Integer and fractional quantum hall effects in lattice magnets

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CHAPTER 1

INTRODUCTION

The subject of this thesis is unconventional phases of matter in strongly correlated materials.

1.1 Strong correlations and topological states of matter

In the course of the past decade or so, a new and exciting field of condensed matter physics has opened up and expanded rapidly. It is the field of topological states of matter, which is centered around a material class called the topological insulators. The birth and subsequent development of this field was precipitated by a simple yet profound question: does the existance of an energy gap uniquely define the insulating state? It was believed that in a way, the atomic insulator (where electrons are uniquely associated to an atomic site and do not move), the band insulator (where an integer number of Bloch bands are filled and separated from empty bands by an energy gap) and, for instance, the vacuum essentially define the same insulating state in the sense that it takes a finite amount of energy to create an excitation in the ground state. However, as was shown in a series of seminal papers [1–5], the mere existance of an energy gap does not uniquely define the insulating state. It turns out that insulating states may be classified according to a global poperty, that for a given Hamiltonian

describing the insulating system, is obtained from the mapping from the Brillouin zone to the space of occupied energy bands corresponding to the Hamiltonian.

This classification is rather different from the way in which we are used to think about distinguishing phases of matter. The traditional way to distinguish phases of matter is due to Landau and assumes the presence of a *local* order parameter which represents the breaking of a symmetry. For instance, the crystalline solid breaks the translational symmetry of the underlying quantum Hamiltonian, while the longe-range magnetic order breaks rotational symmetry. The broken symmetry in a superconductor is related to the more subtle concept of gauge invariance. Hence, distinct phases break different symmetries. In contrast, the additional quantum numbers insulators may acquire in their ground state are given by a topological invariant, a *global* quantity. This invariant does not change when the system is smoothly deformed. The qualification smooth here pertains to the energy gap, which has to remain finite during deformation.

As such, the quantum numbers connected to the topological invariant of the system are insensitive to microscopic details, and the physical properties associated to these quantum numbers are uniquely robust. The fundamental property of a topological insulator material is the presence of gapless boundary or edge excitations at interfaces with topologically distinct systems, such as the vacuum itself. As the topological character cannot change without closing the energy gap, there must be gapless states precisely at the interface between electronic systems with different topology. Examples of this bulk-edge correspondence, which have been famously confirmed in experiment, include the spin-filtered one-dimensional edge states of the Quantum Spin Hall effect [6, 7] and the Dirac cone surface states of three dimensional time-reversal invariant topological insulators [8, 9]. While these two examples, and many others, can be understood from the theory of non-interacting electron band structure, topological states of matter are by no means restricted to non-interacting or weakly interacting systems. An increasing amount of attention is given to material systems where interactions are important. Even more, topology and strong interaction have a long and rich history. Indeed, the fractional quantum Hall effect [10] is a consequence of electron-electron interaction and the quantum Hall liquids hosting this effect are said to be topologically ordered [11]. The work reflected in this thesis is part of the general effort to study and understand the role and consequence of topology in (strongly) correlated materials.

In what follows, the very basis physics of topological states of matter is introduced with a focus on aspects that are relevant to the remainder of this thesis.

1.1.1 Integer and Fractional Quantum Hall effects

In this part of the introduction we review the basics of electrons in a (strong) magnetic field with two purposes in mind. As the second part of this thesis deals explicitly with lattice versions of both integer and fractional quantum Hall effects, some details of the continuum versions will be helpful. In subsequent chapters an understanding will then be developed of how they may be realized in a crystalline solid without external fields. In addition, the quantum Hall effects, in particular the Integer one, are a good starting point to uncover and explain the key role played by topology in electronic structure theory [12].

Previously in this introductory chapter, we have noted that lattice fermion model will be employed to describe electrons in solids. Here we briefly depart from that and consider free electrons subject to a magnetic field without any reference to a periodic crystal lattice. In fact, one of the questions addressed in this thesis is how and in what form do the Integer and in particular the Fractional Quantum Hall effects of the continuum description carry over to the crystal lattice description.

The Hamiltonian for free fermions in two dimensions is simply given by the kinetic energy term as

$$\hat{H} = \frac{1}{2m}\sum_{\alpha}\hat{p}_{\alpha}^{2}, \tag{1.1}$$

where $\hat{p}_\alpha$ is the momentum operator canonically conjugate to the position operator $\hat{r}_\alpha$, $\alpha = x, y$. In a magnetic field given by the vector potential $A_\alpha(\hat{r})$ we make the Peierls substitution, which amounts to

$$\hat{\Pi}_{\alpha} = \hat{p}_{\alpha} - eA_{\alpha}(\hat{r}) = -i\hbar\partial_{\alpha} + |e|A_{\alpha}(\hat{r}). \tag{1.2}$$

This changes the Hamiltonian to simply to $\hat{H} = \sum_\alpha \hat{\Pi}_\alpha^2/2m$. Due to the presence of the vector potential, the operators $\hat{\Pi}_j$ do not commute between themselves but instead are found to obey the canonical commutation relation

$$\begin{aligned}[\hat{\Pi}_{\alpha}, \hat{\Pi}_{\beta}] &= [\hat{p}_{\alpha} + |e|A_{\alpha}(\hat{r}), \hat{p}_{\beta} + |e|A_{\beta}(\hat{r})] \\ &= -i\hbar|e|F_{\alpha\beta}\end{aligned} \tag{1.3}$$

where $F_{\alpha\beta} = \partial_\alpha A_\beta - \partial_\beta A_\alpha$ is the field strength. We are interested in the situation of a uniform magnetic field B perpendicular to the plane in which the electrons live, i.e. the $\hat{z}$ direction. In general the magnetic field is given by $B_\lambda = \epsilon_{\lambda\mu\nu}F_{\mu\nu}/2$, meaning that $F_{\mu\nu} = \epsilon_{\mu\nu\lambda}B_\lambda$. In particular this implies for a uniform field $B_z \equiv B$ in the $\hat{z}$ direction that $[\hat{\Pi}_\alpha, \hat{\Pi}_\beta] = -i\hbar|e|B\epsilon_{\alpha\beta z}$. Defining the fundamental characteristic length scale in the system, the magnetic length, as $l = \sqrt{\hbar/(|e|B)}$, we can write

$$[\hat{\Pi}_{\alpha}, \hat{\Pi}_{\beta}] = -i\hbar^2\epsilon_{\alpha\beta z}/l^2. \tag{1.4}$$

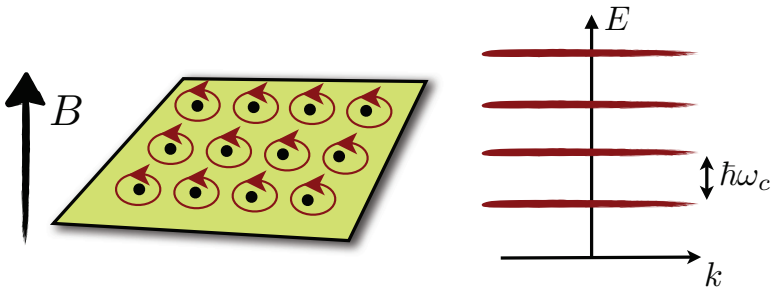

Figure 1.1: (left) Schematic illustration of the (classical) electronic cyclotron orbits in the presence of a magnetic field pointing in the z-direction. (right) Schematic illustration of the electronic Landau levels, i.e. the equidistant quantized energy levels, in the presence of a magnetic field.

Since Hamiltonian consists of the quadrature of operators obeying a canonical commutation relation one can diagonlize the Hamiltonian in the same way as the harmonic oscillator. We define the raising and lowering operators as

$$\hat{a}^\dagger = \frac{l}{\sqrt{2}\hbar}(\hat{\Pi}_x + i\hat{\Pi}_y), \qquad \hat{a} = \frac{l}{\sqrt{2}\hbar}(\hat{\Pi}_x - i\hat{\Pi}_y), \tag{1.5}$$

which obay $[\hat{a}, \hat{a}^\dagger] = 1$, we simple derive that the Hamiltonian takes the form $\hat{H} = \hbar\omega_c(\hat{a}^\dagger\hat{a} + \frac{1}{2})$ with $\omega_c = |e|B/m$ the corresponding frequency. We have thus achieved the diagonalization of the single-particle Hamiltonian, yielding energies $E_n = \hbar\omega_c(n + \frac{1}{2})$. Here n labels the energy levels, which are generally referred to as Landau levels, $n = 0$ corresponding to the lowest Landau level (LLL).

However, to fully characterize the quantum problem and account for all degeneracies, it is helpful to quickly revisit the classical cyclotron orbits. Classicaly, the position of a particle and its velocity in a circular orbit are given by

$$\begin{aligned} \vec{r} &= \vec{R} + r_0(\cos(\omega_c t), \sin(\omega_c t), 0), \\ \vec{v} &= r_0\omega_c(-\sin(\omega_c t), \cos(\omega_c t), 0) \end{aligned} \tag{1.6}$$

where $\vec{R}$ denotes the coordinates of the center of the orbit and r_0 is the radius of the orbit. Here ω_c is the cyclotron frequency of the orbit, which is equal to one used above. Classically momentum and velocity are related by $m_e\vec{v} = \vec{p}$. Using

equation (1.6) we may identify

$$\begin{aligned} \frac{p_x}{m_e\omega_c} &= -r_0\sin(\omega_c t) = \frac{l_B^2 p_x}{\hbar}, \\ \frac{p_y}{m_e\omega_c} &= r_0\cos(\omega_c t) = \frac{l_B^2 p_y}{\hbar} \end{aligned} \tag{1.7}$$

which has the consequence of Eq. (1.6) taking the simply form

$$\vec{R} = \vec{r} - \frac{l^2}{\hbar}(\vec{p}\times\hat{z}). \tag{1.8}$$

This relation between classical variables leads to the definition of the so-called guiding center operators $\hat{R}_x$ and $\hat{R}_y$ in the quantum case as

$$\hat{R}_\alpha = \hat{r}_\alpha - \frac{l^2}{\hbar}(\vec{\Pi}\times\hat{z})_\alpha = \hat{r}_\alpha - \frac{l_B^2}{\hbar}\epsilon^{\alpha\beta z}\hat{\Pi}_\beta. \tag{1.9}$$

These guiding center operators obey the commutation relation

$$[\hat{R}_\alpha, \hat{R}_\beta] = il^2\epsilon^{\alpha\beta z} \tag{1.10}$$

In addition, it is a simple matter to demonstrate that the dynamical momentum operators and guiding center operators commute with one another

$$[\hat{R}_\alpha, \hat{\Pi}_\beta] = [\hat{r}_\alpha - \frac{l^2}{\hbar}\epsilon^{\alpha\mu z}\hat{\Pi}_\mu, \hat{\Pi}_\beta] = i\hbar\delta_{\alpha\beta} + i\hbar\epsilon^{\alpha\mu z}\epsilon^{\mu\beta z} = 0 \tag{1.11}$$

This has the consequence that the guiding center operators commute with the Hamiltonian. One can construct momentum operators canonically conjugate to the guiding center operators, which are defined as

$$\hat{K}_\alpha = \hat{\Pi}_\alpha - \frac{\hbar}{l^2}(\hat{z}\times\hat{\vec{r}})_\alpha = \hat{\Pi}_\alpha - \frac{\hbar}{l^2}\epsilon^{\alpha z\beta}\hat{r}_\beta. \tag{1.12}$$

which are easily found to satisfy $[\hat{R}_\alpha, \hat{K}_\beta] = i\hbar\delta_{\alpha\beta}$. In addition, in the same way as above, the commutator with the dynamical momentum vanishes, $[\hat{\Pi}_\alpha, \hat{K}_\beta] = 0$.

To summarize this brief exposition, the single-particle Hamiltonian may be diagonalized by constructing raising and lowering operators frmo the dynamical momenta and both the guiding center operators and their canonically conjugate momenta commute with the Hamiltonian. For electrons in a uniform magnetic field we expect translational invariance to hold. When constructing operators that implement these translations we cannot use the dynamical momenta as generators, since they do not

commute with the Hamiltonian, i.e. $[\hat{\Pi}_\alpha, \hat{\Pi}_\beta] = -i\hbar^2\epsilon_{\alpha\beta z}/l^2$. The momenta $\hat{K}_\alpha$ do however commute with the Hamiltonian and the operator that implements a translation of a single particle by $\vec{a}$ is

$$\hat{T}(\vec{a}) = e^{ia_\alpha \hat{K}_\alpha/\hbar}. \tag{1.13}$$

The momenta $\hat{K}_\alpha$ do not commute between themselves, which has the profound consequence that different translations do not commute with each other

$$[\hat{T}(\vec{a}), \hat{T}(\vec{b})] = -2\sin\left(\frac{1}{2l^2}\hat{z}\cdot(\vec{a}\times\vec{b})\right)\hat{T}(\vec{a}+\vec{b}). \tag{1.14}$$

This commutation relation is known as the magnetic translation algebra or Girvin-MacDonald-Platzman (GMP) algebra [13] and lies as the heart of Quantum Hall and Fractional Quantum Hall physics [14]. In particular, it is precisely this relation that is responsible for the Aharonov-Bohm phase electrons pick up when encircling magnetic flux.

The GMP algebra can be recast in a different form by first defining a density operator based on the guiding center operators

$$\hat{\rho}(\vec{q}) = e^{iq_\alpha \hat{R}_\alpha}, \tag{1.15}$$

and since the guiding center operators are related to their conjugate momenta by the relation

$$\hat{R}_\alpha = \frac{l^2}{\hbar}\epsilon^{\alpha z\beta}\hat{K}_\beta \tag{1.16}$$

one may easily verify that the density operators thus defined satisfy an algebra equivalent to the one for the translation operators, given specifically by

$$[\hat{\rho}(\vec{q}), \hat{\rho}(\vec{q}')] = -2\sin\left(\frac{1}{2l^2}\hat{z}\cdot(\vec{q}\times\vec{q}')\right)\hat{\rho}(\vec{q}+\vec{q}'). \tag{1.17}$$

Hence, the GMP algebra is also satisfied by density operators constructed from the guiding center operators. Why these play a crucial role in particular for the fractional quantum Hall physics in the presence of interactions may be seen by considering the electron density operators $\bar{\rho}(\vec{p}) = \exp(ip_\alpha \hat{r}_\alpha)$ projected into the lowest Landau level. If $\hat{P}$ is the projector into the LLL, it is a simple matter to verify that

$$\hat{P}e^{ip_\alpha \hat{r}_\alpha}\hat{P} = e^{-q^2l^2/4}\hat{\rho}(\vec{q}). \tag{1.18}$$

We thus draw the consequential conclusion that the GMP algebra is obeyed by density operators when they are projected to the lowest Landau level. It may be argued in a

similar way that this holds for any Landau level labeled by n, however the LLL is the most prominent one, in which the fractional quantum Hall effect is observed.

The GMP algebra is of great importance for the physics of both the integer and the fractional Quantum Hall effect. Neglecting the interactions between electrons we may express the contribution of Landau level n to off-diagonal Hall conductivity in the form of the Kubo formula as [15]

$$\sigma_{xy}^{n} = \frac{e^2\hbar}{im_e^2}\frac{1}{2\pi l^2 N_\phi}\sum_{n'\neq n}\sum_{m,m'}\frac{\langle n,m|\hat{\Pi}_x|n',m'\rangle\langle n',m'|\hat{\Pi}_y|n,m\rangle - (x\leftrightarrow y)}{(E_n - E_{n'})^2}, \tag{1.19}$$

and using the relation $\hat{\Pi}_\alpha = im_e[\hat{H},\hat{r}_\alpha]/\hbar$ together with $P\hat{r}_\alpha P = \hat{R}_\alpha$ for any Landau level, one can derive

$$\sigma_{xy}^{n} = -\frac{ie^2}{2\pi l^2 N_\phi \hbar}\sum_{m}\langle n,m|[\hat{R}_x,\hat{R}_y]|n,m\rangle = \frac{e^2}{h}. \tag{1.20}$$

We conclude that each *filled* Landau level contributes one quantum of e^2/h to the Hall conductivity [16]. This is a direct consequence of the underlying noncommutative GMP algebra.

There is another way in which the GMP algebra is of crucial importance, which concerns the physics of the fractional quantum Hall effect, i.e. the explicit inclusion of Coulomb interactions. An electron-electron interaction of the form $V(\vec{r}_i - \vec{r}_j)$ translates into a Hamiltonian term

$$\sum_{i\neq j} V(\vec{r}_i - \vec{r}_j) \sim \sum_{\vec{q}} V(\vec{q}) \sum_{i<j} e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)} \tag{1.21}$$

where we have taken the system to live on torus geometry, the reciprocal lattice vectors $\vec{q}$ being related to the generators of the torus. The fractional quantum Hall effect is most clearly observed for rather large magnetic fields, in which case the degeneracy of a single Landau level is huge and one may restrict the Hilbert space to the lowest Landau level. The interaction takes the form

$$\sum_{\vec{q}}\sum_{i<j} V(\vec{q})\hat{\rho}_i(\vec{q})\hat{\rho}_j(-\vec{q})e^{-q^2l^2/2}, \tag{1.22}$$

with $\hat{\rho}_i(\vec{q})$ the aforementioned projected density operators. As the Hamiltonian is purely expressed in terms of these density operators, it is certainly not surprising that their algebraic properties and the organization of Hilbert space following from them are fundamental to the physics of the fractional quantum Hall effect. The algebra expressed in equation (1.17) is therefore at the heart of bringing the fractional Quantum

Hall effect from the continuum (electrons in a strong magnetic field) to the lattice (electrons in a periodic crystal with a band structure), which is the subject of part II of this thesis.

1.1.2 Chern Insulators and their generalizations

A key feature of Landau levels that was highlighted above is their contribution to the quantized Hall conductivity $\sigma_{xy} = e^2/h$, when a Landau level is completely filled [16]. Focusing on a single Landau level for the moment, we may express this property in a response equation given by

$$J_i = \sigma_H \epsilon^{ij} E_j, \tag{1.23}$$

where J_i is the current in the i-direction and E_i the i-th electric field component. This can actually be generalized to include the time t component, which gives the response equation

$$J_\mu = \sigma_H \epsilon^{\mu\nu\lambda} \partial_\nu A_\lambda. \tag{1.24}$$

One may functionally integrate this to obtain an effective action of the form

$$S[A_\mu] = \frac{\sigma_H}{2\pi} \int d^2\vec{r}dt \; \epsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda. \tag{1.25}$$

This action describes the fundamental low-energy electromagnetic field theory of the quantum Hall state [17].

One way – perhaps an unsual way – to make a connection to general topological states of matter is to ask the question: are there more states of matter that have an action of this form as their low-energy effective theory? Or, to reformulate this question, are there other insulators that have the same electromagnetic response equation? The answer to this question is "yes", and this affirmative answer is the first step towards a much broader class of distinct insulating states that cannot be adiabatically connected to the trivial atomic insulator.

Imagine we are given a material system governed by the Hamiltonian $\hat{H} = \sum_k \hat{\Psi}^\dagger(\vec{k}) \mathcal{H}(\vec{k}) \hat{\Psi}(\vec{k})$ (suppressing orbital and spin indices for convenience), and we are told that this defines an insulator. Then we may first obtain its Green's function $\mathcal{G}$, given by

$$\mathcal{G}(\omega, \vec{k}) = [\omega + i\delta - \mathcal{H}(\vec{k})]^{-1}, \tag{1.26}$$

and proceed to calculate the following quantity [18]

$$C = \frac{1}{4\pi} \int_{\text{BZ}} d^2k d\omega \; \epsilon^{\mu\nu\lambda} \text{Tr}\,[\mathcal{G}\partial_\mu \mathcal{G}^{-1} \mathcal{G}\partial_\nu \mathcal{G}^{-1} \mathcal{G}\partial_\lambda \mathcal{G}^{-1}], \tag{1.27}$$

where $\partial_\mu \equiv \partial/\partial k_\mu$. It can be proven that C is necessarily an integer [16, 18] and in addition is it clearly a "global" object, as it involves integration over the whole Brillouin zone (BZ). What does C have to do with equation (1.25)? The answer to that question can be expressed in a simple yet profound equation (setting $\hbar = e = 1$ for the moment),

$$\sigma_H = \frac{C}{2\pi}, \tag{1.28}$$

or in words, the integer C is the constant coefficient that multiplies the action and consquently determines the physical response, i.e. the Hall conductivity. As C is restricted to be integer, the Hall conductivity is quantized. For the Quantum Hall state induced by an external magnetic we have $\sigma_H = C = 1$, while in general it may be any number. For ordinary insulators one has $C = 0$.

For the sake of clarity and definiteness we may particularize to the situation of a two-band Hamiltonian, which can be expanded in the space Pauli matrices $\vec{\tau}$ as

$$\mathcal{H}(\vec{k}) = \varepsilon(\vec{k}) I_2 + \vec{d}(\vec{k}) \cdot \vec{\tau}. \tag{1.29}$$

This Hamiltonian has energies $E_\pm(\vec{k}) = \varepsilon(\vec{k}) \pm |\vec{d}(\vec{k})|$, which we assume to correspond to an insulator ($\min E_+(\vec{k}) > \max E_-(\vec{k})$, $\vec{k} \in$ BZ), and since $\varepsilon(\vec{k})$ multiplies the (2×2) identity matrix I_2, the eigenstate structure only depends on $\vec{d}$. Indeed, $\vec{d}(\vec{k})$ contains the information on the topological character of the electronic ground state of the system. Taking the Hamiltonian of equation (1.29) and substituting it into equation (1.27) yields an expression of C in terms of $\vec{d}(\vec{k})$

$$C = \frac{1}{4\pi} \int d^2k \; \epsilon^{\alpha\beta\gamma} \tilde{d}^\alpha \partial_x \tilde{d}^\beta \partial_y \tilde{d}^\gamma. \tag{1.30}$$

Here $\tilde{d}^\alpha(\vec{k}) = d^\alpha(\vec{k})/|\vec{d}(\vec{k})|$ is the normalized $\vec{d}$ vector. The normalized vector $\tilde{d}^\alpha(\vec{k})$ has unit length and thus lives on a sphere, which means we may interpret it as a mapping from the Brillouin zone, a 2-torus T^2, to the sphere S^2. The integrand in equation (1.30) is nothing but the Jacobian of this mapping, which implies that C counts the number of times the image of the mapping wraps around the sphere, which is clearly an integer and cannot change under smooth deformation of the mapping given by $\tilde{\vec{d}}(\vec{k})$. This establishes C as a topological invariant [18]. The integer invariant C is generally referred to as the Chern number, a term borrowed from mathematics. It has become customary to refer to insulators with nonzero C as *Chern insulators*. Chern insulators are systems in the same universality class as the quantum Hall state, and thus fundamentally distinct from "ordinary", or atomic insulators.

As a spoiler for chapter 7, an example of a Chern insulator having $C \neq 0$ is

$$\mathcal{H}(\vec{k}) = \cos k_1 \tau^x + \cos k_2 \tau^y + \cos k_3 \tau^z. \tag{1.31}$$

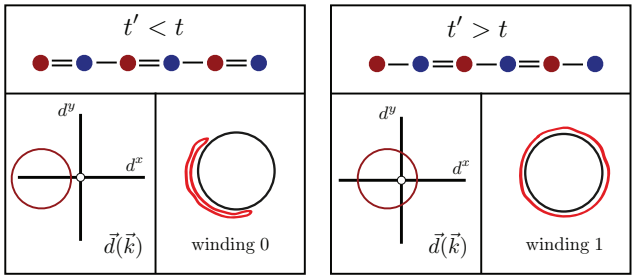

Figure 1.2: The two different topological sectors of the $1D$ Peierls chain discussed in the text. Left, the situation $t' < t$ in which case the d-vector does not wrap around the circle as one traces the $1D$ Brillouin zone (equivalent to a circle). Right, on the other hand, the situation $t' > t$, in which case the d-vector wraps around the circle once.

Here $k_i = \vec{k} \cdot \vec{x}_i$ $(i = 1, 2, 3)$ and $\vec{x}_i$ are lattice vectors of length a making an angle $2\pi/3$ with each other. It corresponds to electrons hopping on the triangular lattice with a flux of $\phi = \pi/2$ threading each triangle. Using equation (1.30) one finds that for this Hamiltonian the insulating round state is characterized by $C = 1$.

At this point a few comments with regard to equation (1.25) are in order. First, by looking at the integrations we notice that this action applies to a two-dimensional $(2D)$ system. Consequently, all considerations above apply to $2D$ systems. Second, it can be checked by looking at the transformation of the electromagnetic field A_μ under time-reversal, that the actions represents a time-reversal symmetry broken state. These observations are a manifestation of the crucial importance of both symmetry and dimensionality in classifying topological phases. The class of systems defined by nonzero C must live in $2D$ and do not require any symmetry. Other topological phases, which can exist in for instance one or three dimensions and have distinct physical properties, often require the presence of a symmetry. To illustrate this we briefly review a famous example in $1D$, the Peierls chain realized in polyacetylene [19].

Imagine a $1D$ chain of atoms with alternating hopping integral t and t', where one is weaker and one is stronger $t > t'$ (or $t < t'$). This is graphically shown in Fig. 1.2, where the two different cases are shown on the right (left) side. The alternation of stronger and weaker bonds mandates a two-site unit cell, with atoms A and B, and the Hamiltonian describing this system can again be expanded in Pauli matrices, now representing the sublattice degree of freedom,

$$\mathcal{H}(k) = \vec{d}(k) \cdot \vec{\tau}, \quad \vec{d}(k) = (t + t' \cos k, \sin k, 0) \tag{1.32}$$

Crucially, since hopping takes place only between A and B atoms, we have $d^z(k) = 0$. This forces the $\vec{d}$ vector to be in the $x-y$ plane and it defines a mapping from the $1D$ Brillouin zone, i.e. the circle, to the $2D$ plane. It is easy to check that for $t \neq t'$ the system is insulating. The topological nature of this insulating state is revealed by taking a closer look that the mapping from the circle to the $x-y$ plane defined by $\vec{d}$. The loop mapped out in the $x-y$ plane either encircles the origin or it does not. In Fig. 1.2, for both $t < t'$ and $t > t'$, the lower left square shows the red loop traced out by the $\vec{d}$-vector as function of $\vec{k}$. The origin is special because there $\vec{d} = 0$ and the insulating gap would vanish. If the loop does not enclose the origin, such as in the left of Fig. 1.2, we can smoothly deform it to a single point, representing the atomic insulator, without closing the energy gap. However, if $\vec{d}(k)$ does enclose the origin, see right side of Fig. 1.2, we cannot do so, and this situation defines a topologically distinct state. In essence, since we must exclude the origin from the plane; we are classifying mappings from the circle to the circle, which are known to come with an integer index: the number of times the image wraps around the target circle. This is schematically depicted in the lower right boxes of Fig. 1.2, where the red "circles" are mapped to the black circles and either wrap around the black circle once (right) or not at all (left). For the Peierls Hamiltonian expressed in equation (1.32) the topological winding number is therefore 1.

How do symmetry and dimensionality manifest themselves? A symmetry constrains the Hamiltonian so that the $\vec{d}$-vector cannot have a z-component. The symmetry is a chiral symmetry and expressed as an anti-commutation relation

$$\{\mathcal{H}, \tau^z\} = 0. \tag{1.33}$$

This relations forces $d^z(k) = 0$ and it furthermore ensures that every state $|\psi\rangle$ of energy E has a partner τ^z at energy $-E$. If $d^z(k)$ was not forced to be zero, but allowed to take arbitrary values, then our argument for distinguishing loops would not hold anymore. Any loop could be smoothly contracted to a point by using the z-component of the $\vec{d}$-vector. In other words, instead of classifying mappings from a circle to a circle, we would be classifying mappings from the circle to the sphere. Mappings of the latter kind are all trivial, as they can always be continuously deformed to a single point on the sphere [20].

Symmetry and dimensionality are fundamental. One of most prominent symmetries permitting a topological classification of insulators in $2D$ and in $3D$ is time-reversal symmetry [1–5, 21, 22]. Up until now, we have discussed topological classifications based on integers. The Chern number C can take any integer value, and the $[d^x(k), d^y(k)]$ vector may in principle encircle the origin any number of times, depending on the form of the Hamiltonian.

Time-reversal symmetry, however, leads to a $\mathbb{Z}_2$ classification, which is to say that there are only two flavors, trivial and nontrivial – topological and non-topological [1–

5]. Real materials belonging to the class of nontrivial systems are then generally refered to as time-reversal invariant topological insulators. Dimensionality is again important. In two dimensions a time-reversal invariant topological state is referred to as the Quantum Spin Hall state [1, 23]. The physical manifestation of the topological nature of the electronic state is the existance of an odd number of spin-filtered counterpropagating edge state pairs. The locking of propagation direction and spin polarization implies the requirement of spin-rotation symmetry breaking, at least partially. Not surprisingly, strong spin-orbit coupling plays a key role in the field of topological insulators. In chapter 10 we will see examples of precisely such two-dimensional Quantum Spin Hall states, where the spin-rotation symmetry breaking comes from electronic interactions. In three dimensions spin-rotation symmetry must be completely broken in order for an insulator to be a topological insulator. The physical consequence of non-trivial topology in three dimensions is the presence of an odd number of two-dimensional Dirac fermions at a sample surface. This is forbidden in a genuinely two-dimensional electronic system [24]. In both two and three dimensions we see that odd and even (edge or surface states) are clearly distinguished when it comes to the physical manifestation of non-trivial topology, which essentially defines the $\mathbb{Z}_2$ classification of time-reversal invariant topological insulators.

Other symmetries giving rise to topologically insulating systems with robust physical properties mandated by their topological character are particle-hole symmetry and the product of time-reversal and particle-hole symmetry, often called sublattice symmetry or chiral symmetry. The robustness follows from the fact that disorder may respect these symmetries and therefore cannot harm the physical consequences of the topological nature of a quantum state. A complete classification based on these three symmetries has been achieved and has resulted in the "periodic table" of topological insulators [21, 22].

1.2 Strongly correlated electrons and electronic degrees of freedom

Generally speaking there are two points of departure for describing electrons in solids. One is to start from the free electron gas and subject the electrons to a weak periodic potential originating from the crystal lattice. Wave functions obtained by solving Schrödinger's equation are perturbed and modified by the periodic potential, which results in the typical band structure of crystalline solids. The other is to picture the electrons as still associated to the atoms of the crystal and construct the electron wave function from corresponding atomic orbital functions. Due to the periodic array of atoms, the atomic wave functions overlap and electrons may tunnel, or "hop", from

atom to atom. The latter approach is referred to as the tight-binding description of electrons, as they are considered to be tightly bound to the atomic sites of the lattice.

Which perspective to adopt depends to a large extent on what objective one has set out to achieve. In this thesis we will work with the tight-binding description, or alternatively called lattice fermion model, as it is the method of preference for addressing materials with strong correlations between electrons from a model Hamiltonian perspective. The prototype of such a model Hamiltonian, designed to capture the essential physics of strongly correlated electrons, is the famous Hubbard model. The Hubbard model is given by the following equation

$$\hat{H}_{\mathrm{HM}} = \sum_{ij} t_{ij} \hat{\psi}^{\dagger}_{i\sigma} \hat{\psi}_{j\sigma} - \mu \sum_{i} \hat{n}_i + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \qquad \textbf{H}\text{ubbard }\textbf{M}\text{odel} \qquad (1.34)$$

and here $\hat{\psi}^{\dagger}_{i\sigma}$ ($\hat{\psi}_{j\sigma}$) are second-quantized operators which create (annihilate) an electron at lattice site i with spin σ, where σ can take the values "$\uparrow$" and "$\downarrow$". The matrix t_{ij} represents the overlap integral of atomic wave functions on site i and site j. In the most simple cases one only considers finite overlap between nearest neighbor sites which is taken to be uniform, i.e. $t_{ij} \to t$. In general however the most important assumption is translational invariance $t_{ij} = t_{-i+j}$. The chemical potential μ controls the particle number, as $\hat{n}_i = \sum_{\sigma} \hat{\psi}^{\dagger}_{i\sigma} \hat{\psi}_{i\sigma}$ is the number operator.

The third term represents the repulsive Coulomb interaction between electrons and assigns an energy penalty of U to two electrons sitting on the same atomic site. Fermi statistics require these electrons to have opposite spin. This form of the interaction term is a substantial simplification as it only takes into account the Coulomb interaction of electrons at the same site. In general, for electrons in close proximity yet different atomic sites there is a repulsive Coulomb force as well, however the screening effect causes the longe-range part of the Coulomb interaction to be weak, which justifies the retaining of only on-site repulsion.

Despite its apparent simplicity, the above Hamiltonian is notoriously hard to solve. Nevertheless, advanced and often involved numerical as well as analytical techniques have achieved considerable progress in applying the Hubbard model to the physical phenomena in real materials. One general approach is to focus on the regime of very strong interaction, i.e. $U \gg t$. In this strong coupling regime doubly occupancy of the same site is very strongly disfavored. In particular at half filling Hilbert space is most conveniently organized by the number of doubly occupancies. The lowest energy sector is the one with no doubly occupied sites. As charge excitations are very expensive in terms of energy, the proper picture of this sector of Hilbert space is that of localized spins. The effective interaction between these localized

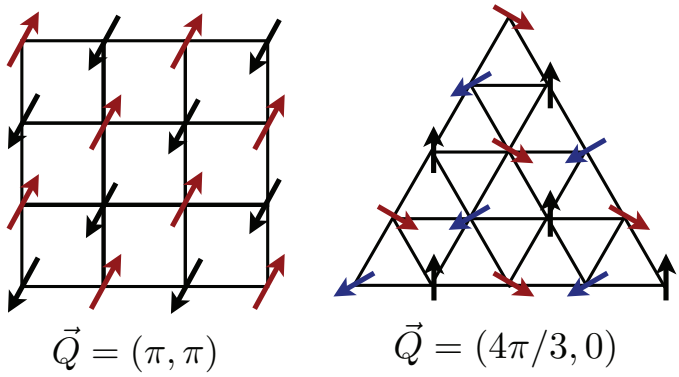

Figure 1.3: Illustration of spin configurations that represent the classical ground state of the Heisenberg spin model on the square lattice (left) and the triangular lattice (right). On the square lattice spins are anti-parallel on neighboring sites, realizing the collinear anti-ferromagnet. Due to frustration of the triangular lattice the spins do not order in a anti-parallel collinear pattern, but make an angle of $2\pi/3$ with one another.

spins is captured by the Heisenberg Hamiltonian which takes the form

$$\hat{H}_{\text{HB}} = \sum_{ij} J_{ij} \vec{s}_i \cdot \vec{s}_j \qquad \textbf{H}\text{eisen}\textbf{b}\text{erg Hamiltonian} \tag{1.35}$$

where the spin operators $\vec{s}_i$ are given in terms of fermions as

$$\vec{s}_i = \hat{\psi}^\dagger_{i\sigma} \vec{\sigma}_{\sigma\sigma'} \hat{\psi}_{i\sigma'}, \tag{1.36}$$

where the the vector $\vec{\sigma}$ represents the spin Pauli matrices, i.e. $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$. That the effective interaction between spins should have this form may be understood by considering virtual processes out of and back into the singly occupied subspace. If electrons on neighboring sites occupy opposite spin states, virtual processes with amplitude $\sim t^2/U \simeq J$ are allowed by the Pauli principle and electrons can lower their energy in this way. Hence, in the general case one has $J_{ij} = J = +|J|$ and the effective interaction is anti-ferromagnetic. A virtual process of this kind is also referred to as a superexchange process, and the Heisenberg Hamiltonian is alternatively named superexchange Hamiltonian. In strong coupling and at half filling the system is an insulator, as there are no charge excitations, and the Heisenberg Hamiltonian pertains solely to the magnetic state of the system. The canonical approach that leads

to an understanding of the magnetic ground state is to consider the electron spin $\vec{s}_i$ as a very large spin, i.e. $|\vec{s}_i| \gg 1$, and treat it a classical spin. The latter means that we disregard for the moment that it actually represents an operator acting on a finite dimensional Hilbert space, but instead picture it as a classical $O(3)$ vector pointing in any direction in space. Particularizing to the simple square crystal lattice, and keeping only nearest neighbor magnetic interactions ($J \sum \vec{S}_i \cdot \vec{S}_j$), it is straightforward to deduce that the (classical) energy on each bond is minimized by anti-parallel spin, i.e. $J\vec{S}_i \cdot \vec{S}_j = -JS^2$ if $\vec{S}_i = -\vec{S}_j$, S being the magnitude of the spin. On the square this leads to the anti-ferromagnetic spin state, as depicted in Fig. 1.3.

The situation is different for a different crystal lattice, the triangular lattice (see Fig. 1.3). Due to lattice connectedness it is not possible to have spins on all neighboring sites aligned anti-parallel consistently. This is an example of frustration: the energy cannot be simultaneously minimized on each and every bond. The solution to this problem is for the spins to arrange so as to optimally relieve the frustration, in this particular case by making angles of $2\pi/3$ with each other. This noncollinear but coplanar order is thus a consequence of frustration.

The example of the triangular lattice already hints at the key role the crystal structure plays in the manifestation of magnetism in real materials. Even more complicated behaviour is expected and observed for kagome lattice compounds, or compounds which approximately realize a kagome structure. The kagome lattice consists of corner sharing triangles, which directly results in a macroscopic degeneracy of (classical) magnetic ground states. From the triangular lattice we learned that on each triangle the spins are coplanar but make an angle of $2\pi/3$. For corner sharing triangles this does not fix all spins and a huge number of configurations satisfying the energetic constraints exist. This is reflected in thermodynamic quantities and leads to exotic phenomena such as spin-liquid behaviour.

Even though the pictorial representation of spins as classical arrows such as in Fig. 3.3 provides an intuitive understanding of the magnetism observed in materials, one should not forget that the electron spin is a quintessentially quantum mechanical object. The assumption of large spin, $|\vec{s}_i| \gg 1$, is not at all justified for the electron spin, which has length $1/2$. Quantum corrections need to be taken into account and the general recepy to do that is spin-wave analysis. Spin-waves are collective excitations on top of the ordered classical state, in the same way as lattice distortions (*phonons*) are collective modes corresponding to the ordered crystal. Depending on the lattice structure, quantum fluctuations may either give corrections to the classical state, or completely invalidate the classical description and necessitate new physical concepts. Away from half filling, when one cannot think of all sites as being occupied by precisely a single electron, hopping processes become possible again, as their will be empty sites (for either electrons or holes). In this case the Heisenberg Hamiltonian

needs to be supplemented with a hopping term

$$\hat{H}_{\mathrm{DLU}} = \sum_{ij} t_{ij} \hat{P} \hat{\psi}^{\dagger}_{i\sigma} \hat{\psi}_{j\sigma} \hat{P} + \hat{H}_{\mathrm{HB}}, \qquad \textbf{D}\text{oped } \textbf{L}\text{arge } \textbf{U} \text{ Model} \tag{1.37}$$

and the projection operators $\hat{P}$ make sure that doubly occupied sites are excluded.

The most drastic simplification of the Hubbard model given in equation 1.34 is its single-band nature. Orbital degeneracy is however ubiquitous in real materials and neglecting the orbital degree of freedom of electron wave-functions can be a major distortion of reality. In some cases that may be legitimate and sufficient to capture the essential features, as for instance in many cuprates, where only the $d_{x^2-y^2}$ orbital is close to the Fermi level. In many cases however, in particular widely studied d-electron systems, orbital degeneracy is an unavoidable source of complicated behaviour.

A prime example of the relevance of orbital physics are the Mn and Co ions. The Mn may exist in a Mn^{4+} or Mn^{3+} valence state. In the latter case the t_{2g} orbital manifold contains three electrons and is separated from the the e_g orbitals by a cubic crystal field originating from the local octahedral oxygen environment. Hund's rule coupling aligns the three spins in the t_{2g} sector, effectively creating a larger $S = 3/2$ localized "core" spin, and putting the remaining electron in an e_g orbital. The splitting between e_g and t_{2g} is generally large, justifying the assumption of localized t_{2g} spins. This particular physical picture will reappear many times in the remainder of this thesis. Figure 1.4 schematically summarizes these considerations for d-electrons in a cubic environment.

A simple model Hamtiltonian that captures the essentials of an e_g electron interacting with a large localized spin is given by the Kondo-Lattice or Double-Exchange Hamiltonian,

$$\hat{H}_{\mathrm{KLM}} = \sum_{ij} t_{ij} \hat{\psi}^{\dagger}_{i\sigma} \hat{\psi}_{j\sigma} + J_{\mathrm{Kondo}} \sum_{i} \vec{\mathcal{S}}_i \cdot \vec{s}_i, \qquad \textbf{K}\text{ondo } \textbf{L}\text{attice } \textbf{M}\text{odel} \tag{1.38}$$

which explicitly couples an electron spin $\vec{s}_i$ to a "core" spin $\vec{\mathcal{S}}_i$ on every site i. Even though this simplified version does not even take into account the orbital flavor of itinerant electron, it certainly derives from orbtal physics. This double-exchange model has proven very successful in particular in describing Mn based materials, where large J_{Kondo} leads to wide range of ferromagnetic metal in the phase diagram. The ferromagnetic tendency build into this model, as opposed to the anti-ferromagnetic interaction of the Heisenberg model, and the corresponding transition to a ferromagnetic metal is intimitely related to the observed colossal negative magnetoresistance in these materials. The Kondo-Lattice model of equation (1.38) is at the heart of Part I of thesis. In Chapter 2 the Kondo-Lattice model will be discussed in more details

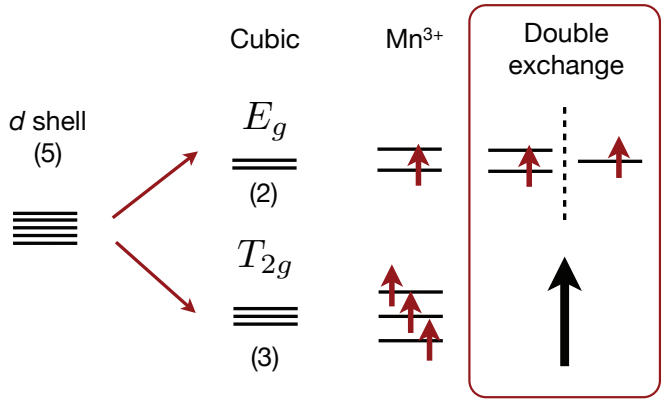

Figure 1.4: Illustration of the significance of electronic orbital degrees of freedom. The five-fold degenerate d-levels are split by the crystal field with cubic symmetry into an E_g and a T_{2g} manifold, two-fold and three-fold degenerate, respectively. In a manganese ion, three electrons occupy the T_{2g} manifold, with their spins aligned by Hund's coupling. The itinerant electron(s) in the E_g manifold effectively "see" a spin of length $3/2$, as is shown on the right in the red box. Depending on the strength of the coupling to this localized spin, the itinerant electrons can be either both aligned and anti-aligned, the latter costing energy, or can only be aligned (very strong coupling).

and different approaches to apply and study it in specific cases will be presented. Then, in Chapters 3 and 4 the Kondo-Lattice model and its derivative version, the Double-Exchange model will be the starting point for addressing the physics of interacting local moments and itinerant electons on the honeycomb and checkerboard lattice, respectively. It will be demonstrated how lattice topology and competing ordering tendencies (ferromagnetic vs. antiferromagntic) lead to a rich magnetic and electronic phase diagram.

Increasing the degree of complexity and taking full account of orbital degeneracy leads to an involved Hamiltonian with a number of distinct interaction terms. It is precisely such a Hamiltonian that will be the object of study in Part II of this thesis. Due to the spatial anisotropy of p- and d-orbitals, the overlap integrals between them depend both on the orbital and the *direction* of hopping, contrary to the s-orbitals. Hopping between a d_{xz} and a d_{xy} orbital is different in the x-direction than it is in the z-direction. Even more, electrons may also hop from one d_{xz} state to a d_{xy} state via ligand oxygen orbitals. Hence, the kinetic part of the Hamiltonian is now given

by

$$\hat{H}_{\text{MOK}} = \sum_{ij} t_{ij}^{\gamma\gamma'} \hat{\psi}^\dagger_{i\gamma\sigma} \hat{\psi}_{j\gamma'\sigma}, \qquad \textbf{M}\text{ulti }\textbf{O}\text{ribtal }\textbf{K}\text{inetic Hamiltonian} \tag{1.39}$$

(summation of Greek indices implied), where γ (γ') denote the orbital degree of freedom. Taking the simple cubic lattice as an example, and assuming only nearest neighbor hopping, we must distinguish three different matrices, $t_{\hat{x}}^{\gamma\gamma'}$, $t_{\hat{y}}^{\gamma\gamma'}$ and $t_{\hat{z}}^{\gamma\gamma'}$. They represent hopping in the x, y and z directions, respectively, and are generally all different yet related by symmetry.

The repulsive on-site Coulomb interactions can be expressed by the following Hamiltonian

$$\begin{aligned}\hat{H}_{\text{C}} = U \sum_i \hat{n}_{i\gamma\uparrow}\hat{n}_{i\gamma\downarrow} + (U' - J/2) \sum_{i,\gamma<\gamma'} \hat{n}_{i\gamma}\hat{n}_{i\gamma'} - 2J \sum_{i,\gamma<\gamma'} \vec{s}_{i\gamma} \cdot \vec{s}_{i\gamma'} \\ + J' \sum_{i,\gamma<\gamma'} \left(\hat{\psi}^\dagger_{i\gamma\uparrow}\hat{\psi}^\dagger_{i\gamma\downarrow}\hat{\psi}_{i\gamma'\downarrow}\hat{\psi}_{i\gamma'\uparrow} + \text{hc} \right) \qquad \textbf{C}\text{oulomb Hamiltonian}\end{aligned} \tag{1.40}$$

The various terms represent (i) the intra-orbital Coulomb repulsion, given by a Hubbard U, energetically penalizing two electrons occupying the same orbital with opposite spin quantum numbers, (ii) the inter-orbital Coulomb repulsion, given by $U' - J/2$, energetically penalizing two electrons on the same site but in different orbitals, (iii) Hund's rule coulpling, given by J, favoring alignment of electron spins occupying different orbitals, and (iv) the pair hopping term, given by J', changing the orbital flavor of a doubly occupied orbital.

Together with the kinetic term this interaction Hamiltonian constitutes a rather involved model of interacting electrons in solids. One may again assume very strong coupling and diagonalize the interaction Hamiltonian first, after which perturbatively including the hopping Hamiltonian generally yields a spin-orbital superexchange Hamiltonian. The latter will be $SU(2)$ invariant in the spin sector, but will depend in a non-symmetric way in the orbital degree of freedom, which is consequence of the intrinsic spatial anisotropy of the orbitals. An alternative approach is to employ a mean-field decoupling of the Coulomb Hamiltonian. This is the method of choice used in Part II of this thesis.

1.3 This thesis

Based on this general introduction to two important concepts, i.e. strong electron correlations and topology, we give a brief overview of the content of this thesis.

Part I of this thesis reports on a study of the Kondo-Lattice model, i.e. the model that describes interacting spins and electrons, on the honeycomb (chapter 3) and checkerboard (chapter 4) lattices. The honeycomb lattice is a two-dimensional bipartite lattice, while the checkerboard lattice is two-dimensional spin-ice lattice and hence frustrated.

Part II deals with the question whether coupling between localized magnetic moments and itinerant electrons can lead to lattice Quantum Hall effects. The specific focus will be on looking into model systems which can exhibit Fractional Quantum Hall effects and the importance of electronic orbital degrees of freedom will be addressed.

Part III provides a symmetry classification of density wave orders emerging from electronic interactions, with the aim of obtaining insight into the possibilities of realizing interaction-induced topological states of matter. Chapter 8 will introduce the subject and will summarize the main results and conclusions of chapters 9 and 10. Chapter 11 summarizes once again from a slightly different perspective.