A Topological Approach to the Charge Density Wave

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Author: Sam Kuypers *Student number*: 10650253
Supervisor: dr. J. van Wezel *Second assessor*: prof. dr. J.S. Caux

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Faculteit Natuurwetenschappen, Wiskunde & Informatica
Instituut voor Theoretische Fysica Amsterdam

UNIVERSITEIT VAN AMSTERDAM

Abstract

In this paper a one-dimensional material with topological order, namely the charge density wave, is discussed. A review of the relevant theoretical background is provided. A method is proposed for finding the Chern numbers for the charge density wave. This method allows one to approximate the Hamiltonian of the charge density wave in such a way that the eigenstates can be determined, so that the Chern numbers can be calculated.

Acknowledgements

I would like to thank Dr. Jasper van Wezel for introducing me to this fascinating field of physics and for the guidance he has given me throughout my research. Furthermore, I would like to thank Ana Silva for her help in reviewing my work and prof. Dr. Caux for his role as second assessor.

Populaire Wetenschappelijk introductie

De moderne mens heeft in het dagelijks leven veel te maken met elektriciteit. Alles van huishoudelijke apparatuur tot mobiele telefoons wordt aangedreven door elektrische stroom. In deze scriptie gaat het echter niet over de elektrische stroom zelf, maar over de materialen die stroom geleiden. Het bestuderen van geleiders, isolatoren en andere vaste stoffen is waar het vakgebied gecondenseerde materie over gaat.

Over het algemeen zijn materialen geleiders of isolatoren. Geleiders laten makkelijk een stroom door, terwijl isolatoren dat maar moeizaam of totaal niet doen. Echter is er vrij recent een nieuwe vorm van materie ontdekt die zowel isoleert als geleid. Over het oppervlakte van dit soort materialen kan een stroom lopen terwijl de binnenkant van het materiaal isoleert. Materialen met deze eigenschappen noemt men topologische isolatoren.

Topologische isolatoren zijn een excentrieke vorm van materie. De theorie achter deze materialen is reeds bekend, echter in het vorige decennium zijn voor het eerst pas waarnemingen gedaan van topologische isolatoren. We kennen steeds meer materialen die en als geleider en als isolator werken. Accurate modellen voor hoe dit soort materialen zich gedragen, worden steeds belangrijker. Dit zodat wij in de toekomst hiervoor toepassingen kunnen vinden.

Het doel van deze scriptie is om een wiskundige methode te formuleren voor het bepalen van de hoeveelheid stroom die door dit soort materialen heen gaat. Dit wordt gedaan door te bestuderen hoe de parameter ruimte van het materiaal zich gedraagt. De parameter ruimte is een abstracte wiskundige ruimte van het systeem. De structuur, ofwel de topologie, van de parameter ruimte bepaald of een materiaal een topologische isolator is.

Contents

CHAPTER 1

Introduction

For many years, phases of matter have been described using Landau theory. It was thought that all phases of matter could be described by the symmetries of the ground state of a system. However, since the discovery of the integer quantum Hall effect, it has become clear that Landau theory does not describe all possible phases of matter. A new kind of order has since been introduced called topological order. Topological order becomes apparent whenever the parameter space of a quantum mechanical system is non-trivial.

An example of materials with topological order are topological insulators. Such materials have a Fermi energy that lies in a band gap, and should thus be insulators under most conditions. However, when they are subjected to a slowly varying potential they allow for quantised transport of charge. This transport occurs at the boundary of the material, while the bulk remains insulating. The number of particles transported through the topological insulator can be linked to a Chern number. The Chern number reflects the non-trivial topology of parameter space.

In the following text one such system with topological order will be studied. This system is called the charge density wave: a one-dimensional crystal with phonon distortions The phonon distortions open up a band gap in the material. Under the right conditions, the Fermi energy of the system lies within this band gap and the material becomes insulating. The charge density wave allows for a current to flow at the boundaries of the material, but the bulk remains insulating.

Charge density waves have been studied by physicists using computation. The goal of this thesis was to see if analytical methods existed through which the Chern number can be calculated. This thesis will propose an analytical method for calculating the Chern number of the charge density wave, and discuss possible shortcomings of this method.

CHAPTER 2

Solid State Physics

A complete understanding of the material that is discussed in this thesis requires some background knowledge in condensed-matter physics, specifically in the field of topological insulators. An introduction into these fields is provided in the following two chapters.

2.1 The hopping Hamiltonian

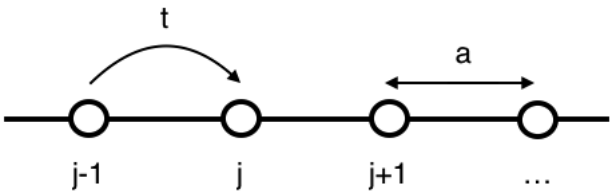

Figure 2.1: A periodic lattice with spacing a and hopping amplitude t. The index j denotes the j^{th} atom in the chain.

Let us consider an array of identical atoms so ordered that they form a one-dimensional chain with a lattice constant a (see figure 2.1) [18]. It is assumed that the electrons are fairly localised and can therefore only occupy a single lattice site (in this case an atom). In order to avoid boundary effects, we impose the periodic boundary condition $|j + N\rangle = |j\rangle$, with N representing the number of atoms in the chain and j the j^{th} site of the lattice. The distance x is given by aj, and the total length L of the chain equals Na. By letting $N \to \infty$ a large chain is approximated. Furthermore, we take into account that the electrons can jump from one site to the next. This is done

with a so-called hopping amplitude t, which is the energy it costs an electron to tunnel from one site to the next.

A simplified model for such a quantum mechanical system is the Hubbard model. The Hubbard model is a useful basis for studying the CDW; for our purposes, some simplifications will be made of this model in this subsection. The usefulness of this model comes from the fact that we can write the eigenstate of this Hamiltonian in terms of the vacuum state $|\Omega\rangle$ and fermion creation operators [7]

$$|\psi\rangle = \left[\Pi_i c_{i,\downarrow}^\dagger\right] \left[\Pi_j c_{j,\uparrow}^\dagger\right] |\Omega\rangle \,. \tag{2.1}$$

With $c_j^\dagger$ and c_j being the fermion creation- and annihilation operators, which abide by the following anticommutation relations

$$\{c_{i,\sigma}^\dagger c_{j,\tau}\} = \delta_{ij}\delta_{\sigma\tau}, \quad \{c_{i,\sigma}^\dagger c_{j,\tau}^\dagger\} = 0, \quad \{c_{i,\sigma} c_{j,\tau}\} = 0, \tag{2.2}$$

here $\{A, B\} = AB + BA$. As an example, consider the wave function of two electrons: one at position x with spin up, and one at position y with spin down. This would then be denoted as

$$|x\uparrow, y\downarrow\rangle = c_{x,\uparrow}^\dagger c_{y,\downarrow}^\dagger |\Omega\rangle \,. \tag{2.3}$$

Using second quantisation, the Hamiltonian for the Hubbard model can be written as [7]

$$\hat{H} = \sum_{<j,i>} \sum_{\sigma=\downarrow,\uparrow} (-t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} - t_{ji} c_{i,\sigma}^\dagger c_{j,\sigma}) + \sum_{i=1}^{N} U_i c_{i,\uparrow}^\dagger c_{i,\uparrow} c_{i,\downarrow}^\dagger c_{i,\downarrow}. \tag{2.4}$$

Here the first term is called the hopping Hamiltonian, the factor t_{xy} is the hopping amplitude, and $< j, i >$ stands for a sum over nearest neighbours. The second term of the Hamiltonian is the spin-interaction term. When two electrons with opposite spin are on the same lattice site x the system gains energy U_x.

For the purpose of this thesis, it will not be necessary to consider the effects of spin. Therefore, the spin-interaction terms of the above Hamiltonian will be neglected. Furthermore, because we are dealing with an arrangement of identical atoms, the hopping probability t_{ij} will become

$$t_{ij} = \begin{cases} t/2 & \text{if } i \text{ and } j \text{ are nearest neighbours,} \\ 0 & \text{in all other cases.} \end{cases} \tag{2.5}$$

Using these simplifications, the Hamiltonian that we will be working with, henceforth called the hopping Hamiltonian, becomes [18]

$$\hat{H} = -\frac{t}{2} \sum_j (c_j^\dagger c_{j+1} + h.c.). \tag{2.6}$$

2.2 Bloch waves

The symmetries of a physical system can usually be exploited in order to simplify a problem. For this reason, it will be useful to examine the translational symmetry of the Hamiltonian in Eq. 2.6. It is evident that under the transformation $x \to x + a$, with a being the lattice constant, the energy remains invariant. Therefore, the so-called translation operator [8]

$$T_a \left|\psi(x)\right\rangle = \left|\psi(x+a)\right\rangle, \tag{2.7}$$

commutes with the Hamiltonian. This means that we can chose a basis such that $|\psi_{nk}\rangle$ simultaneously diagonalises both T_a and $\hat{H}$.

The eigenvalue of the translation operator turns out to be [8]

$$T_a \left|\psi_{nk}(x)\right\rangle = \left|\psi_{nk}(x+a)\right\rangle = \exp(ika)\left|\psi_{nk}(x)\right\rangle, \tag{2.8}$$

with k being the quasi-momentum, also referred to as the wave number (a proof of this fact is provided in appendix A.1). Thus, it is possible to write this vector in terms of Bloch waves, defined as [8]

$$\left|\psi_{nk}(x)\right\rangle = \exp(ikx)\left|u_n(x)\right\rangle, \tag{2.9}$$

where $|u_n(x)\rangle$ has the same periodicity as the unit cell $|u_n(x+a)\rangle = |u_n(x)\rangle$. The method of writing the eigenstate of the Hamiltonian in terms of Bloch waves is not only applicable to the aforementioned Hamiltonian (equation 2.6); it applies to any Hamiltonian that commutes with the translation operator.

2.3 Metals and Insulators

In the outlined model the eigenvalue problem will be solved using the Fourier transformation [18]

$$c_j = \frac{1}{\sqrt{N}} \sum_k \exp\left(-aijk\right) c_k. \tag{2.10}$$

Here, a represents the lattice constant, i the imaginary number, k the wave number and N the number of atoms on the chain. Because the lattice is periodic with the lattice constant a, the wave number k is well defined in the region $(-\pi/a, \pi/a)$ [18]. Wave numbers outside of this region repeat themselfs such that k-space is a d-dimensional torus **??**. Furthermore, due to the periodic boundary condition $x = x + L$, the spacing between wave numbers is $2\pi/Na$.

Returning to the Hamiltonian, let us invoke the identity [8]

$$\frac{1}{N}\sum_{j}\exp\left(aij(k-k')\right)=\delta_{k,k'}, \tag{2.11}$$

from which it can be obtained that the Hamiltonian becomes [18]

$$\hat{H}=-t\sum_{k}\cos\left(ka\right)c_{k}^{\dagger}c_{k}. \tag{2.12}$$

Having performed the Fourier transformation, we have effectively solved the eigenvalue problem of the Hamiltonian. For if we now write our eigenstate as a product of momentum creation- and annihilation operators working on the vacuum state $|k\rangle = c_k^\dagger |\Omega\rangle$, we find that

$$\hat{H}\left|k\right\rangle=-t\cos\left(ka\right)\left|k\right\rangle. \tag{2.13}$$

Using this result, it can be clarified how metals and insulators differ. There is evidently only a small range of energies that electrons can occupy. Due to the Pauli exclusion principle, electrons cannot occupy the same energy eigenstate. Thus, when the chemical energy of the system lies in a region with no allowed energies (see left side of figure 2.2), electrons cannot be excited to the next energy level. The material is therefore insulating. When the chemical energy lies in a region with energy bands (see right side of figure 2.2) electrons can be easily excited (for instance, by thermal fluctuations) to higher energy states. In this case the material is a metal.

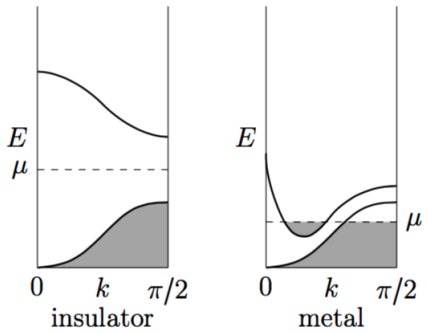

Figure 2.2: Two graphs of energy bands, with E representing energy and k the wave number [6]. The graph on the left shows an insulator with a chemical potential μ in between bands, while the right graph shows a metal with a chemical potential inside energy bands.

In this thesis materials are discussed that act like insulators, in that they have a Fermi energy in a bandgap, but nonetheless conduct electrons.

They do this when a slowly varying potential is applied to the system. In the following chapter, the physics of such materials is reviewed.

CHAPTER 3

Chern Insulators

This chapter will discuss the theory behind Chern, or topological, insulators. Chern insulators are insulators that, under the right conditions, allow for the quantised transport of particles. The number of particles transported is called the Chern number. The Chern number is a result of the non-trivial topology of the parameter space of a quantum mechanical system.

3.1 The Berry phase

The topological order of a material can be described using the Berry phase, which will be introduced in the following subsection. Subsequently, the connection between the Berry phase and the quantised current will be derived.

3.1.1 Berry's phase as an example of holomony

Berry's phase is an example of holomony in quantum mechanics [5]. In differential geometry, holomony is the angle by which a vector quantity is rotated while it is transported parallel to some curved surface. Michael Berry uses a classical example of holomony to draw the analogy between Berry's phase, a quantum mechanical phase he discovered, and the parallel transport that occurs during excursions over closed loops on spheres [2]. His example goes as follows: consider an arrow with its origin at the north pole of a globe, angled tangential to the globe (see figure 3.1). Let the arrow move down along a line of longitude such that at every point it remains tangential to the globe. The arrow will move down until it reaches the equator, after which it will move along the equator to another line of longitude. Through this new line of longitude, let it now move up to the north pole again. The arrow has been transported over a closed loop along the sphere, and at no point in time was it not tangential to the sphere. What one finds, however,

is that the arrow has picked up a phase. This is evident because the arrow is no longer pointing in its direction (see figure 3.1).

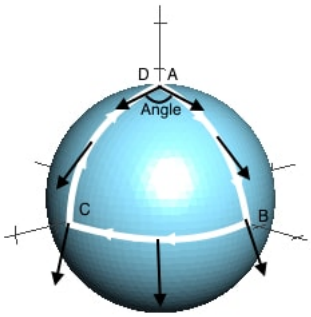

Figure 3.1: The closed loop over the sphere goes from A, B, C to D. The white arrows show the direction of the path taken. The black arrows are tangential to the surface at every point. It can be seen that the black arrows are rotated after the loop is completed.

Berry's phase is different to the aforementioned example in that it does not result from a loop in real space. It is rather the result of closed loops in the parameter space of quantum systems. Such loops occur whenever the environment of a quantum mechanical system is gradually changed in such a way that after a time T the system restores to its initial condition. During such processes, the initial and final wave functions are the same up to some phase factor.

3.1.2 Berry's phase as a consequence of adiabetic theorem

In the following section, the derivation of the Berry phase will be shown. This will be done in accordance with Berry's original paper [1], as well as with the paper by Xiao et al. [3]. Let us start by considering a quantum mechanical system with a Hamiltonian $\hat{H}$ that depends on time t through a set of parameters. Let these parameters be represented by $\boldsymbol{\xi}(t)$. For brevity this will be contracted to $\boldsymbol{\xi} = \boldsymbol{\xi}(t)$. The state $|\psi(t)\rangle$ of this system will evolve through time according to Schrödinger's equation

$$\hat{H}(\boldsymbol{\xi})\,|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle\,. \tag{3.1}$$

Let us now presume that the system's environment is gradually changed. If this change is gradual enough, a basis can be used such that, at any point in time, $\hat{H}(\boldsymbol{\xi})$ is diagonal. That is, for all n (assuming the basis is discrete),

$$\hat{H}(\boldsymbol{\xi}) \left|n(\boldsymbol{\xi})\right\rangle = \epsilon_n \left|n(\boldsymbol{\xi})\right\rangle \tag{3.2}$$

is satisfied. When a system that is initially prepared in the state $|n(\boldsymbol{\xi}(0))\rangle$ is adiabatically evolved from $t = 0$ to $t = T$, it follows from the adiabatic theorem that at time $t = T$ the system is given by [1]

$$\left|\psi_n(T)\right\rangle = \exp\left\{-\frac{i}{\hbar}\int_0^T E_n(\boldsymbol{\xi}(t))dt\right\} \exp(i\gamma_n(T)) \left|n(\boldsymbol{\xi}(T))\right\rangle . \tag{3.3}$$

Here, the second exponential is the Berry phase[1]. To find an expression for the Berry phase, we use Eq. 3.1 and 3.3 to obtain that [3]

$$\gamma_n(T) = \int_0^T i \left\langle n(\boldsymbol{\xi})\right| \frac{\partial}{\partial t} \left|n(\boldsymbol{\xi})\right\rangle dt. \tag{3.4}$$

Gradually changing the system can be seen as an excursion over a trajectory in parameter space, defined through $\boldsymbol{\xi}(t)$. When a system evolves in such a way that after time T it returns to its inital condition, the trajectory in parameter space becomes a loop, which shall be denoted as $\mathcal{L}$. By performing a change of variables in Eq. 3.4 it thus becomes [1]

$$\gamma_n(\mathcal{L}) = \oint_{\mathcal{L}} i \left\langle n(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}} n(\boldsymbol{\xi})\right\rangle \cdot d\boldsymbol{\xi}. \tag{3.5}$$

Here the quantity $i \left\langle n(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}} n(\boldsymbol{\xi})\right\rangle$ is called the Berry connection and shall henceforth be written as $\mathcal{A}_n(\boldsymbol{\xi})$. Evidently, Eq. 3.5 is only dependent on the path taken through parameter space. This highlights the geometric property of the Berry phase.

In order for the Berry phase to be an observable quantity, it must be both real and gauge-invariant. We shall concern ourselves only with the gauge-invariance of the Berry phase here (for a proof that the Berry phase is a real number, see appendix A.2).

It can be readily deduced that Eq. 3.4 is not gauge-invariant. By performing the gauge transformation [3]

$$\left|\psi_n(\boldsymbol{\xi})\right\rangle \rightarrow \exp(i\Lambda(\boldsymbol{\xi})) \left|\psi_n(\boldsymbol{\xi})\right\rangle , \tag{3.6}$$

[1]Michael Berry originally discovered the Berry phase while studying stationary quantum states. He considered the possibility that the phase differences between such systems could be a consequence of the adiabatic theorem [2]

the Berry phase transforms as

$$\gamma_n \to \gamma_n + \Lambda(\boldsymbol{\xi}(0)) - \Lambda(\boldsymbol{\xi}(T)). \tag{3.7}$$

Hence, a suitable $\Lambda(\boldsymbol{\xi})$ can be chosen such that the Berry phase will be transformed to zero. However, with the condition that we have a loop in parameter space, $\boldsymbol{\xi}(0) = \boldsymbol{\xi}(T)$, such gauge transformations are no longer possible due to the single-valuedness of the gauge [3]

$$\Lambda(\boldsymbol{\xi}(0)) - \Lambda(\boldsymbol{\xi}(T)) = 2\pi n, \qquad n \in \mathbb{Z}. \tag{3.8}$$

It follows that in such instances the Berry phase cannot be transformed and is thus gauge-variant.

3.1.3 The Berry curvature and classical electromagnetism

There exist some similarities between the mathematics of classical electromagnetism and that of the Berry phase, which will be clarified here. These similarities have been shown to exist by [1], [3] and [4]. First, let us again consider equation 3.5. As noted before, the line integral of the Berry connection over some closed curve is a measurable quantity, but the local Berry connection is not, because it is not gauge-invariant. Vector fields with such properties have been studied in classical electromagnetism, where they are known as the magnetic vector potential. To exploit these commonalities, let us apply Stokes' theorem to Eq. 3.5 in order to get [4]

$$\gamma_n(\mathcal{L}) = \iint_{\mathcal{S}} \nabla_{\boldsymbol{\xi}} \times \mathcal{A}_n(\boldsymbol{\xi}) \cdot d\mathbf{S}. \tag{3.9}$$

Here $\mathcal{S}$ is a surface that has as its boundary the closed loop $\mathcal{L}$. $d\mathbf{S}$ is an infinitesimal element of the surface $\mathcal{S}$ that is oriented perpendicular to this surface. The vector $\nabla_{\boldsymbol{\xi}} \times \mathcal{A}_n(\boldsymbol{\xi})$ in Eq. 3.9 will henceforth be referred to as the Berry curvature and will be denoted as $\boldsymbol{\Omega}_n(\boldsymbol{\xi})$. Simplifing Eq. 3.9 gives us [3]

$$\gamma_n(\mathcal{L}) = \iint_{\mathcal{S}} \boldsymbol{\Omega}_n(\boldsymbol{\xi}) \cdot d\mathbf{A}. \tag{3.10}$$

From Eq. 3.10 it becomes clear that the Berry phase can be interpreted as the Berry curvature flux through the surface $\mathcal{S}$. The sources of the Berry curvature are the degeneracies of the of the wave function[1].

The Berry curvature can also be expressed as a sum over states. Let us consider the Berry curvature once more, this time working out an explicit expression using the instantaneous eigenstates of the Hamiltonian [1]

$$\boldsymbol{\Omega}_n(\boldsymbol{\xi}) = -i\nabla_{\boldsymbol{\xi}} \times \langle n(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}} n(\boldsymbol{\xi})\rangle \,. \tag{3.11}$$

By working out the cross-product and using the identity operator, this expression can be rewritten as a sum over states. Some obvious abbreviations in notation will be made here [1]

$$\boldsymbol{\Omega}_n(\boldsymbol{\xi}) = -i \sum_{m\neq n} \langle \nabla n|m\rangle \times \langle m|\nabla n\rangle \,. \tag{3.12}$$

By invoking the second Hellmann-Feynman theorem [3] (for a derivation of this theorem see appendix A),

$$\frac{\langle m|\, \nabla \hat{H}\, |n\rangle}{(\epsilon_m - \epsilon_n)} = \langle m|\nabla n\rangle \,, \tag{3.13}$$

the expression for the Berry curvature can be simplified to [1]

$$\boldsymbol{\Omega}_n(\boldsymbol{\xi}) = -i \sum_{n\neq m} \frac{\langle n(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}} \hat{H}|m(\boldsymbol{\xi})\rangle \times \langle m(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}} \hat{H}|n(\boldsymbol{\xi})\rangle}{(\epsilon_m(\boldsymbol{\xi}) - \epsilon_n(\boldsymbol{\xi}))^2}. \tag{3.14}$$

To further apply our knowledge of electromagnetism, we can introduce the Berry curvature as a second-order tensor [4]

$$\Omega^n_{\mu\nu} = \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu, \tag{3.15}$$

which is explicitly given by

$$\Omega^n_{\mu\nu} = -2\Im \left\langle \frac{\partial n(\boldsymbol{\xi})}{\partial \xi^\mu} \,\middle|\, \frac{\partial n(\boldsymbol{\xi})}{\partial \xi^\nu} \right\rangle . \tag{3.16}$$

The relation between the tensor form and the Berry curvature vector is $\Omega^n_{ij} = \epsilon_{ijk}(\boldsymbol{\Omega}_n)_k$ with ϵ_{ija} being the Levi-Cevita tensor [3]. The tensor form of the Berry curvature is the form that will be most used in this study of Chern insulators.

It must be stressed that the similarities between classical electromagnetism and the Berry phase are purely mathematical in nature. The vector $\boldsymbol{\xi}$ is not necessarily three-dimensional, nor does it always denote coordinates in real space. Whenever the Berry phase is proportional to some magnetic flux it is only so because of the specifities of the system; it does not hold in general.

The Berry phase is geometric property of the parameter space of a quantum mechanical system. As such, it can be used to quantify the topology of parameter space. This is precisely what the Berry is used for in the study of Chern insulators. In the next section the Berry phase will be used to determine the current that can flow through a Chern insulator.

3.2 Quantised current

In the following section, the Berry phase will be connected to Chern insulators. It will be shown that in certain materials that are generally considerd insulators, it is possible to induce a current. This current is quantised, as will be shown in the upcoming subsection. Furthermore, using the Berry phase it will be shown that quantisation of the current is result of the topology of the parameter space of the material.

3.2.1 Derivation of the quantised current

The question we pose is: do certain insulators allow for a current under the condition that the potential is slowly varying? To answer this question, let us consider a quantum system that is a one-dimensional band insulator. Per definition, such an insulator has a Fermi energy that lies in between two energy bands. Let us apply a potential which is periodic in time t with period T, and in position x with period L. It was Thouless who showed that for such a system a current can be induced [15].

Because the system is periodic even with perturbation, it becomes useful to work with Bloch representation. The instantaneous eigenstates of the Hamiltonian are then given by $\exp(ikx)\,|u_{nk}(t)\rangle$, with k being the wave number. If the potential varies slowly enough, the adiabatic approximation can be used. Disregarding an irrelevant phase factor, the expression for the wavefunction is [3]

$$|\psi_{nk}\rangle \approx |u_{nk}\rangle - i\hbar \sum_{n' \neq n} \frac{|u_{n'k}\rangle \langle u_{n'k}|\partial_t u_{nk}\rangle}{(\epsilon_{n'} - \epsilon_n)}. \tag{3.17}$$

We will now use the following formal relationship between the Hamiltonian and the velocity operator [10]

$$v_n = \frac{1}{\hbar} \langle \psi | \partial \hat{H}/\partial k | \psi \rangle \,, \tag{3.18}$$

where $\hat{H}$ is the Hamiltonian of the system and $\hbar$ is the reduced Placnk constant. Thus, up to the same order as Eq. 3.17, the average velocity is

given by [3]

$$v_n = \frac{\partial \epsilon_n(k)}{\hbar \partial k} + \sum_{m \neq n} \left[\frac{\langle u_n | \partial_k \hat{H} | u_m \rangle \langle u_m | \partial_t u_n \rangle}{(\epsilon_m - \epsilon_n)} - h.c. \right]. \tag{3.19}$$

By using both the second Hellmann-Feynman theorem and the identity operator $\sum_m |\psi_m\rangle \langle \psi_m| = \mathbb{1}$, the expression becomes

$$v_n = \frac{\partial \epsilon_n(k)}{\hbar \partial k} - i[\langle \partial_k u_n | \partial_t u_n \rangle - \langle \partial_t u_n | \partial_k u_n \rangle]. \tag{3.20}$$

Observe that the second term in this equation is equal to the Berry curvature tensor Ω_{kt}. Thus, it is possible to symplify Eq. 3.20 as

$$v_n = \frac{\partial \epsilon_n(k)}{\hbar \partial k} - \Omega^n_{kt}. \tag{3.21}$$

Integrating Eq. 3.21 over the BZ, the first term disappears due to the periodicty of the system, and we are left with only the second-order term. Summing over all filled bands will therefore give us that the induced current is [3]

$$j = -\sum_n \int_{BZ} \Omega_{kt} \frac{dk}{2\pi}. \tag{3.22}$$

We are interested in the number of particles that are tansported after a period of time, T, has elapsed. For a single band we then find that the number of transported particles is given by [15]

$$c_n = -\int_0^T dt \int_{BZ} \Omega_{kt} \frac{dk}{2\pi}. \tag{3.23}$$

By integrating the Berry curvature over the BZ, we find the induced current in a Chern insulator. From the above derivation it is not clear why the particles transported should be an integer number. In the next section, the link between the Chern number and the above expression will be made, thus proving that the number of particles transported is an integer.

3.2.2 The Chern number

In the previous section it has been shown that the current in a Chern insulator is given by integrating the Berry curvature over the BZ. Such a surface integral can be related to a line integral over the boundary of that surface through Stokes' theorem. The BZ of a crystal, being a torus, does not have

a boundary; it follows that the integral of the Berry curvature over the BZ should be zero [20].

However, the previous argument does not apply when the topology of the parameter space is non-trivial. This occurs in systems where the gauge is not well behaved over the whole BZ. In such instances it is necessary to divide the BZ into sections, such that the gauge is well defined everywhere. The boundary between two such regions necessarily has a phase discrepancy, for otherwise the gauge could have been well defined over the whole BZ. Because of this phase discrepancy, an integer called the Chern number can be assigned to the system, representing the non-trivial topology of the parameter space of the system.

For the following derivation of the Chern number, let us assume that the BZ of a system can be divided into two regions, denoted as $\mathcal{S}_1$ and $\mathcal{S}_2$. At the boundary of these two regions, the phase discrepancy is [20]

$$|\psi_1\rangle = \exp(i\chi(\boldsymbol{\xi}))\,|\psi_2\rangle\,. \tag{3.24}$$

Here $|\psi_1\rangle$ represents the wave function in $\mathcal{S}_1$, and $|\psi_2\rangle$ represents the wave function in $\mathcal{S}_2$. Thus, the difference in the Berry connection between areas $\mathcal{S}_1$ and $\mathcal{S}_2$ at the boundary becomes [20]

$$\mathcal{A}_1(\boldsymbol{\xi}) = i\,\langle\psi_1|\partial_{\boldsymbol{\xi}}\psi_1\rangle = i\,\langle\psi_2|\partial_{\boldsymbol{\xi}}\psi_2\rangle - \nabla_{\boldsymbol{\xi}}\chi(\boldsymbol{\xi}) = \mathcal{A}_2 - \nabla_{\boldsymbol{\xi}}\chi(\boldsymbol{\xi}). \tag{3.25}$$

Using the difference in the Berry connection at the boundary, it will now be shown that the Berry phase must be an integer. By using Eq. 3.9 and applying Stokes' theorem, the Berry phase for the system is [20]

$$\gamma_n(\mathcal{L}) = \iint_{\mathcal{S}_1} \nabla_{\boldsymbol{\xi}} \times \mathcal{A}_1(\boldsymbol{\xi}) \cdot d\mathbf{S} + \iint_{\mathcal{S}_2} \nabla_{\boldsymbol{\xi}} \times \mathcal{A}_2(\boldsymbol{\xi}) \cdot d\mathbf{S} \tag{3.26}$$

$$= \oint_{\partial\mathcal{S}_1} \mathcal{A}_1(\boldsymbol{\xi}) \cdot d\boldsymbol{\xi} + \oint_{\partial\mathcal{S}_2} \mathcal{A}_2(\boldsymbol{\xi}) \cdot d\boldsymbol{\xi} \tag{3.27}$$

Since the BZ is a torus, and is thus without a boundary, it follows that $\partial\mathcal{S}_1 = -\partial\mathcal{S}_2$. This enables us to simplify the above equation as [20]

$$\gamma_n(\mathcal{L}) = \oint_{\partial\mathcal{S}_1} [\mathcal{A}_1(\boldsymbol{\xi}) - \mathcal{A}_2(\boldsymbol{\xi})] \cdot d\boldsymbol{\xi} \tag{3.28}$$

$$= -\oint_{\partial\mathcal{S}_1} \nabla_{\boldsymbol{\xi}}\chi(\boldsymbol{\xi}) \cdot d\boldsymbol{\xi}. \tag{3.29}$$

One can imagine $\nabla_{\boldsymbol{\xi}}\chi(\boldsymbol{\xi})$ as an arrow rotating while it moves along the curve $\partial\mathcal{S}_1$. The above integral represents the amount in radians that the arrow is rotated during its excursion over the curve [10]. Because of the single-valuedness of $\chi(\boldsymbol{\xi})$, the arrow will have to return to its initial value when it comes back to its starting point. Evidently the Berry phase has to be an integer times 2π.

3.2.3 Chern number in the two-level system

The simplest possible example of a system where the Berry phase manifests itself is in the two-level Hamiltonian. This system is a practical example of how the Chern number is a representation of the non-trivial topology of parameter space.

The two-level Hamiltonian is [6]

$$\hat{H}(\mathbf{k}) = \begin{pmatrix} h_0 + h_z & h_x - ih_y \\ h_x + ih_y & h_0 - h_z \end{pmatrix}. \tag{3.30}$$

Using the Pauli matrices, Eq. 3.30 can be rewritten as [6]

$$\hat{H}(\mathbf{k}) = h^{\mu}(\mathbf{k})\sigma_{\mu} = \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma} + \sigma_0 h_0, \tag{3.31}$$

with the Pauli vector $\boldsymbol{\sigma}$ and the matrix σ_0 being equal to the two-by-two identity operator $\mathbb{1}$. The energies of the two-level Hamiltonian are [6]

$$E_{\pm} = h_0 \pm \|\mathbf{h}\|. \tag{3.32}$$

The eigenstates for this Hamiltonian can be obtained by writing the vector $\mathbf{h}$ in spherical coordinates, $\mathbf{h} = (h\cos(\phi)\sin(\theta), h\sin(\phi)\sin(\theta), h\cos(\theta))$. Here θ represents the azimuthal angle and ϕ the polar angle. The eigenstates, as functions of θ and ϕ, are [3]

$$|\psi_-\rangle = \begin{pmatrix} \sin(\theta/2)e^{-i\phi} \\ -\cos(\theta/2) \end{pmatrix}, \qquad |\psi_+\rangle = \begin{pmatrix} \cos(\theta/2)e^{-i\phi} \\ \sin(\theta/2) \end{pmatrix}. \tag{3.33}$$

Using the enegry eigenstates of the Hamiltonian, the Berry connection can be determined. For the lowest eneregy eigenstate, the two vector components of the Berry connection are [3]

$$\mathcal{A}_{\theta} = \langle\psi_-|\partial_{\theta}\psi_-\rangle = 0, \qquad \mathcal{A}_{\phi} = \langle\psi_-|\partial_{\phi}\psi_-\rangle = \sin^2(\theta/2). \tag{3.34}$$

As stated previously, we shall look at the non-trivial topology of parameter space. As such, we shall only be concerned with the lower energy eigenstate. When evaluating the lower energy eigenstate at $\theta \to 0$, the phase of the wave function becomes ill-defined. By performing the gauge transformation [6]

$$|\psi_-\rangle \to \exp(i\phi)\,|\psi_-\rangle, \tag{3.35}$$

the ambiguity of the phase at $\theta \to 0$ can be lifted; but doing so will only shift the ill-defined region to $\theta \to \pi$. Thus, the wave function cannot be

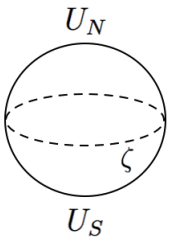

Figure 3.2: The regions U_N and U_S where the phase is well defined can be seen here [6]. The curve that represents the boundary of these regions is denoted as ζ.

both smooth and well defined over the whole BZ. In order to ensure the wave function is well defined at every point, it is necessary to divide the sphere into two regions, denoted here as U_N and U_S (see figure 3.2).

At the boundary ζ, where regions U_N and U_S meet, there is a discrepancy in the Berry connection $\mathcal{A}_{U_S} - \mathcal{A}_{U_N} = \boldsymbol{\nabla}\phi$. This discrepancy results in the Chern number becoming

$$c_1 = \frac{1}{2\pi} \oint_\zeta \boldsymbol{\nabla}\phi \cdot d\hat{\boldsymbol{\phi}}, \tag{3.36}$$

with $\hat{\boldsymbol{\phi}}$ being the unit vector in the direction of the polar angle. Therefore, the Chern number of the lowest energy band is $c_1 = 1$.

This derivation illustrates how the Chern number results from the phase discrepancy at the boundary of the two regions U_N and U_S, thus clarifying the relationship between the topology of the parameter space of the quantum mechanical system and the resulting Chern number.

3.3 Integer Quantum Hall Effect

The charge density wave can be mapped onto the integer quantum Hall effect (IQHE), a system that has been studied extensively. The setup of the IQHE consists of a two-dimensional electron gas moving in a plane, with a magnetic field applied perpendicular to this plane. The plane is defined by $0 < x < L_x$ and $0 < y < L_y$. There is also an electric field applied tangential to the plane. In the low temperature limit, the magnetic field will quantise the energy of the system into so-called Landau levels. The low temperature limit assures that the material will be an insulator, because the gaps between the Landau levels are much larger than the thermal excitations of the electrons. The name 'integer quantum Hall effect' derives from the fact that the conductivity of the system is quantised $\sigma_{xy} = (pe/2\pi\hbar)$ with $p \in \mathbb{N}$.

3.3.1 Landau levels

The Landau levels can be derived using the Hamiltonian for a system with a freely moving electron in an applied magnetic field [9]

$$\hat{H} = \frac{1}{2m}\left[(p_x - eH_0 y)^2 + p_y^2\right] + eE_0 y. \tag{3.37}$$

Here p_i represents the momentum operators of spacial direction i; e represents the charge of the electron; and H_0 and E_0 represent the magnitudes of the magnetic and electric fields respectively. For the magnetic field, the Landau gauge is used. For this system, p_x commutes with the Hamiltonian and is thus a constant of the motion. This allows the energy eigenstate of this system to be written as [9]

$$\exp(ik_x x)\phi_n(y - y'), \tag{3.38}$$

with ϕ_n representing the n^{th} energy eigenstate of the simple harmonic oscillator. The centre of this eigenstate is shifted to the new origin $y' = \hbar k_x / eH_0$, with k_x being the wave number in the x-direction. Here ω_c is the angular frequency eH_0/m. The energy of this Hamiltonian is given by [9]

$$\epsilon_{n,k} = (n + \frac{1}{2})\omega_c \hbar + \frac{1}{2} m (E_0/H_0)^2 + eE_0 y'. \tag{3.39}$$

The boundary conditions will now be imposed on these functions. Because the electrons are restricted from leaving the plane, the centre of the wave function needs to be within the area $S = L_x L_y$. This condition means that k_x is quantised [19]

$$k_x(m) = 2\pi m / L_x, \tag{3.40}$$

with $m \in \mathbb{N}$. Furthermore, because $0 < y' < L_y$, a second condition is that $0 < m < \Phi/\Phi_0$. Here $\Phi_0 = 2\pi\hbar/e$ and $\Phi = H_0 L_x L_y$ [19]. Because of this, we can write the centre of the wavefunction as [16]

$$y'_m = L_y \frac{\Phi_0}{\Phi} m. \tag{3.41}$$

3.3.2 Laughlin's argument

Laughlin has proposed an argument for the quantisation of the conductivity in the QHE, based on fundamental physical principles. Using gauge arguments, Laughlin proved the quantisation of the Hall conductances. The

following subsection will describe his proof, sometimes called Laughlin's argument.

Let us again consider a two-dimensional, non-interacting electron gas, with the slight alteration that the surface $0 < x < L_x$, $0 < y < L_x$ will now be made into a loop. This will be done by imposing the condition $(x, y) = (x, y + L_y)$. Note that the magnetic field is still perpenducular to every point on this loop (see figure 3.3). The Hamiltonian for this loop is similar to Eq. 3.37.

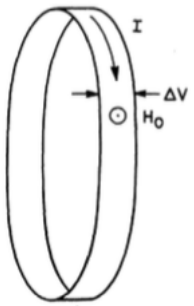

Figure 3.3: A loop with at every point a magnetic field perpendicular to it aswell as an applied electric field ΔV [9]. The current in this diagram is denoted with I.

To determine the current of the system, Laughlin used the formula [9]

$$I = -\frac{\Delta\epsilon_{n,k}}{\Phi_0}. \tag{3.42}$$

As noted before, Eq. 3.37 has solutions ϕ_n centred around $y_m = \hbar k_x(m)/eH_0$. The centre of these solutions is not gauge-invariant. Let us consider the gauge transformation that adds the vector $\Delta A\hat{x}$ to our original vector potential. Here $\hat{x}$ represents the unit vector in the x-direction of the material, such that this new gauge penetrates the loop through its centre. The change in the centre of the wave function is [9]

$$y_n \to y_n - L_x L_y \frac{\Delta A}{\Phi}. \tag{3.43}$$

However, not all ΔA are allowed. Only when ΔA is a multiple of $-\Phi_0/L_x$ does the system remain unchanged by the gauge transformation. For example, the gauge transformation $\Delta A = -\Phi_0/L_x$ transforms the centre of the n^{th} wave function as [16]

$$y_m \to y_m + L_y \frac{\Phi_0}{\Phi} = y_{m+1}. \tag{3.44}$$

It is evident that this gauge tranformation essentially shifts every particle from position m to $m+1$. It follows that the gauge transformation transports some charge through the loop. Seeing as the energy is purely electric, it is evident that $\Delta\epsilon_{n,k} = peV$, with p being the number of charged particles transported through the system. Using Eq. 3.45 this results in [9]

$$I = p\frac{e^2V}{2\pi\hbar}. \tag{3.45}$$

From this result it follows that $\sigma_{xy} = (pe/2\pi\hbar)$. Thus, it has been shown how the IQHE can be explained through gauge arguments.

3.3.3 Topology of the integer quantum Hall effect

Laughlin's argument has been extended by Halperin [17], who noted that Laughlin's argument points to the existence of a gapless edge state. This preludes the Chern number approach, since the Chern number can be thought of as proving the existence of edge states in a material. However, from the above derivation it is not instantly clear that the quantisation of the resistivity of the IQHE is topological in nature. This fact was first shown by Thouless, Kohmoto, Nightingale and den Nijs [11].

The Chern number for the IQHE has been derived by making use of the Nakabo-Kubo formula. This formula comes from linear response theory; for a derivation of the formula see source [16]. The Nakabo-Kubo formula is

$$\sigma_{xy} = -ie^2\hbar \sum_{\epsilon_\alpha<E_f} \sum_{E_f<\epsilon_\beta} \frac{(v_y)_{\alpha\beta}(v_x)_{\beta\alpha} - (v_x)_{\alpha\beta}(v_y)_{\beta\alpha}}{(\epsilon_\alpha - \epsilon_\beta)^2}, \tag{3.46}$$

with E_f being the Fermi energy and v_x and v_y the velocity operators [10]. This formula can be related to the Berry curvature by using the formal definitions of the velocity operators [10]

$$(v_i)_{\alpha\beta} = \frac{1}{\hbar}\left\langle \alpha|\partial\hat{H}/\partial k_i|\beta\right\rangle. \tag{3.47}$$

Using this formal relationship and invoking the second Hellmann-Feynman theorem, Eq. 3.46 becomes [10]

$$\sigma_{xy} = -i\frac{e^2}{\hbar} \sum_{\epsilon_\alpha<E_f} \sum_{E_f<\epsilon_\beta} \left(\left\langle \frac{\partial u^\alpha}{\partial k_2} \middle| \beta \right\rangle \left\langle \beta \middle| \frac{\partial u^\alpha}{\partial k_1} \right\rangle - \left\langle \frac{\partial u^\alpha}{\partial k_1} \middle| \beta \right\rangle \left\langle \beta \middle| \frac{\partial u^\alpha}{\partial k_2} \right\rangle \right). \tag{3.48}$$

Here, $|u^\alpha\rangle$ are the Bloch waves, with α denoting the quantum number related to energy. By further applying the identity operator, the expression becomes

$$\sigma_{xy}^{(\alpha)} = \left(\frac{e^2}{2\pi\hbar}\right) \frac{1}{2\pi i} \int_{BZ} d^2k \left[\nabla_k \times \mathcal{A}_\alpha(k_1, k_2)\right]_3 , \tag{3.49}$$

with $[...]_3$ denoting the third vector component, the Berry connection being $\mathcal{A}(k_1, k_2) = \langle u^\alpha | \nabla_k u^\alpha \rangle$, and ∇_k being the vector with elements $\partial/\partial k_1$ and $\partial/\partial k_2$. As has been shown in a previous section, this integral can be linked to a Chern number p. Thus, the conductivity becomes [10]

$$\sigma_{xy} = \frac{e^2}{2\pi\hbar} p. \tag{3.50}$$

This result is in agreement with that obtained in the previous section through Laughlin's argument. It shows the topological nature of the IQHE.

CHAPTER 4

Charge Density Wave

The charge density wave (CDW) is a one-dimensional crystal with phonon distortions that modulate the positions of the atoms, with the result that the atoms are no longer evenly spaced. The crystal is still invariant under discrete translations, but the length of these translations is enlarged. Because of this, the size of the unit cell is extended and the Brillouin zone is reduced in length, and a gap opens up in the energy bands of the system. Thus, under the right conditions, the CDW is insulating.

This chapter begins with a description of the charge density wave. It will show that the CDW has topological order, and that a slowly varying potential can therefore induce a current. The question of this research project was whether an analytical method of determining the Chern numbers for the CDW exists. This chapter will continue by proposing such an analytical method, and conclude with a discussion of possible shortcomings.

4.1 Rice-Mele model

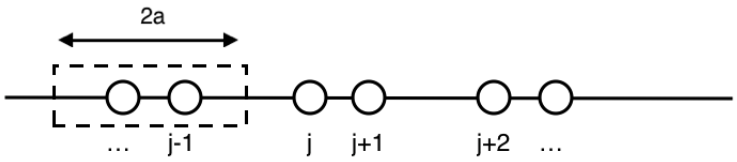

Figure 4.1: Shifted atoms

In order to understand the CDW let us first consider the Rice-Mele model. The Rice-Mele model is an altered version of the Hamiltonian discussed in the

previous section. Let us consider again Eq. 2.6. This time, an extra term is added to the Hamiltonian that represents phonon-electron interactions. These interactions slightly shift the positions of the atoms in the chain either to the right or to the left so that pairs of atoms are formed (see figure). The amount that the atoms are shifted is dependent on the magnitude of the phonon-electron interactions δt. The Hamiltonian for the Rice-Mele model is [3]

$$\hat{H} = \frac{1}{2}\sum_{j}\left\{[\delta t(-1)^j - t]c_j^\dagger c_{j+1} + h.c.\right\}. \tag{4.1}$$

The eigenvalue problem of this Hamiltonian can again be solved by using the Fourier transformation from Eq. 4.3. Doing so yields the Hamiltonian

$$\begin{aligned}\hat{H} = \sum_{k=-\pi/2a}^{\pi/2a} \{i\delta t[\sin(ak)c_{k+\pi/a}^\dagger c_k - \sin(ak)c_k^\dagger c_{k+\pi/a}] \\ + t[\cos(ak)c_k^\dagger c_k - \cos(ak)c_{k+\pi/a}^\dagger c_{k+\pi/a}]\}.\end{aligned} \tag{4.2}$$

For a step-by-step derivation of this Fourier transformation, see appendix A.4.

The Hamiltonian from Eq. 4.2 is somewhat complex to evaluate as it is. In order to simplify this equation, the Bogoliubov-DeGennes Hamiltonian can be used [18]

$$\hat{H} = \sum_{k=-\pi/2a}^{\pi/2a} \begin{pmatrix} c_k^\dagger & c_{k+\pi/a}^\dagger \end{pmatrix} \mathcal{H}(k) \begin{pmatrix} c_k \\ c_{k+\pi/a} \end{pmatrix}, \tag{4.3}$$

$$\mathcal{H}(k) = \begin{pmatrix} t\cos(ak) & i\delta t\sin(ak) \\ -i\delta t\sin(ak) & -t\cos(ak) \end{pmatrix}. \tag{4.4}$$

The eigenvalue problem of Eq. 4.3 is now reduced to finding the eigenvalue of $\mathcal{H}(k)$. The energy of this Hamiltonian is

$$E_\pm(k) = \pm\sqrt{t^2\cos^2(ak) + \delta t^2\sin^2(ak)}. \tag{4.5}$$

There are two important things to note about the Rice-Mele model. Firstly, as mentioned in the introduction to this chapter, a gap opens in the energy bands (see figure 4.2). This can be shown by evaluating Eq. 4.5 at the points $k = \pm\pi/a$. The gap is a result of the off-diagonal elements in $\mathcal{H}(k)$, which represent the interactions between different bands. The energy gap ensures that if the crystal is half filled with electrons, it will be insulating. Secondly, the density of electrons in the material becomes a cosinus [13]. This fact will be used to slide the charge density wave.

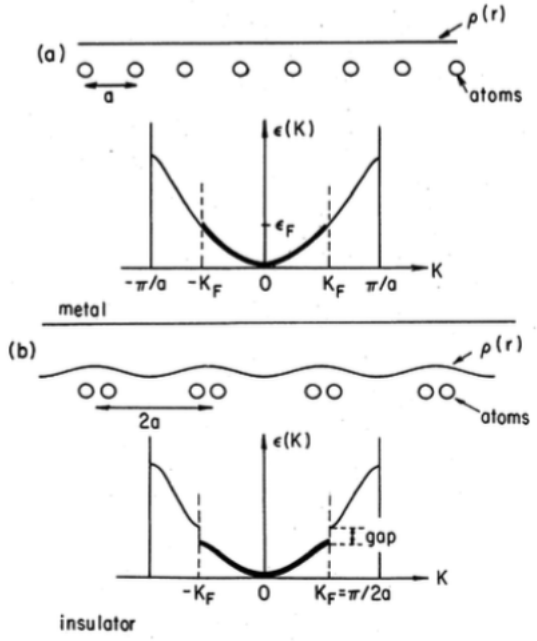

Figure 4.2: In figure (a) we see the energy of the charge density wave without phonon interactions [13]. In figure (b) we see the gap opening up and the BZ being reduced in size due to the phonon interactions. Furthermore, we see that the charge density becomes a cosinus in figure (b).

4.2 General Hamiltonian for the charge density wave

The Rice-Mele model demonstrates all of the important phenomena that are emblematic of the charge density wave. However, there is a more general formulation of the charge density wave that will be employed in this thesis. This model has been used in the study of CDWs before and originates in a paper by Flicker and van Wezel [14]. The Hamiltonian for this general charge density wave is [14]

$$\hat{H} = \frac{1}{2}\sum_{j}\Big\{[\delta t\cos\left(ajQ_n+\phi\right)-t]c_j^{\dagger}c_{j+1}+h.c.\Big\}; \tag{4.6}$$

here $Q_n = (2\pi/an)$, and ϕ is some arbitrary phase. For higher integers n, the number of atoms that cluster together becomes larger. Therefore, the unit cell of the system is enlarged in order to accommodate the new translationial symmetry of the system. An enlarged unit cell means a reduced Broullin zone in k-space. The physical interpretation of Q_n is that it is the length of the reduced BZ of the system.

Let us consider for what scenerios the CDW is insulating. First, let us denote the total number of electrons that can occupy the charge density wave with N_{tot}. When the BZ is reduced in length, the density of states remains unchanged. Because of this, when the length of the BZ is reduced by the fraction $1/q$ with $q \in \mathbb{N}$, the number of atoms that can occupy the lowest energy band is N_{tot}/q. The same holds true for the second-lowest energy band, but in order to fill the second-lowest energy band completely $2N_{tot}/q$ electrons are needed. Thus, for energy band p there are pN_{tot}/q electrons needed to fill up the band. Here p/q is called the filling fraction of the CDW [14].

The way in which charge can be transported through the charge density wave is by varying phase ϕ, such that after a certain time T the difference in ϕ is 2π. This is called sliding the charge density wave (see figure 4.3).

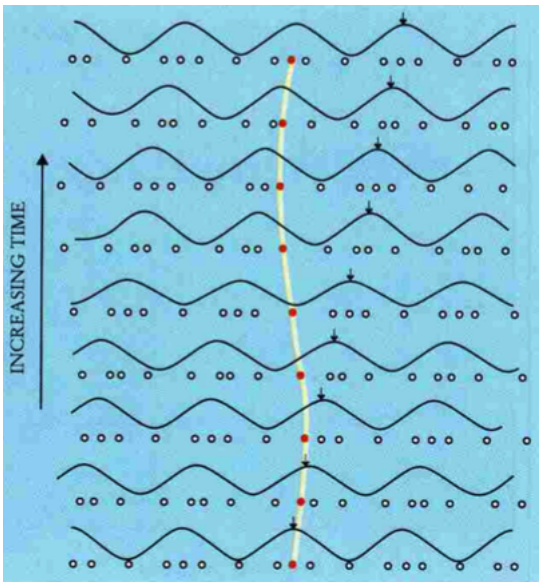

Figure 4.3: A charge density wave with a phase that is slowly changed through time [12]. It can be seen that after the phase has changed by 2π, the modulated atoms return to their initial position, but some charge has been transported.

4.2.1 Chern number for 1/3-filling

Let us look at the Chern number for the CDW with $n = 3$ and thus with $Q_3 = 2\pi/3a$ (the 1/2-filling fraction Hamiltonian will be discussed in a later section). The outline of determining the Chern number is as follows: first,

the energy eigenstates of the Hamiltonian need to be determined. Next an explicit expression of the Berry curvature tensor will be derived using the energy eigenstates. Finally the Berry curvature will be integrated over the BZ to yield the Chern number.

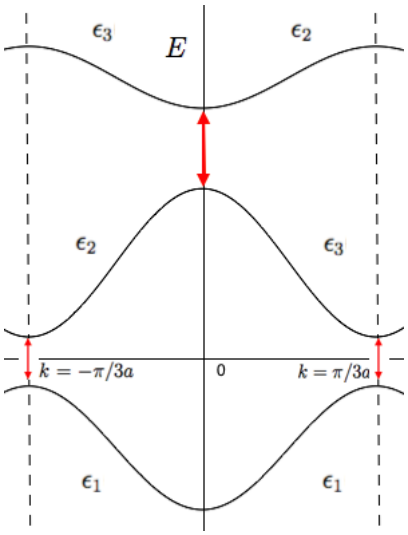

Figure 4.4: The figure represents energy bands of the charge density wave for $Q_3 = 2\pi/3a$. The graph show the energy plotted against the wave number k. The red arrows represent the points at which different bands interact with one another. Here ϵ_1, ϵ_2 and ϵ_3 denote the functions from 4.8. The symbols ϵ_1, ϵ_2 and ϵ_3 are so positioned that it can be seen at which points these functions should cross if there were no interactions between bands.

As such, let us start by finding the eigenvalues for our Hamiltonian. Using 4.6 and Fourier tranforming it, it can be shown that the Bogoliubov-DeGennes Hamiltonian is given by

$$\mathcal{H}(k,\phi) = \begin{pmatrix} \epsilon_1(k) & \delta t_1(k)e^{i\phi} & \delta t_2^*(k)e^{-i\phi} \\ \delta t_1^*(k)e^{-i\phi} & \epsilon_2(k) & \delta t_3(k)e^{i\phi} \\ \delta t_2(k)e^{i\phi} & \delta t_3^*(k)e^{-i\phi} & \epsilon_3(k) \end{pmatrix}, \tag{4.7}$$

with

$$\delta t_1(k) = \frac{\delta t}{2}\left[e^{-ia(k+Q_3)} + e^{iak}\right], \qquad \epsilon_1(k) = -t\cos(ak), \tag{4.8}$$

$$\delta t_2(k) = \frac{\delta t}{2}\left[e^{-iak} + e^{ia(k-Q_3)}\right], \qquad \epsilon_2(k) = -t\cos(ak + aQ_3), \tag{4.9}$$

$$\delta t_3(k) = \frac{\delta t}{2}\left[e^{-ia(k+2Q_3)} + e^{ia(k+Q_3)}\right], \quad \epsilon_3(k) = -t\cos(ak + 2aQ_3). \tag{4.10}$$

The matrix in Eq. 4.7 is quite complex. To avoid the difficulty of finding the exact eigenstates of this Hamiltonian, the system will be approximated. For this approximation, two facts are used:

- The points at which the diagonal elements of the matrix $\mathcal{H}(k,\phi)$ are degenerate act like sources of Berry curvature [3], and therefore determine the Chern number. Other points in the Brillouin zone are not of importance to the Berry curvature.
- The lowest diagonal energy ϵ_1 is degenerate at the points $k = -\pi/3a$ and $k = \pi/3a$.

Thus, the proposed method of finding the Chern number is as follows: firstly, determine the energy eigenstate at the points that are of importance for the Berry curvature. Secondly, define a smooth function between these points. Thus, an expression for the energy eigenstate has been found and the Berry curvature can be determined.

In order to find the energy eigenstates of Eq. 4.7 at the points $k = \pm\pi/a$, a further approximation is used. The degeneracies of the diagonal elements of Eq. 4.7 are lifted by the off-diagonal elements; thus, the off-diagonal elements are only of importance at the points $k = \pm\pi/a$. For example, near the point $k = -\pi/3a$ it is possible to write Eq. 4.7 as

$$\mathcal{H}(-\pi/3a,\phi) \approx \begin{pmatrix} \epsilon_1(-\pi/3a) & \delta t_1(-\pi/3a)e^{i\phi} & 0 \\ \delta t_1^*(-\pi/3a)e^{-i\phi} & \epsilon_2(-\pi/3a) & 0 \\ 0 & 0 & \epsilon_3(-\pi/3a) \end{pmatrix}. \quad (4.11)$$

We can do this because $\epsilon_1(-\pi/3a)$ and $\epsilon_2(-\pi/3a)$ are equal to one another at these points. Because we are determining the 1/3-filling fraction case, we are only interested in the lowest energy eigenstates. For the matrix 4.11, the eigenstate with the lowest energy is

$$|\psi(-a\pi/3)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{-i\phi}e^{i\pi/3} \\ 0 \end{pmatrix}. \quad (4.12)$$

The other point of interest is $k = \pi/3a$. By approximating the matrix such that only the off-diagonal terms δt_2 and δt_2^* are taken into account, it can be shown that the lowest energy eigenstate at this point is

$$|\psi(a\pi/3)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -e^{i\phi}e^{-i\pi/3} \end{pmatrix}. \quad (4.13)$$

In between these points the wave function should restore to being

$$|\psi(k)\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \tag{4.14}$$

because the interactions will no longer be of interest and the matrix will simply be diagonal.

A problem arises due to gauge freedom. Both Eq. 4.12 and Eq. 4.13 are determined up to a phase factor. Because of this, we will partition the BZ into two sections: $\mathcal{S}_1 = [-\pi/3a, 0]$ and $\mathcal{S}_2 = [0, \pi/3a]$. As such, let us write the wave functions in these regions as

$$|\psi_1(k,\phi)\rangle = \begin{pmatrix} \alpha_1(k) \\ \beta_1(k)e^{-i\phi}e^{i\pi/3} \\ \gamma_1(k) \end{pmatrix}, \quad |\psi_2(k,\phi)\rangle = \begin{pmatrix} \alpha_2(k) \\ \beta_2(k) \\ \gamma_2(k)e^{i\phi}e^{-i\pi/3} \end{pmatrix}. \tag{4.15}$$

Here $|\psi_1\rangle$ is the lowest energy eigenstate in region $\mathcal{S}_1$, and $|\psi_2\rangle$ is the lowest energy eigenstate in the region $\mathcal{S}_2$. Because of the normalisation condition on the wave function, α can be determined when β and γ are given. As such, we will only concern ourselves with β and γ. The values of these functions in the relevant regions are given in the table below.

	$k = -\pi/3a$	$k = 0$
β_1	$-1/\sqrt{2}$	0
γ_1	0	0

	$k = 0$	$k = \pi/3a$
β_2	0	0
γ_2	0	$-1/\sqrt{2}$

(4.16)

By using Eq. (3.23) the Chern number is given by

$$c_1 = \int_0^{2\pi} d\phi \int_{-\pi/3}^{\pi/3} \frac{dk}{2\pi} \Omega_{k\phi}. \tag{4.17}$$

Now the energy eigenstates from Eq. 4.15 can be used to find an expression for the Berry curvature $\Omega_{k\phi}$. The Berry curvature is explicitly given by

$$\Omega_{k\phi} = -2\Im \langle \partial_k \psi_- | \partial_\phi \psi_- \rangle . \tag{4.18}$$

Performing the calculation, a Chern number results

$$c_1 = \int_0^{2\pi} d\phi \int_{-\pi/3a}^{\pi/3a} \frac{dk}{2\pi} \Omega_{k\phi} \tag{4.19}$$

$$= -\beta_1^2(k)\Big|_{-\pi/3a}^{0} + \gamma_2^2(k)\Big|_0^{\pi/3a} \tag{4.20}$$

$$= -1 \tag{4.21}$$

Disregarding a minus sign, the result is in agreement with the values known from the literature [14].

4.2.2 Chern number for 2/3-filling

Having found the Chern number for the 1/3-filling case, let us now apply the proposed method to the 2/3-filling case. The matrix is again given by Eq. 4.7. This time we will look at the second-lowest energy eigenstate. As such, there will be only three points at which the off-diagonal terms need to be taken into account (see figure 4.2.1). These interactions play a role near the points $k = -\pi/3a$, $k = 0$ and $k = \pi/3a$. The first and last points are simply the same interactions from the previous section; only now they are the higher energy state. Because of this, the eigenstates are

$$|\psi(-\frac{\pi}{3a})\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{-i\phi}e^{i\pi/3} \\ 0 \end{pmatrix}, \qquad |\psi(\frac{\pi}{3a})\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ e^{i\phi}e^{-i\pi/3} \end{pmatrix}. \tag{4.22}$$

For brevity we will again use the symbol $|\psi\rangle$ here; however, here $|\psi\rangle$ represents the eigenstate of the second energy band. The degeneracy at point $k = 0$ results from the crossing of bands ϵ_2 and ϵ_3. Thus, the matrix at $k = 0$ is approximated as

$$\mathcal{H}(0,\phi) \approx \begin{pmatrix} \epsilon_1(0) & 0 & 0 \\ 0 & \epsilon_2(0) & \delta t_3(0)e^{i\phi} \\ 0 & \delta t_3^*(0)e^{-i\phi} & \epsilon_3(0) \end{pmatrix}. \tag{4.23}$$

Thus, it is evident that the eigenstate is

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -e^{-i\phi}e^{-i\pi/3} \end{pmatrix}. \tag{4.24}$$

Now that the second energy eigenstate has been determined for the relevant points, the Berry curvature can be calculated. As before, it will be necessary to devide the BZ up into different regions; in this instance, four regions are required. For a step-by-step derivation of the boundary conditions see appendix A.5. We can thus define the following functions:

$$|\psi_1\rangle = \begin{pmatrix} \alpha_1 \\ \beta_1 e^{-i\phi}e^{i\pi/3} \\ 0 \end{pmatrix}, \qquad |\psi_2\rangle = \begin{pmatrix} 0 \\ \alpha_2 \\ \beta_2 e^{-i\phi}e^{-i\pi/3} \end{pmatrix}, \tag{4.25}$$

$$|\psi_3\rangle = \begin{pmatrix} 0 \\ \beta_3 e^{i\phi}e^{i\pi/3} \\ \alpha_3 \end{pmatrix}, \qquad |\psi_4\rangle = \begin{pmatrix} \alpha_4 \\ 0 \\ \beta_4 e^{i\phi}e^{-i\pi/3} \end{pmatrix}, \tag{4.26}$$

with $|\psi_i\rangle$ being the second-lowest energy eigenstate in the i$^{\text{th}}$ region, and α being fully defined through the normalisation condition on $|\psi(k,\phi)\rangle$. The values of the functions β_1, β_2, β_3 and β_4 are given in the table below.

	$k=-\pi/3a$	$k=-\pi/6a$	$k=0$	$k=\pi/6a$	$k=\pi/3a$
β_1	$1/\sqrt{2}$	1	0	0	0
β_2	0	0	$-1/\sqrt{2}$	0	0
β_3	0	0	$1/\sqrt{2}$	0	0
β_4	0	0	0	1	$1/\sqrt{2}$

(4.27)

Using these facts, it can be show that the Chern number integral is given by

$$c_2 = \int_0^{2\pi} d\phi \int_{-\pi/3a}^{\pi/3a} \frac{dk}{2\pi} \Omega_{k\phi} \tag{4.28}$$

$$= \beta_1^2(k)\Big|_{-\pi/3a}^{-\pi/6a} + \beta_2^2(k)\Big|_{-\pi/6a}^{0} - \beta_2^2(k)\Big|_{0}^{\pi/6a} - \beta_2^2(k)\Big|_{\pi/6a}^{\pi/3a} \tag{4.29}$$

$$= 2 \tag{4.30}$$

This result is again in agreement with the Chern number values found in the literature [14]. Again, a minus sign appears to be missing, but the relative minus sign between c_1 and c_2 is correct.

4.2.3 Chern number for 1/2-filling

We will now return to the 1/2-filling CDW. It will be shown that this system does not have a Chern number.

The Hamiltonian from Eq. 4.6 can be evaluated using $Q_2 = \pi/a$. Using a Fourier transformation, the Bogoliubov-DeGennes Hamiltonian becomes

$$\mathcal{H}(k,\phi) = \begin{pmatrix} t\cos(ak) & i\delta t \sin(ak)\cos(\phi) \\ -i\delta t \sin(ak)\cos(\phi) & -t\cos(ak). \end{pmatrix} \tag{4.31}$$

The energy of this Hamiltonian can be shown to be

$$E_\pm = \pm\sqrt{t^2\cos^2(ak) + \delta t^2 \sin^2(ak)\cos^2(\phi)}. \tag{4.32}$$

It is evident that for the values $k = \pm\pi/2a$ and $\phi = \pm\pi/2$, the energy gap between the two surfaces closes. This means that for $n = 2$ the CDW is not an insulator and therefore cannot be a topological insulator either. Further confirmation of this fact is that when the Berry curvature from Eq. 3.14 is used to determine the Chern number, there are points at which the Berry curvature is infinity. This is precisely because the energy gap closes. As such, a Chern number for this case can not be calculated.

4.3 Discussion

In this chapter, a method for determining the Chern number in a CDW has been proposed. The method consists of several layers of approximations. First of all, the off-diagonal terms in the hamiltonian are only taken into account at points where the diagonal elements are degenerate. Subsequently, the energy eigenstates of the hamiltonian are determined at these precise points. The idea of the approximation is that these points act like sources for the Berry curvature and thus are the most vital to determining the Chern number.

The second layer of approximation occurs when, having found the energy eigenstates at all these different points, a smooth function is defined in between these points. However, when determining the eigenstates of the Hamiltonian, there is a freedom to chose the phase of the wave function. Thus, several regions are defined where the phases differ. The Berry curvature is integrated seperately in each of these regions. Having done so, the Chern number has been determined.

It seems that the above described method yields the right answer for at least two filling fractions. However, at many instances in the method, the gauge freedom is used. Thus it could be that the answers are correct only because there are many degrees of freedom in the system.

CHAPTER 5

Conclusion

This paper discussed Chern insulators and methods of determining the Chern numbers of charge density waves. First, an introduction to condensed matter physics was provided, using the Hubbard model. Furthermore it was shown that materials that have a Fermi energy that lies in a band gap are generally insulating. The thesis continued by discussing the theory behind topological insulators. Which are materials that also have a Fermi energy that lies in a band gap, but in which a current can nonetheless be induced. The number of particles transported throught the system has been linked to the systems topology through a Chern number. The Chern number was explained through the Berry phase. The general background of the project was closed by discussion of the integer quantum Hall Effect.

After the relevant background material was introduced, the charge density wave was discussed. Charge density waves are one-dimensional crystals of which the position of the atoms is modulated. This modulations reduces the length of the Brillouin zone and opens a band gap in the material. Thus when the charge density wave has the right number of electrons in it, it becomes insulating. Following this, methods for determining the Chern number of the charge density wave have been proposed. The method proposed allows one to approximate the Hamiltonian of the charge density wave. The energy eigenstate of the approximated Hamiltonian can be found and thus the Chern number can be calculated. This has been done in order to gain a deeper understanding of the workings of the charge density wave.

The proposed method goes as follows: firstly, determine the wave function at all places where there are degenerate states. Next, define regions that have smooth functions such that the Berry curvature can be calculated there. This method appears to work in at least two instances. Possible shortcomings of the method have been discussed, which include that there might be two many freedoms in the system.

APPENDIX A

First Appendix

A.1 Bloch waves

The following derivation originates from the book Solid State Physics [8]. Consider the vector $|\psi(x)\rangle$, which is an eigenvector of the Hamiltonian. As stated before, it should also be an eigenvector of the the translation operator

$$T_R \, |\psi(x)\rangle = c(R) \, |\psi(x)\rangle \, . \tag{A.1}$$

Here R and R' being a multiple of the lattice constant a. It can be readily deduced that the translation operators have the properties

$$T_R T_{R'} \, |\psi(x)\rangle = c(R) T_{R'} \, |\psi(x)\rangle = c(R)c(R') \, |\psi(x)\rangle \, , \tag{A.2}$$
$$T_R T_{R'} \, |\psi(x)\rangle = T_{R+R'} \, |\psi(x)\rangle = c(R+R') \, |\psi(x)\rangle \, . \tag{A.3}$$

When the translation operator commutes with the Hamiltonian of a system, the effects of the translations cannot be observed

$$\langle \psi(x+R) | \psi(r+R) \rangle = \langle \psi(x) | c^\dagger(R) c(R) | \psi(x) \rangle = \langle \psi(x) | \psi(x) \rangle \, . \tag{A.4}$$

The properties that the eigenvalues of the translation operator must adhere to are

$$c(R+R') = c(R)c(R'), \qquad \|c(R)\|^2 = 1. \tag{A.5}$$

It follows from these conditions that the eigenvalue of the translation operator is

$$c(R) = \exp(iRk). \tag{A.6}$$

Here k being the wave number.

A.2 Proof that the Berry connection is a real quantity

It is important that the Berry connection is a real number, in order for the Berry phase to be an observable quantity. It is assumed that the reader is familiar with the short-hand notation used here.

The normalisation condition on the eigenstate ensures that the Berry connection is real [5]. Note that the Berry connection is given by

$$-\Im \langle n|\nabla n\rangle \,. \tag{A.7}$$

Now, given the fact that the $\langle n|n\rangle = 1$, it follows that

$$\nabla \langle n|n\rangle = 0 \tag{A.8}$$

$$\rightarrow \langle n|\nabla n\rangle = -\langle \nabla n|n\rangle \tag{A.9}$$

$$\rightarrow \langle n|\nabla n\rangle^{\dagger} = -\langle n|\nabla n\rangle \,. \tag{A.10}$$

Thus, $\langle n|\nabla n\rangle$ is a purely imaginary number, and $A.7$ is purely real.

A.3 Second Hellmann-Feynman theorem

The following derivation comes from [21]. The fact that $|n\rangle$ is an instantaneous basis for $\hat{H}$, i.e.

$$\hat{H}\,|n\rangle = \epsilon_n\,|n\rangle\,, \tag{A.11}$$

allows us to prove the aforementioned identity. First, by applying the gradient to both sides of Eq. $A.11$, the expression becomes

$$(\nabla \hat{H})\,|n\rangle + \hat{H}\,|\nabla n\rangle = (\nabla \epsilon_n)\,|n\rangle + \epsilon_n\,|\nabla n\rangle\,. \tag{A.12}$$

Multiplying both sides of the equation with $\langle m|$, where $m \neq n$,

$$\langle m|\nabla \hat{H}|n\rangle + \langle m|\epsilon_m|n\rangle = \langle m|(\nabla \epsilon_n)|n\rangle + \epsilon_n\,\langle m|\nabla n\rangle\,. \tag{A.13}$$

Simplifying the equation thus gives us the aforementioned identity

$$\frac{\langle m|\,\nabla \hat{H}\,|n\rangle}{(\epsilon_m - \epsilon_n)} = \langle m|\nabla n\rangle\,, \qquad\qquad (m \neq n). \tag{A.14}$$

A.4 Rice-Mele model in k-space

The Rice-Mele model has a Hamiltonian that consists of a hopping term and phonon-interaction term

$$\hat{H} = \hat{H}_{hop} + \hat{H}_{int}. \tag{A.15}$$

In the following section, $\hat{H}_{int}$ will be Fourier transformed.

$$\hat{H}_{int} = \frac{\delta t}{2} \sum_j [(-1)^j c_j^\dagger c_{j+1} + h.c.] \tag{A.16}$$

First, note that $(-1)^j = \exp(aQ_2 ij)$, with $Q_2 = \pi/a$. By performing the Fourier transformation 4.3, this gives

$$\hat{H}_{int} = \frac{\delta t}{2N} \sum_{k,k',j} \left\{ c_k^\dagger c_{k'} \exp[aij(k - k' + Q_2)] \exp(-aik') + h.c. \right\}. \tag{A.17}$$

Invoking the identity $\sum_j \exp[aij(k - k' + Q_2)] = N\delta(k - k' + Q_2)$, yields the equation

$$\hat{H} = \frac{\delta t}{2} \sum_k \left\{ \exp[-ai(k + Q_2)] c_k^\dagger c_{k+Q_2} + h.c. \right\}. \tag{A.18}$$

Thus, the whole Hamiltonian in k-space becomes

$$\hat{H} = \sum_{k \in BZ} \left\{ \frac{\delta t}{2} \exp[-i(ak + \pi)] c_k^\dagger c_{k+Q_2} + t \cos(ak) c_k^\dagger c_k + h.c. \right\}. \tag{A.19}$$

It is not straightforward that this Hamiltonian is hermitian. By changing the summation bounds from $k \in \{-\pi/a, \pi/a\}$ to $k \in \{-\pi/2a, \pi/2a\}$ it is obtained that

$$\begin{aligned} \hat{H} = \sum_{k=-\pi/2a}^{\pi/2a} \{ & i\delta t[\sin(ak) c_{k+\pi/a}^\dagger c_k - \sin(ak) c_k^\dagger c_{k+\pi/a}] \\ & + t[\cos(ak) c_k^\dagger c_k - \cos(ak) c_{k+\pi/a}^\dagger c_{k+\pi/a}] \}. \end{aligned} \tag{A.20}$$

A.5 Boundary conditions on the energy eigenstates

The energy eigenstates of the second energy band of the charge density wave at the points $k = -\pi/3a$, $k = 0$ and $k = \pi/3a$ have been derived in chapter 4. Because of the fact that for other points in the BZ the off-diagonal elements of the Hamiltonian are left out of consideration, the Hamiltonian will consist out of merely the diagonal elements. This means that the energie eigenstates are given by

$$|\epsilon_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\epsilon_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\epsilon_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{A.21}$$

For $k = -\pi/6a$ the eigenstate becomes $|\epsilon_2\rangle$ and for $k = \pi/6a$ the eigenstate becomes $|\epsilon_3\rangle$. We now have the energy eigenstates at all necessary points. Using the gauge freedom the functions can be connected as follows:

$$|\psi(-\frac{\pi}{3a})\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{-i\phi}e^{i\pi/3} \\ 0 \end{pmatrix} \quad \rightarrow |\psi(-\frac{\pi}{6a})\rangle = \begin{pmatrix} 0 \\ e^{-i\phi}e^{i\pi/3} \\ 0 \end{pmatrix}. \tag{A.22}$$

For the second region

$$|\psi(-\frac{\pi}{6a})\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \rightarrow \quad |\psi(0)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -e^{-i\phi} \end{pmatrix}. \tag{A.23}$$

For the third region we find

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ e^{i\phi}e^{i\pi/3a} \\ 1 \end{pmatrix} \rightarrow \quad |\psi(\frac{\pi}{6a})\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{A.24}$$

For the fourth region

$$|\psi(\frac{\pi}{6a})\rangle = \begin{pmatrix} 0 \\ 0 \\ e^{i\phi}e^{-i\pi/3a} \end{pmatrix} \rightarrow \quad |\psi(\frac{\pi}{3a})\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ e^{i\phi}e^{-i\pi/3a} \end{pmatrix}. \tag{A.25}$$

Using these facts the choices for the values in table 4.27 can be shown to be the correct ones.

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