler law for the square lattice by expressing the velocity in terms of the stress acting on a dislocation. While the resulting expression has a similar form as for the hexagonal lattice, and is a valid expression for the dislocation velocity under the imposition of an external displacement field, it is not immediately clear how to relate it to the stress tensor and derive an explicit mobility. This is a very interesting results since it shows that this method of deriving the dislocation mobility might be applicable only in the one-mode approximation.

This approach has provided insight into the theoretical calculations that connect the phase-field crystal description of dislocation dynamics to that of continuum mechanics. However, whether it is possible to connect these descriptions explicitly remains an open question. An alternative approach to the calculation done in this thesis, which by definition would have allowed us to find an expression for the Peach-Koehler law in a square lattice, would be to only use the first harmonic in the Fourier expansion. In this approximation, only the first term in the expression for the stress, Eq. (4.49) would be present, and only the first of the two sums would be present in Eq. (4.77). Then the derivation of the mobility would be algebraically identical to the work done previously to derive the mobility in the hexagonal lattice. The obvious downside to this approach is that the one-mode harmonic Fourier expansion is a poor approximation of the phase field for the square lattice. As such, the approximation of the mobility obtained by such a method would not be very good. A different idea would be to find two independent expressions for the dislocation velocity of the defect, one expression using only the first harmonics and a second expression using only the second harmonics. For each of these harmonics, the defect velocity's derivation will be identical to that of the hexagonal lattice. The two expressions for the velocity could then be added together, each weighted by

the amplitude of the respective harmonic, allowing us to substitute in the stress tensor. However, this approach assumes that the defect velocity we obtain from using either of the harmonics is the same, which seems doubtful given that the tetradic product sum for the two kinds of reciprocal vectors is different [9].

In summary, this thesis represents the first attempt to generalize the framework of exact analytical calculation of the Peach-Koehler law to a PFC model including higher order Fourier modes. The result shows that the generalization is not straightforward and that more research is needed to find this connection explicitly, and we have proposed a few potential strategies.

Appendix A

Lattice geometry

A.1 Reciprocal lattice vectors

Say we have some lattice with basis vectors $\mathbf{a}_1 = a_0(0,1)$, $\mathbf{a}_2 = a_0(1,0)$. The phase field of the lattice should be periodic $\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{a})$. Taking the Fourier transform of both sides we find

$$\psi(\mathbf{q}) = \int dr^3 \psi(\mathbf{r}) \mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} = \int d^3\mathbf{r}\psi(\mathbf{r}+\mathbf{a})e^{-i\mathbf{q}\cdot\mathbf{r}} \tag{A.1}$$

We can define $\mathbf{r}' = \mathbf{r}+\mathbf{a}$, which gives us $d\mathbf{r} = d\mathbf{r}'$. The equation above become

$$\int d^3\mathbf{r}\psi(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}} = \int d^3\mathbf{r}'\psi(\mathbf{r}')e^{-i\mathbf{q}\cdot(\mathbf{r}'-\mathbf{a})} \tag{A.2}$$

$$= e^{i\mathbf{q}\cdot\mathbf{a}} \int d^3\mathbf{r}'\psi(\mathbf{r}')e^{-i\mathbf{q}\cdot\mathbf{r}'}. \tag{A.3}$$

Since $\mathbf{r}'$ is just a dummy variable in the above integral, the integral in the expression above must be equal to to integral we started out with. Hence $e^{i\mathbf{q}\cdot\mathbf{a}} = 1$ which implies $\mathbf{q}\cdot\mathbf{a} = 2\pi N$ where N is some integer. For the square lattice this gives us that any vector of the form

$$\mathbf{q} = \frac{2\pi}{a_0}(k,l) \tag{A.4}$$

will be a reciprocal lattice vector, if k and l are integers The reciprocal lattice vectors $\frac{2\pi}{a_0}(1,0)$, $\frac{2\pi}{a_0}(-1,0)$, $\frac{2\pi}{a_0}(0,-1)$ and $\frac{2\pi}{a_0}(0,1)$ are often referred to as the first harmonics, while $\frac{2\pi}{a_0}(1,1)$, $\frac{2\pi}{a_0}(1,-1)$, $\frac{2\pi}{a_0}(-1,1)$ and $\frac{2\pi}{a_0}(-1,-1)$ are referred to as the second harmonics.

A.2 Lattice vectors and moments

Say we have some set of lattice vectors

$$Q = \{\boldsymbol{q}^{(n)}\}_{n=1}^{N}. \tag{A.5}$$

From this set we can construct something called the p'th moment tensor

$$\boldsymbol{Q} = \sum_{n=1}^{N} \boldsymbol{q}^{(n)} \underbrace{\otimes \ldots \otimes}_{p \ times} \boldsymbol{q}^{(n)} \tag{A.6}$$

or in index notation

$$Q_{i_1 \ldots i_p} = \sum_{n=1}^{N} q_{i_1}^{(n)} \ldots q_{i_p}^{(n)}. \tag{A.7}$$

Looking at the reciprocal vectors of the square lattice, including only the first two harmonics, we get

$$Q = \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ -1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} -1 \\ 1 \end{pmatrix} \begin{pmatrix} -1 \\ -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right\}. \tag{A.8}$$

We get the following components of the second moment tensor of this set

$$\begin{aligned} Q_{11} &= 6 \\ Q_{12} &= 0 \\ Q_{21} &= 0 \\ Q_{22} &= 6 \end{aligned} \tag{A.9}$$

which we can write as

$$Q_{ij} = 6\delta_{ij}. \tag{A.10}$$

This turns out to be an example of a general phenomena; if you have some set of lattice vectors which has B-fold rotational symmetry, the p'th order moment is zero if p is odd and isotropic if p is even [1]. Isotropic tensors are defined by not having their components changed when you rotate the coordinate system. For rank two tensors the unique isotropic tensor is the Kronecker delta. By B-fold rotational symmetry we mean that there are B different angles you can rotate the set of lattice vectors by and obtain the same set of vectors. For instance, the square lattice has $B = 4$ because rotation about the origin of every vector in the set by $\pi/2$, π, $3\pi/4$ and 2π all leave the set unchanged. Because the only isotropic rank two tensor is the Kronecker delta, we know that the second order moment has to be proportional to the Kronecker delta

$$Q_{ij} = \sum_{n=1}^{N} q_i^{(n)} q_j^{(n)} \propto \delta_{ij}. \tag{A.11}$$

If we assume that all vectors in the set have the same length we can take the trace to obtain

$$N q_0^2 = 2 \tag{A.12}$$

so the proportionality constant is $\frac{N q_0^2}{2}$ and we get

$$\sum_{n=1}^{N} q_i^{(n)} q_j^{(n)} = \frac{N q_0^2}{2} \delta_{ij}. \tag{A.13}$$

In the above example of the square lattice the vectors did not all have the same length. We can then split the set Q into sets of vectors which has uniform length respectively, apply the result to each set separately and sum the result. In the example above this would give

$$\sum_{n=1}^{N} q_i^{(n)} q_j^{(n)} = \frac{N}{4}(p_0^2 + k_0^2)\delta_{ij}. \tag{A.14}$$

Appendix B

Phase Field Crystal

B.1 Computing a time derivative

The aim of this section is to prove the identity

$$D^{(n)}\partial_t\delta^{(2)}(\eta_n) = -\epsilon_{kl}\partial_k J_l. \tag{B.1}$$

We use the notation $\eta_{n,1} = \Re[\eta_n]$ and $\eta_{n,2} = \Im[\eta_n]$. Evaluating the left hand side of the equation above gives

$$\epsilon_{kl}\partial_k\eta_{n,1}\partial_l\eta_{n,2}\partial_t\delta^{(2)}(\eta_n) = \epsilon_{kl}\partial_k\eta_{n,1}\partial_l\eta_{n,2}\frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,1}}\partial_t\eta_{n,1} + \epsilon_{kl}\partial_k\eta_{n,1}\partial_l\eta_{n,2}\frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,2}}\partial_t\eta_{n,2}. \tag{B.2}$$

Turning to the right hand side we have

$$\begin{aligned}
\epsilon_{kl}J_l\partial_k\delta^{(2)}(\eta_n) \quad &= \epsilon_{kl}\Im[\partial_t\eta_n\partial_l\bar{\eta}_n]\left(\frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,1}}\partial_k\eta_{n,1} + \frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,2}}\partial_k\eta_{n,2}\right) \\
&= \epsilon_{kl}\Im[(\partial_t\eta_{n,1} + i\partial_t\eta_{n,2})(\partial_l\eta_{n,1} - i\partial_l\eta_{n,2})\left(\frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,1}}\partial_k\eta_{n,1} + \frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,2}}\partial_k\eta_{n,2}\right) \\
&= \epsilon_{kl}(\partial_t\eta_{n,2}\partial_l\eta_{n,1} - \partial_t\eta_{n,1}\partial_l\eta_{n,2})\left(\frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,1}}\partial_k\eta_{n,1} + \frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,2}}\partial_k\eta_{n,2}\right).
\end{aligned} \tag{B.3}$$

When the expressions inside the brackets are multiplied out, any symmetric tensors will vanish since they are contracted with the Levi-Civita symbol. Hence we are left with

$$= \epsilon_{kl}\partial_t\eta_{n,2}\partial_l\eta_{n,1}\frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,2}}\partial_k\eta_{n,2} - \epsilon_{kl}\partial_t\eta_{n,1}\partial_l\eta_{n,2}\frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,1}}\partial_k\eta_{n,1}. \tag{B.4}$$

The k and l indices can be permuted in the first term provided we change the sign. Hence we obtain

$$= -\epsilon_{kl}\partial_t\eta_{n,2}\partial_k\eta_{n,1}\frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,2}}\partial_l\eta_{n,2} - \epsilon_{kl}\partial_t\eta_{n,1}\partial_l\eta_{n,2}\frac{\partial\delta^{(2)}(\eta_n)}{\partial\eta_{n,1}}\partial_k\eta_{n,1}. \tag{B.5}$$

B.2 Stress algebra

We want to evaluate the expression

$$-2\langle \mathcal{L}_1\mathcal{L}_2 A \sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}(\mathcal{L}_1+\mathcal{L}_2)\partial_{ij} A \sum e^{i\mathbf{p}^{(n)}(\mathbf{r}-\mathbf{u})}\rangle. \tag{B.6}$$

We start by considering

$$\mathcal{L}_1\mathcal{L}_2 A \sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}. \tag{B.7}$$

Since derivatives commute we can also express this as

$$\mathcal{L}_2\mathcal{L}_1 A \sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}. \tag{B.8}$$

We then get

$$\mathcal{L}_2(\partial_{ii}+1)A \sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} \tag{B.9}$$

$$= \mathcal{L}_2\big[\partial_i\big(A\sum ip_j^{(n)}\partial_i(r_j-u_j)e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}\big) + A\sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}\big] \tag{B.10}$$

$$= \mathcal{L}_2\big[A\sum(ip_j^{(n)}ip_k^{(n)}\partial_i(r_j-u_j)\partial_i(r_k-u_k) + ip_j^{(n)}\partial_{ii}(r_j-u_j)+1)e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}\big] \tag{B.11}$$

$$= \mathcal{L}_2\big[A\sum((-1)p_j^{(n)}p_k^{(n)}\delta_{ij}\delta_{ik} + p_j^{(n)}p_k^{(n)}\delta_{ij}\partial_i u_k + p_j^{(n)}p_k^{(n)}\delta_{ik}\partial_i u_j + 1)e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}\big]. \tag{B.12}$$

Using that $\mathbf{p}^{(n)}\cdot\mathbf{p}^{(n)} = 1$ we get

$$2\mathcal{L}_2\big[A\sum p_i^{(n)}p_k^{(n)}\partial_i u_k e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}\big] \tag{B.13}$$

$$= 2(2+\partial_{ll})A\sum p_i^{(n)}p_k^{(n)}\partial_i u_k e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} \tag{B.14}$$

$$= 2A\sum\big[2(p_i^{(n)}p_k^{(n)}\partial_i u_k) + p_i^{(n)}p_k^{(n)}ip_a^{(n)}\partial_i u_k\partial_l(r_a-u_a)\partial_l\big]e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} \tag{B.15}$$

$$= 2A\sum\big[2(p_i^{(n)}p_k^{(n)}\partial_i u_k) + p_i^{(n)}p_k^{(n)}ip_l^{(n)}ip_b^{(n)}\partial_i u_k\partial_l(r_b-u_b)\big]e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} \tag{B.16}$$

$$= 2A\sum p_i^{(n)}p_k^{(n)}\partial_i u_k e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}. \tag{B.17}$$

Using parts of the calculations above we also have

$$\partial_{ij}\mathcal{L}_1 A\sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} \tag{B.18}$$

$$= \partial_{ij}(1+\partial_{kk})A\sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} \tag{B.19}$$

$$= \partial_{ij}\big[A\sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} + \partial_k\big(A\sum ip_a^{(n)}\partial_k(r_a-u_a)e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}\big)\big] \tag{B.20}$$

$$= \partial_{ij}\big[A\sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} + A\sum ip_a^{(n)}ip_c^{(n)}\partial_k(r_a-u_a)\partial_k(r_c-u_c)e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}\big] \tag{B.21}$$

$$= \partial_{ij}A\sum\big[1-p_a^{(n)}p_c^{(n)}\delta_{ka}\delta_{kc}+p_a^{(n)}p_c^{(n)}\partial_k u_a\delta_{kc}+p_a^{(n)}p_c^{(n)}\partial_k u_c\delta_{ka}\big]e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} \tag{B.22}$$

$$= \partial_{ij}A\sum\big[1+2p_a^{(n)}p_c^{(n)}\partial_k u_a e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}\big] \tag{B.23}$$

and

$$\partial_{ij}\mathcal{L}_2 A\sum e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})} \tag{B.24}$$

$$= \partial_{ij}A\sum\big[1+2p_a^{(n)}p_c^{(n)}\partial_a u_c\big]e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})}. \tag{B.25}$$

Having gathered these ingredients we can now evaluate the expressions we started with

$$\langle(\mathcal{L}_2\mathcal{L}_2 A\sum_n e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})(\mathcal{L}_1+\mathcal{L}_2)\partial_{ij}A\sum_m e^{i\mathbf{p}^{(m)}\cdot(\mathbf{r}-\mathbf{u})}\rangle \tag{B.26}$$

$$2A^2\sum_{n,m}(p_i^{(n)}p_k^{(n)}\partial_i u_k e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})\partial_{ij}\big[(1+2p_a^{(m)}p_c^{(m)}\partial_a u_c)e^{i\mathbf{p}^{(m)}\cdot(\mathbf{r}-\mathbf{u})}\big] \tag{B.27}$$

$$= 2A^2\sum_{n,m}\langle(p_i^{(n)}p_k^{(n)}\partial_i u_k e^{i\mathbf{p}^{(n)}\cdot(\mathbf{r}-\mathbf{u})})(-2p_a^{(m)}p_c^{(m)}p_i^{(m)}p_j^{(m)}-p_i^{(m)}p_j^{(m)}-2p_a^{(m)}p_c^{(m)}p_i^{(m)}p_j^{(m)})e^{i\mathbf{p}^{(m)}\cdot(\mathbf{r}-\mathbf{u})}\rangle \tag{B.28}$$

$$= -2A^2\sum_{n,m}\langle p_a^{(n)}p_c^{(n)}p_i^{(m)}p_j^{(m)}\partial_a u_c\langle e^{i(\mathbf{p}^{(n)}+\mathbf{p}^{(m)})\cdot(\mathbf{r}-\mathbf{u})}\rangle\rangle. \tag{B.29}$$

Using that $\langle e^{i(\mathbf{p}^{(n)}+\mathbf{p}^{(m)})\cdot(\mathbf{r}-\mathbf{u})}\rangle\rangle = \delta_{n-m}$ and that we can reorganize the sum such that a sum over m is the same as a sum over $-m$ we get that the above is equal to

$$= -2A^2\sum_n p_a^{(n)}p_c^{(n)}p_i^{(n)}p_j^{(n)}\partial_a u_c. \tag{B.30}$$

Bibliography

[1] Hudong Chen and Steven Orszag. Moment isotropy and discrete rotational symmetry of two-dimensional lattice vectors. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 369(1944):2176–2183, 2011.

[2] KR Elder and Martin Grant. Modeling elastic and plastic deformations in nonequilibrium processing using phase field crystals. *Physical Review E*, 70(5):051605, 2004.

[3] Tae-Hwan Jang, Seung-Hwan Do, Minseong Lee, Hui Wu, Craig M. Brown, Andrew D. Christianson, Sang-Wook Cheong, and Jae-Hoon Park. Physical properties of the quasi-two-dimensional square lattice antiferromagnet $ba_2fesi_2o_7$. *Phys. Rev. B*, 104:214434, Dec 2021.

[4] Lev Davidovich Landau, Evgenij M Lifšic, Evegnii Mikhailovich Lifshitz, Arnold Markovich Kosevich, and Lev Petrovich Pitaevskii. *Theory of elasticity: volume 7*, volume 7. Elsevier, 1986.

[5] Tamer A Moniem. All optical active high decoder using integrated 2d square lattice photonic crystals. *Journal of Modern Optics*, 62(19):1643–1649, 2015.

[6] Marco Salvalaglio and Ken R Elder. Coarse-grained modeling of crystals by the amplitude expansion of the phase-field crystal model: an overview. *Modelling and Simulation in Materials Science and Engineering*, 2022.

[7] Audun Skaugen, Luiza Angheluta, and Jorge Viñals. Dislocation dynamics and crystal plasticity in the phase-field crystal model. *Phys. Rev. B*, 97(5):054113, February 2018.

[8] Vidar Skogvoll, Luiza Angheluta, Audun Skaugen, Marco Salvalaglio, and Jorge Viñals. A phase field crystal theory of the kinematics of dislocation lines. *Journal of the Mechanics and Physics of Solids*, 166:104932, September 2022.

[9] Vidar Skogvoll, Audun Skaugen, and Luiza Angheluta. Stress in ordered systems: Ginzburg-landau-type density field theory. *Physical Review B*, 103(22):224107, 2021.

[10] Vidar Skogvoll, Audun Skaugen, Luiza Angheluta, and Jorge Viñals. Dislocation nucleation in the phase-field crystal model. *Physical Review B*, 103(1):014107, 2021.