

Topological insulators

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Chapter 1

The Su-Schrieffer-Heeger (SSH) model

The basic concepts of topological insulators are best understood via a concrete model. In this chapter we discuss the simplest such physical system, the Su-Schrieffer-Heeger (SSH) model[8] of polyacetylene, describing spinless fermions hopping on a 1D lattice with staggered hopping amplitudes. Along the way, we introduce important concepts, as the single-particle Hamiltonian, the difference between bulk and boundary, adiabatic phases and their connection to observables, a symmetry (chiral symmetry) that restricts the values of these phases, and bulk–boundary correspondance.



Figure 1.1: Geometry of the SSH model. A 1D chain with two atoms in the unit cell (circled by dashed line). The hopping amplitudes are staggered: w (double line) and v (single line). The long chain consists of the left edge (blue shaded background), the translationally invariant bulk (no background) and the right edge (green shaded background). The hopping amplitudes at the edges are subject to disorder, in the bulk, however, are fixed. .

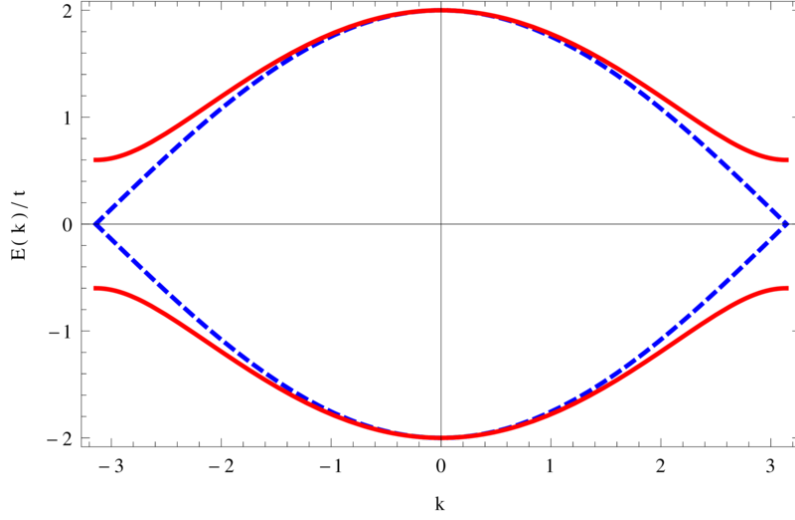


Figure 1.2: Bandstructure of polyacetylene in the case of $\delta t = 0$ (dashed blue line) and $\delta t = \pm 0.3t$ (red solid line) .

1.1 Hamiltonian

1.1.1 NN hopping chain

We consider spinless fermions hopping on a chain (1D lattice) with $M = 2N$ sites. The operator \hat{c}_r^\dagger creates a fermion on site $r = 0, \dots, M$. The Hamiltonian of the model reads

$$\hat{H} = \sum_{r=1}^M t_r \hat{c}_r^\dagger \hat{c}_{r+1} + h.c., \quad (1.1)$$

where t_r is the position-dependent hopping amplitude. We use periodic boundary conditions, i.e., $c_{2N+1} \equiv c_1$, but an open chain can still be realized by setting $t_{2N} = 0$. The special feature of this model Hamiltonian is that it has no onsite potential terms.

We assume that there are many fermions already on the chain, as is usually the case in real solid state physics systems. To take this into account, we use a grand canonical Hamiltonian, whereby we fix the number of fermions using the chemical potential μ :

$$\hat{H} = \sum_{r=1}^M t_r \hat{c}_r^\dagger \hat{c}_{r+1} + h.c. - \mu \sum_r \hat{c}_r^\dagger \hat{c}_r. \quad (1.2)$$

In the absence of interactions, this still is a single-particle Hamiltonian, and its ground state can be simply obtained by occupying all negative energy states and leaving all positive energy states unoccupied. For simplicity, we will work at 0 temperature, and

thus it is the ground state of this Hamiltonian that we will be interested in, and so the chemical potential plays the role of a Fermi energy.

We set the chemical potential to $\mu = 0$. In the absence of onsite potentials the choice $\mu = 0$ ensures that in the ground state, $M/2$ electrons will be in the system, since, as we will show below, $M/2$ eigenstates of \hat{H} have negative energy. This is a very natural choice for a real physical polymer where every atom brings 1 conduction electron: altogether, the chain will contain $M/2$ electrons of each spin. (The SSH model we consider here does not include spin, and so refers to, both species (both spins) of electrons, excluding any terms that couple the two species.)

Finally, since we are going to use staggered hopping amplitudes (i.e., alternate between weak and strong hopping), we use different notation for hopping over even and odd links, $t_{2n} = v_n$; $t_{2n+1} = w_n$. The grand canonical Hamiltonian of the SSH model then reads

$$\hat{H} = \sum_{n=1}^N \left(v_n \hat{c}_{2n-1}^\dagger \hat{c}_{2n} + w_n \hat{c}_{2n}^\dagger \hat{c}_{2n+1} + h.c. \right) \quad (1.3)$$

Single particle Hamiltonian

Although we have written the Hamiltonian for the chain in second quantized form, there are no interaction terms here: this is a *free Hamiltonian*, quadratic in the fermionic operators:

$$\hat{H} = \sum_{r=1}^M \hat{c}_r^\dagger H_{rs} \hat{c}_s. \quad (1.4)$$

The Hamiltonian noninteracting, and is therefore diagonalizable by a basis transformation on the single particle operators:

$$\hat{H} = \sum_{\alpha=1}^M E_\alpha \hat{\gamma}_\alpha^\dagger \hat{\gamma}_\alpha; \quad (1.5)$$

$$\hat{\gamma}_\alpha = \sum_{r=1}^M \Psi_{\alpha,r}^* \hat{c}_r. \quad (1.6)$$

Here the complex coefficients $\Psi_{\alpha,r}$ are determined by the eigenvectors of the $M \times M$ Hermitian matrix H ,

$$\sum_s H_{rs} \Psi_{\alpha,s} = E_\alpha \Psi_{\alpha,r}. \quad (1.7)$$

Since we have a noninteracting system, we can use the language of single-particle quantum mechanics, wherever it is more convenient. This is defined by

$$|r\rangle = \hat{c}_r |0\rangle ; \quad (1.8)$$

$$\hat{H} = \sum_{r=1}^M H_{rs} |r\rangle \langle s| ; \quad (1.9)$$

$$(1.10)$$

The energy eigenstates are vectors in the single-particle Hilbert space defined by

$$\hat{H} |\alpha\rangle = E_\alpha |\alpha\rangle . \quad (1.11)$$

In the ground state of \hat{H} , all negative energy eigenstates of H will be occupied (occupying these decreases the energy), positive energy eigenstates will be unoccupied.

1.1.2 Bulk and boundary

As every solid-state system, the long chain of the SSH model has a *bulk* and a *boundary*. The boundary in this case are the two ends, or “edges” of the chain, indicated by shading in Fig. 1.1.

The bulk, the long middle part of the chain, is taken to be translationally invariant. Since the chain is taken to be “long”, for most of the energy eigenstates it is a good approximation to just use periodic boundary conditions. In that sense, the bulk quasi-momentum k is a good quantum number, and the bulk has a well defined dispersion relation. Since we are concerned with insulators, we want the bulk to have an energy gap Δ around 0. Since we are using the grand canonical Hamiltonian, the Fermi energy is always at $E = 0$.

The two ends of the chain, the edges, cannot be translational invariant, as they contain the termination: we also allow them to have disorder. Where the border between “edge” and “bulk” should be taken (i.e., how many sites should be counted as “edges”) is a bit like the difference between quantum and classical world in the Copenhagen interpretation: the border can be shifted according to computational power, but should have no influence on the results as long as the bulk is long enough (compared to the typical size of edge states, proportional to $1/\sqrt{\Delta}$).

1.2 Staggered hopping makes the bulk an insulator

The SSH model only describes a band insulator if, in the large N limit, there is a finite energy gap Δ separating the highest energy bulk occupied state and the lowest energy bulk unoccupied state. For this gap to open, we need at least two bulk energy bands,

and so a unit cell that comprises two sites. It is for this reason that we use staggered hopping amplitudes, and so the bulk has translational invariance only with respect to displacement by integer multiples of 2. In the bulk, the hopping amplitudes read

$$t_{2n} = v; \quad t_{2n+1} = w = |w| e^{i\phi}. \quad (1.12)$$

Actually, using a higher level model, one can show that such a staggering occurs spontaneously in a solid state system, e.g., polyacetylene, by what is known as the Peierls instability. As seen in Fig. 1.2, it reduces the energy of the ground state, since it decreases the energies of all occupied states and increases the energies of the empty states.

1.2.1 Sublattice structure

In a chain with staggered hopping amplitudes, the practical choice for a unit cell includes two sites per cell. For simplicity we assume that the total number of sites is even, $M = 2N$, and introduce *cell index* $n = 1, \dots, N$ and *sublattice index* $j = 1, 2$ (or $j = A, B$) according to $\hat{c}_{n,j} = \hat{c}_{2n+j-2}$. In an even more concise notation, we can group the fermion creation operators on site n together in a formal vector,

$$\hat{\mathbf{c}}_n^\dagger = (\hat{c}_{n,1}^\dagger, \hat{c}_{n,2}^\dagger) = (\hat{c}_{2n-1}^\dagger, \hat{c}_{2n}^\dagger). \quad (1.13)$$

Rewriting the Hamiltonian in these operators, we have

$$\hat{H} = \sum_{n=1}^N \left(v_n \hat{c}_{n,1}^\dagger \hat{c}_{n,2} + w_n \hat{c}_{n,2}^\dagger \hat{c}_{n+1,1} + h.c. \right) = \sum_{m=1}^N \hat{\mathbf{c}}_m^\dagger H_{mn} \hat{\mathbf{c}}_n. \quad (1.14)$$

Here each H_{mn} is itself a 2×2 matrix. We can use the terminology of the hopping model, and call $U_n = H_{nn}$ the onsite potentials, and $T_n = H_{n,n+1}$ the hopping matrices. All the H_{mn} , where $|m - n| > 1$, vanish: this can always be achieved for a finite range hopping model by choosing a large enough unit cell. As an example, the Hamiltonian of a 1D chain of 6 cells (12 sites) reads

$$H = \begin{pmatrix} U_1 & T_1 & 0 & 0 & 0 & T_6^\dagger \\ T_1^\dagger & U_2 & T_2 & 0 & 0 & 0 \\ 0 & T_2^\dagger & U & T_3 & 0 & 0 \\ 0 & 0 & T_3^\dagger & U & T_4 & 0 \\ 0 & 0 & 0 & T_4^\dagger & U & T_4 \\ T_6 & 0 & 0 & 0 & T_5^\dagger & U_6 \end{pmatrix}. \quad (1.15)$$

This includes an open chain, if $T_6 = 0$, and a closed chain with no ends, only bulk, if $T_n = T$ and $U_n = U$.

The “onsite potential” matrices U_n and hopping amplitudes T_n read

$$U_n = \begin{pmatrix} 0 & v_n \\ v_n^* & 0 \end{pmatrix} = \text{Re } v_n \sigma_x - \text{Im } v_n \sigma_y, \quad (1.16)$$

$$T_n = \begin{pmatrix} 0 & 0 \\ w_n & 0 \end{pmatrix} = w_n (\sigma_x - i \sigma_y) / 2, \quad (1.17)$$

using the Pauli matrices

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.18)$$

In the translation invariant bulk, we can look for eigenstates of the $2N \times 2N$ matrix H in the form of $\Psi_{2n+j-2}(k) = e^{i2\pi kn/N} \Psi_j(k)$. The 2-component *Bloch vectors* $\Psi(k)$ are eigenvectors of the 2×2 matrix $H(k)$, defined as

$$H(k) = U + e^{-ik} T^\dagger + e^{ik} T = U + (T + T^\dagger) \cos k + i(T - T^\dagger) \sin k \quad (1.19)$$

The bulk Hamiltonian can be written in terms of the Pauli matrices as

$$H(k) = h_x(k) \sigma_x + h_y(k) \sigma_y + h_z(k) \sigma_z = \mathbf{h}(k) \cdot \boldsymbol{\sigma}; \quad (1.20)$$

$$h_x(k) = \text{Re } v + |w| \cos(k + \phi); \quad (1.21)$$

$$h_y(k) = -\text{Im } v + |w| \sin(k + \phi); \quad (1.22)$$

$$h_z(k) = 0. \quad (1.23)$$

The dispersion relation of the bulk can be read off from relations (1.23) easily, using the fact that $H(k)^2 = E(k)^2 \sigma_0$ because of the anticommutation relations of the Pauli matrices. We have

$$E(k) = |v + e^{-ik} w^*| = \sqrt{|v|^2 + |w|^2 + 2|v||w| \cos(k + \arg v + \arg w)} \quad (1.24)$$

The dispersion relation is plotted in Fig. 1.2. The minimum of the dispersion relation is $\Delta = |v| - |w|$, which shows that staggering does indeed open a gap.

Although the dispersion relation is useful to read off a number of physical properties of the stationary states (e.g., their group velocity), it does not contain all the information. Stationary states do not only have an energy eigenvalue, but also an internal structure (they are represented by the vectors in Hilbert space). The SSH model is a simple two-band model, and so the “internal structure” of the eigenstates with momentum k is simply given by the direction in which the vector $\mathbf{h}(k)$ of Eq. (1.23) points (the energy is given by the magnitude of $\mathbf{h}(k)$; for details see section 2.1.1). We are thus led to consider the path of the endpoint of $\mathbf{h}(k)$, as k goes through the Brillouin Zone. This is a circle of radius $|w|$ on the h_x, h_y plane, with center v^* . The fact that this is a closed path is a generic feature, following from periodicity of the Brillouin zone, $H(k = -\pi) = H(k = \pi)$. That this path lies on one plane, is a remarkable feature of the model, following from the fact that no sublattice potential (σ_z term) was allowed in the Hamiltonian, and therefore $h_z(k) = h_0(k) = 0$. We explore this further in the next section.

1.2.2 Chiral symmetry

The Hamiltonian of the SSH model, including bulk and boundary, Eq. (1.3) is *bipartite*. By this we mean that we can assign each site one of the sublattice indices A or B , such that the Hamiltonian includes no transitions between sites with the same index. In this case, this sublattice index is the same as the index denoted by j in the previous section. Formally, we can define the projectors on the sublattices using the notation of Eq. (1.10) as

$$P_A = \sum_{r=2n} |r\rangle \langle r|; \quad (1.25)$$

$$P_B = \sum_{r=2n+1} |r\rangle \langle r|. \quad (1.26)$$

We define the “coloring” operator

$$\Sigma_z = P_A - P_B. \quad (1.27)$$

The matrix elements of Σ_z vanish, $\langle r | \Sigma_z | s \rangle = 0$, if sites r and s are in different unit cells (even within a unit cell if $r \neq s$, but this is not important here). In that sense the operator Σ_z is *local*, i.e., it does not mix sites between unit cells. Therefore it can be represented in terms of a matrix acting within each unit cell:

$$\Sigma_z = \sigma_z \oplus \sigma_z \oplus \dots \oplus \sigma_z = \bigoplus_{n=1}^N \sigma_z. \quad (1.28)$$

Thus Σ_z inherits its algebra from σ_z ,

$$\Sigma_z^\dagger \Sigma_z = 1; \quad (1.29)$$

$$\Sigma_z^2 = 1; \quad (1.30)$$

There are no onsite terms in the Hamiltonian, and therefore, independent of the values of the hopping amplitudes t_j , the operator Σ_z anticommutes with the Hamiltonian:

$$\Sigma_z H \Sigma_z = -H. \quad (1.31)$$

This anticommutation relation holds for the same chiral symmetry operator if the hopping amplitudes depend on the position. The properties of locality, unitarity, hermiticity, and the anticommutation relation (1.31) together ensure that Σ_z is a unitary representation of *chiral symmetry*.

If chiral symmetry is to be useful for topological protection, as we are going to use it later on, it has to be robust. Many of the parameters of a Hamiltonian are subject to (local) disorder. In the SSH model, this is the case with the hopping amplitudes. We can

formally gather all parameters subject to disorder in a vector ξ . Instead of talking about the symmetries of a Hamiltonian H , we should rather refer to symmetries of a set of Hamiltonians $\{H(\xi)\}$, for all ξ from some ensemble. We can then claim that this set has chiral symmetry represented by Σ_z if all Hamiltonians in the set have chiral symmetry.

It can happen that a Hamiltonian is not bipartite, but only because of an unlucky choice of coordinates. Therefore, in the definition of chiral symmetry, before applying the “coloring operator” Σ_z , we can allow for a basis transformation via a unitary matrix U , independent of ξ , and local (not exchanging sites between unit cells). We then define

$$\Gamma = U^\dagger \Sigma_z U. \quad (1.32)$$

The relations of locality, unitarity, hermiticity, and the anticommutation relation can be transcribed from (1.31):

$$\Gamma = \sum_{n=1}^N \Gamma_n; \quad (1.33)$$

$$\Gamma^\dagger = \Gamma = \Gamma^{-1}; \quad (1.34)$$

$$\Gamma H \Gamma = -H. \quad (1.35)$$

We included the requirement that Γ should take a direct sum form in the sense of Eq. (1.28). It can be shown that if there is a local, ξ -independent operator Γ such that Eqs. (1.33), (1.34), (1.35) hold, one can always construct a basis transformation unitary operator U to have chiral symmetry represented by Σ_z .

A straightforward consequence of chiral symmetry is that the spectrum of H is symmetric. For eigenstates $|\psi_n\rangle$ of H , we have

$$H |\psi_n\rangle = E_n |\psi_n\rangle; \quad (1.36)$$

$$H \Gamma |\psi_n\rangle = -\Gamma H |\psi_n\rangle = -\Gamma E_n |\psi_n\rangle = -E_n \Gamma |\psi_n\rangle. \quad (1.37)$$

For any eigenstate of the SSH model with nonzero energy, flipping the sign of the wavefunction on the odd sites gives another eigenstate with opposite energy. Since these eigenstates have different energy, their wavefunctions have to be orthogonal. This implies that every nonzero energy eigenstate of H has equal support on both sublattices. In contrast, 0 energy eigenstates can be their own chiral symmetric partners: these are eigenstates of Σ_z , and therefore have support on only one sublattice.

1.2.3 Bulk winding number

The path of the endpoint of $\mathbf{h}(k)$, as k goes through the Brillouin Zone, is a closed path on the h_x, h_y plane, and the origin, $\mathbf{h} = 0$, cannot be on the path (there is no gap if $\mathbf{h} = 0$). To a closed path on the plane that does not contain the origin, we can associate a

winding number ν . This is the number of times the path encircles the origin, the winding of the complex number $h_x(k) + ih_y(k)$ as the wavenumber k is swept across the Brillouin Zone, $k = -\pi \rightarrow \pi$. To write this in a compact formula, note that $H(k)$ is off-diagonal for any k :

$$H(k) = \begin{pmatrix} 0 & h(k) \\ h^*(k) & 0 \end{pmatrix}; \quad h(k) = h_x(k) - ih_y(k). \quad (1.38)$$

The winding of $\mathbf{h}(k)$ is the same as the winding number of the complex number $h(k)$. This can be written as an integral, using the complex logarithm function, $\log(|h| e^{i \arg h}) = \log |h| + i \arg h$. It is easy to check that

$$\nu = \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk \frac{d}{dk} \log h(k). \quad (1.39)$$

The above integral is always real, since $|h(k = -\pi)| = |h(k = \pi)|$.

In general, for 1D chains with more complex unit cells, and a higher number of bands, say, $2n$, the above formula generalizes in the following way. We fix a basis where chiral symmetry is represented by $\Sigma_z = \text{diag}(\underbrace{1, \dots, 1}_n, \underbrace{-1, \dots, -1}_n)$. In this basis $H(k)$ has the

block off-diagonal form above, with $h(k)$ a $n \times n$ matrix. Without proof, we remark that replacing $\log h(k)$ with $\log \det h(k)$ in the formula above gives a topological invariant, the winding number ν .

For the SSH model the winding number is either $\nu = 1$ in the case of large intercell hopping, $|w| > |v|$, or $\nu = 0$ for small intercell hopping, $|w| < |v|$. To change the winding number, we need to either a) pull the path through the origin in the h_x, h_y plane, or b) lift it out of the plane and put it back on the plane at a different position. Method a) means closing the bulk gap. Method b) requires breaking chiral symmetry. These options are illustrated in Fig. 1.3

This brings us to the notion of *adiabatic equivalence* of bulk Hamiltonians. Two bulk insulators are adiabatically connected if one can be deformed into the other via a continuously changed parameter, while respecting the symmetries of the system, and without closing the bulk gap around $E = 0$. Actually, using adiabatic equivalence we can now also extend the topological classification based on the winding number above to of chiral symmetric 1D Hamiltonians without translation invariance.

1.3 Edge states

Now consider a finite open chain. To keep it simple, the only point where translational invariance is broken is where the chain is opened, $w_N = 0$. The spectrum of such a chain of 20 unit cells is shown as the parameters of the system are varied in Fig. 1.4. Notice

from the spectra that whenever the bulk winding number is nonzero, and the gap is large enough, there is a pair of low energy eigenstates whose wavefunctions are localized at the edges (here defined as having less than 10 % probability between $4 < m < 16$). For a general formulation of why these *edge states* appear, we need to gather more tools. For now, it is worthwhile to do a “quick trick”: adiabatic deformation into the fully dimerized limit.

1.3.1 Fully dimerized limit

There are two limiting cases where the SSH model becomes particularly simple and the edge states appear in a straightforward way: if the intercell hopping is set to zero, $w = 0$, or if the intercell hopping vanishes, $v = 0$. In both cases, the nonzero hopping amplitudes can be set to 1. In these “fully dimerized cases” the SSH chain falls apart to a sequence of disconnected dimers, as shown in Fig. 1.5.

The bulk of the fully dimerized limit has energy eigenstates that are the even (energy $E = +1$) and odd (energy $E = -1$) superpositions of the two sites forming a dimer. In the trivial, $v = 1$ case, the bulk Hamiltonian reads $H(k) = \sigma_x$, independent of the wavenumber k , and each unit cell is a dimer. In that case, the winding number is $\nu = 0$. In the nontrivial, $v = 0$ case, the bulk Hamiltonian is $H = \sigma_x \cos k + \sigma_y \sin k$, and each

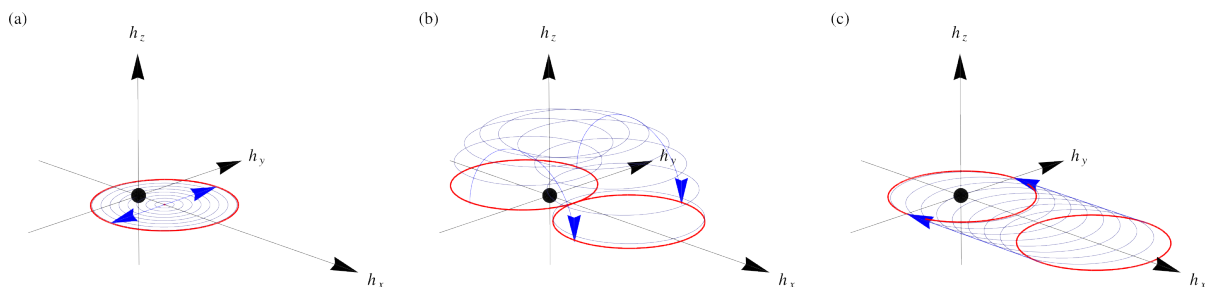


Figure 1.3: The endpoints of the vector $\mathbf{h}(k)$ as k goes across the Brillouin Zone (red or blue closed circles), for various parameter settings in the SSH model. In a), intracell hopping v is set to 0.5, and intercell hopping is gradually increased from 0 to 1 (outermost red circle). In the process, the bulk gap was closed and reopened, as the origin (black point) is included in some of the blue circles. The winding number changed from 0 to 1. In b), keeping $w = 1$, we increase the intracell hopping from 0.5 to 2.5, but avoid closing the bulk gap by introducing a sublattice potential, $H_{\text{sublattice}} = u\sigma_z$. We do this by tuning a parameter θ from 0 to π , and setting $v = 1.5 - \cos \theta$, and $u = \sin \theta$. At the end of the process, $\theta = 0$, there is no sublattice potential, so chiral symmetry is restored, but the winding number is 0 again. In c), we gradually decrease intracell hopping v to 0 so that the winding number again changes to 1. In the process, the bulk gap closes and reopens.

dimer is shared between two neighboring unit cells. In this nontrivial case, the winding number is $\nu = 1$. In both cases, $H(k)^2 = 1$, showing that the bulk has flat bands, with zero group velocity. This indicates that the energy eigenstates are localized, which is clearly the case: each eigenstate resides on its own dimer.

At the ends of an open, nontrivial fully dimerized chain, there is one 0 energy edge state (one on each end of the chain, two in total). When the edge is created by setting an intercell hopping amplitude to 0, in the nontrivial case, at each edge, a dimer is cut into two monomers, one half of which is left “inside” the chain. Since no onsite potentials are allowed (these would break chiral symmetry), the energy eigenstates on these monomers have 0 energy. In contrast, a trivial fully dimerized chain already has edges built into the Hamiltonian, and therefore has no 0 energy edge states.

1.3.2 Adiabatic deformation

Although the fully dimerized limits represent two very special cases of the SSH model, they are exhaustive in the sense that any generic SSH Hamiltonian is adiabatically connected to either the one or the other. To see what we mean by “adiabatically connected”, consider a generic insulating SSH Hamiltonian, with a translationally invariant bulk (with staggered hopping amplitudes) and two open ends, with arbitrary end regions. Now consider continuously decreasing the weaker hopping amplitude to 0, then changing the phase of the stronger hopping amplitude to 0, then changing the magnitude of the

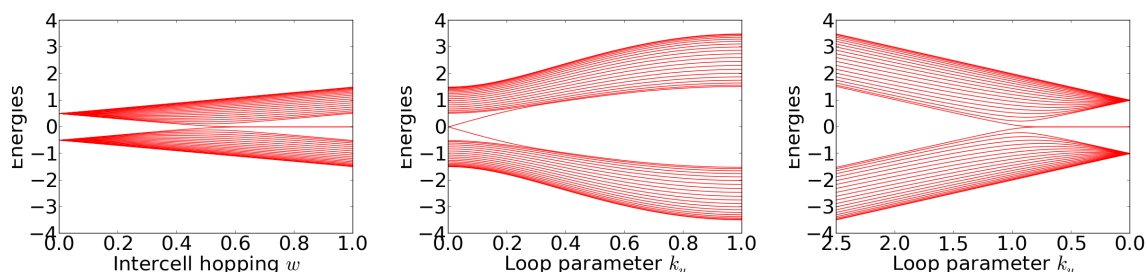


Figure 1.4: Spectra of finite open SSH chains of 40 sites (20 cells), as parameters are changed according to Fig. 1.3. In a), when the bulk gap closes and reopens, the winding number becomes 1, and a pair of midgap states appears, which for a large enough gap are localized onto the edges (blue dots indicate states whose support is 90% on $0 < m < 4$). In b), because of the extra sublattice potential, $H_{\text{sublattice}} = u\sigma_z$, the edge state energies are changed: increased (decreased) on the left (right) edge, as indicated by the blue (green) circles, until these states merge into the bulk. At the end of the cycle on b), the winding number is 0 again, and no midgap states are left. In c), as the winding number is changed back to 1, a pair of midgap states again appear, which for large gaps are again localized on the edges (blue dots).

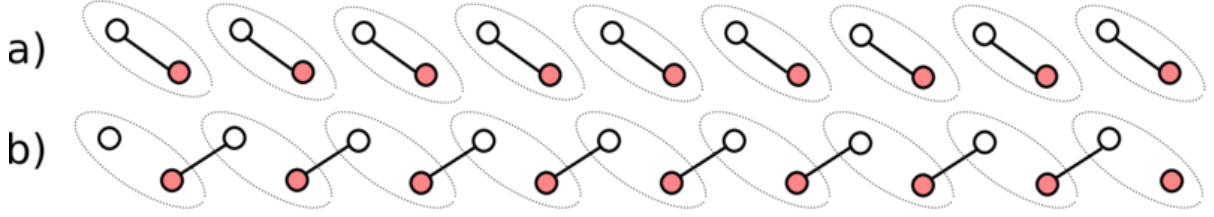


Figure 1.5: Fully dimerized limits of the SSH model. A 1D chain with a) no intercell hopping, “trivial” or b) no intracell hopping, “nontrivial”, consists of disconnected dimers. In the trivial case, a), every energy eigenstate is an even or an odd superposition of two sites at the same unit cell. In the nontrivial case, b), there are also isolated cells, 1 site per edge, that must contain 0 energy eigenstates, as there are no onsite potentials. .

stronger hopping amplitude to 1. This process changes the bulk to either to the trivial $v = 1, w = 0$, or the nontrivial $v = 0, w = 1$ fully dimerized limit. During these changes, the bulk gap was not closed, and thus by definition this constitutes an adiabatic deformation of H . Finally, to arrive to the fully dimerized limit, the hopping amplitudes at the edge regions can be set to continue the pattern of the bulk up until the very end. This continuous change in the system parameters obviously cannot affect the bulk gap, and is therefore adiabatic.

It is worthwhile to note that the adiabatic deformation of the Hamiltonian is understood to be a fictitious process, and not take place in time. Therefore we do not need to care about how fast the parameters are changed, whether the adiabatic approximation holds or not. Since the bulk gap stays open during the whole deformation process, one could perform it at a rate that is slow enough to ensure adiabaticity.

The 0 energy edge states at the left (right) end only have support on sublattice A (B), and so are eigenstates of the chiral symmetry operator Σ_z . Later in the course, we will see that this property also holds away from the fully dimerized limit. With a nonzero intercell hopping v , the edge states are not confined to the very last unit cells on the chain any more. However, since the bulk gap still exists, the edge states, are exponentially localized at the edges. They still are eigenstates of Σ_z , with support only on one sublattice. This can be seen in Fig. 1.4 b), where, upon switching on a sublattice potential, the energies of the edge states at the two edges are changed in opposite directions.

1.3.3 Edge states between different domains

Edge states do not only occur at the ends of an open chain, but also at interfaces between different insulating domains of the same chain. This can be understood via the fully dimerized limit, Fig. 1.6. There are two types of domain walls here: those containing single isolated sites, which host 0 energy states on a single sublattice (no onsite potentials are allowed), and those containing trimers. On a trimer, the odd superposition of the

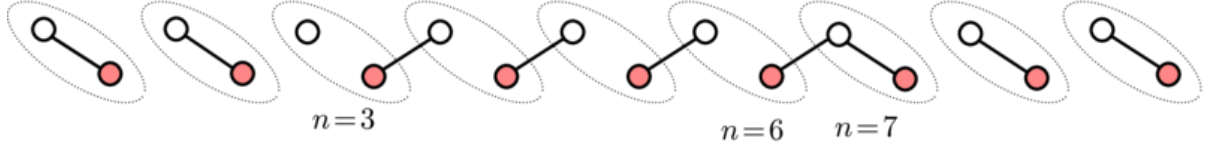


Figure 1.6: A long, fully dimerized SSH chain with 3 domains. The boundaries between the domains, the “domain walls”, host 0 energy eigenstates. These can be localized on a single site, as for the domain wall at $n = 3$, or on a superposition of sites, as the odd superposition of the ends of the trimer shared between the $n = 6$ and $n = 7$ unit cells. .

two end sites form a zero energy eigenstate. In the the example of Fig. 1.6, this is

$$\hat{H}(|6, B\rangle - |7, B\rangle) = 0, \quad (1.40)$$

where $|6, B\rangle = |12\rangle$ is the state where the single occupied site is that in unit cell $n = 6$, on sublattice B . Note that, just as the edge states at the ends of the chain, these zero energy states at the interfaces are also localized on one sublattice.

From a perfect dimerized phase without domains it is only possible to germinate an even number of interfaces. This means that if one encounters a domain wall with a localized state on one sublattice then there will be another domain wall somewhere in the system with a localized state on the opposite sublattice.

Switching on the intracell hopping v changes the wavefunctions of the edge states at the domain walls and gives them “evanescent tails” that decay exponentially into the bulks. If two domain walls were close enough to each other, at a distance of L unit cells, the two edge states on the walls can hybridize, form “bonding” and “anti-bonding” states. Their energies are of the order of their overlap, $\pm e^{-L\Delta}$, where Δ is the bulk gap in dimensionless units. At half filling, of these only the negative energy eigenstate will be occupied. This state hosts a single electron, however, its wavefunction is localized with equal weight on the two domain walls. Hence each domain wall, when well separated from other domain walls and the ends of the chain, will carry half an electronic charge. This “fractionalization” of a charge to two spatially separated parts is also a distinct feature of topological insulators.

Chapter 2

Berry phase and polarization

The SSH model was a concrete example for a 1D topological insulator. We have seen how the bulk–boundary correspondence works: At the interfaces between two bulks with different topological invariants, there were low energy states protected by the global chiral symmetry. These low energy midgap states are 0 dimensional: they extend slightly into the bulks, with exponentially decaying tails, but other than that, they just are there, and do nothing spectacular. (Although closely related edge states in a topological superconductor wire can be used for quantum information processing).

In higher dimensional topological insulators, edge states can have a wider range of properties. In two dimensions, they can propagate along the 1D edge, and their propagation is reflectionless. Higher dimensional lattice systems have more complicated topological invariants than the winding number in the SSH model. The first step towards understanding these invariants is the adiabatic Berry phase.

2.1 Berry phase, Berry connection, Berry curvature

We introduce the Berry phase in the most general setting, and use examples to illustrate its properties.

2.1.1 Fixing the gauge

Take a physical system with parameters $\mathbf{R} = (R_1, R_2, \dots, R_N)$, that are real numbers. We denote the Hamiltonian by $H(\mathbf{R})$, and its eigenstates, ordered according to the energies $E_n(\mathbf{R})$, by $|n(\mathbf{R})\rangle$:

$$H(\mathbf{R}) |n(\mathbf{R})\rangle = E_n(\mathbf{R}) |n(\mathbf{R})\rangle. \quad (2.1)$$

We call $\{|n(\mathbf{R})\rangle\}$ the *snapshot basis*. The above definition requires fixing the arbitrary phase prefactor for every $|n(\mathbf{R})\rangle$. This is *gauge fixing*, and since this is very important for what follows, let's see how it works for a specific example.

Spin-1/2: No “nice” global gauge

A simple but important example is the most general 2-level Hamiltonian,

$$H(\mathbf{R}) = h_0(\mathbf{R})\sigma_0 + h_1(\mathbf{R})\sigma_x + h_2(\mathbf{R})\sigma_y + h_3(\mathbf{R})\sigma_z = h_0(\mathbf{R})\sigma_0 + \mathbf{h}(\mathbf{R})\boldsymbol{\sigma}, \quad (2.2)$$

with real functions $h_j(\mathbf{R})$. The value of h_0 does not affect the eigenstate $|n(\mathbf{R})\rangle$, and therefore we set it to 0 for simplicity. Because of the anticommutation relations of the Pauli matrices, the Hamiltonian squares to a multiple of the identity operator, $H(\mathbf{R})^2 = \mathbf{h}^2 \in \mathbb{R}$, and so the spectrum of $H(\mathbf{R})$ is symmetric: For any choice of \mathbf{R} it is $\pm\sqrt{\mathbf{h}^2}$. We want to characterize the eigenstates, and so the value of the energy is irrelevant: we introduce the unit vector

$$\hat{\mathbf{h}} = \mathbf{h}/\sqrt{\mathbf{h}^2}. \quad (2.3)$$

The endpoints of $\hat{\mathbf{h}}$ map out the surface of a unit sphere, called the Bloch sphere, shown in Fig. 2.1. One point on the sphere can be parametrized by the usual spherical angles $\theta \in [0, \pi)$ and $\varphi \in [0, 2\pi)$, as

$$\cos \theta = \hat{h}_3; \quad (2.4)$$

$$e^{i\varphi} = \frac{\hat{h}_1 + i\hat{h}_2}{\sqrt{\hat{h}_1^2 + \hat{h}_2^2}}. \quad (2.5)$$

The eigenstate with $E = +|\mathbf{h}|$ of the corresponding Hamiltonian is:

$$|n(\hat{\mathbf{h}})\rangle = |\hat{\mathbf{h}}\rangle = e^{i\alpha(\theta, \varphi)} \begin{pmatrix} e^{-i\varphi/2} \cos \theta/2 \\ e^{i\varphi/2} \sin \theta/2 \end{pmatrix}. \quad (2.6)$$

We explicitly pulled out the free phase factor in front of the vector. Fixing this phase factor corresponds to fixing a gauge. The eigenstate with $E = -|\mathbf{h}|$ is $|n(-\hat{\mathbf{h}})\rangle$.

Consider fixing $\alpha = 0$. This is appealing because both θ and φ carry factors of $1/2$. However, fixing θ , let us make a full circle in parameter space: $\varphi = 0 \rightarrow 2\pi$. We should come back to the same Hilbert space vector, and we do, but we also pick up a phase of -1 . We can either say that this choice of gauge led to a discontinuity at $\varphi = 0$, or that our representation is not single-valued. One might think that there are ways to fix this, however.

Let us fix $\alpha = \varphi/2$. This gives an additional factor of -1 as we make the circle in φ , and so it seems we have a continuous, single valued representation:

$$|\hat{\mathbf{h}}\rangle_S = \begin{pmatrix} \cos \theta/2 \\ e^{i\varphi} \sin \theta/2 \end{pmatrix}. \quad (2.7)$$

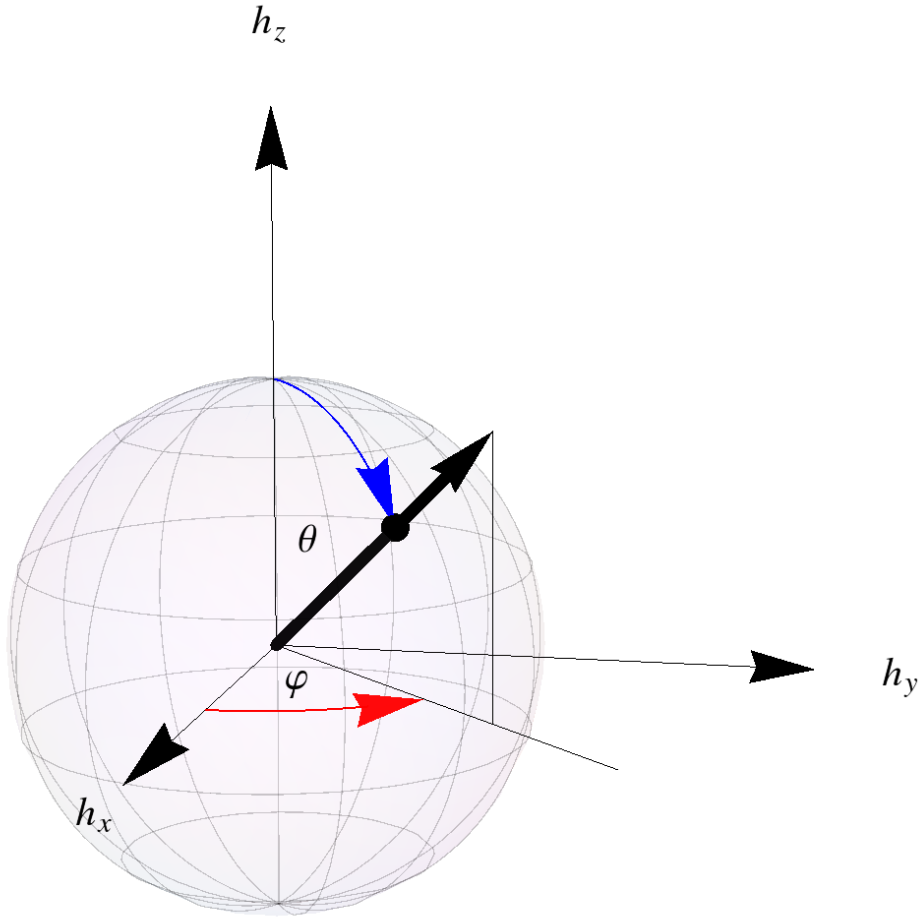


Figure 2.1: The Bloch sphere. A generic traceless two-level Hamiltonian is a linear combination of Pauli matrices, $H = \mathbf{h}\boldsymbol{\sigma}$. This can be identified with a point in \mathbb{R}^3 . The eigenenergies are given by the distance of the point from the origin, the eigenstates depend only on the direction of the vector \mathbf{h} , i.e., on the angles θ and ϕ , as defined in Eq. (2.5) .

There are two tricky points, however: the North Pole, $\theta = 0$, and the South Pole, $\theta = \pi$. At the North Pole, $|(0, 0, 1)\rangle_S = (1, 0)$ no problems. At the South Pole, however, $|(0, 0, -1)\rangle_S = (0, e^{i\varphi})$, whose value depends on which direction we approach the pole from.

We can try to solve the problem at the South Pole by choosing $\alpha = -\varphi/2$, which gives us

$$|\hat{\mathbf{h}}\rangle_N = \begin{pmatrix} e^{-i\varphi} \cos \theta/2 \\ \sin \theta/2 \end{pmatrix}. \quad (2.8)$$

As you can probably already see, this representation runs into trouble at the North Pole: $|(0, 0, 1)\rangle = (e^{-i\varphi}, 0)$.

We can try to overcome the problems at the Poles by taking linear combinations of $|\hat{\mathbf{h}}\rangle_N$ and $|\hat{\mathbf{h}}\rangle_S$, with prefactors that vanish at the North and South Poles, respectively. A family of options is:

$$|\hat{\mathbf{h}}\rangle_\chi = \cos \frac{\theta}{2} |\hat{\mathbf{h}}\rangle_S + e^{i\chi} \sin \frac{\theta}{2} |\hat{\mathbf{h}}\rangle_N \quad (2.9)$$

$$= \begin{pmatrix} \cos \frac{\theta}{2} (\cos \frac{\theta}{2} + \sin \frac{\theta}{2} e^{i\chi} e^{-i\varphi}) \\ \sin \frac{\theta}{2} e^{i\varphi} (\cos \frac{\theta}{2} + \sin \frac{\theta}{2} e^{i\chi} e^{-i\varphi}) \end{pmatrix}. \quad (2.10)$$

This is single valued everywhere, solves the problems at the Poles. However, it has its own problems at $\theta = \pi/2$, $\varphi = \chi \pm \pi$: there, its norm disappears.

It is not all that surprising that we could not find a well-behaved gauge: there is none.

2.1.2 Adiabatic phase

Coming back to a general Hamiltonian, Eq. (2.1), we assume that a part of its spectrum is discrete: there is an $n \in \mathbb{N}$ such that the “gaps” $E_n(\mathbf{R}) - E_{n-1}(\mathbf{R})$ and $E_{n+1}(\mathbf{R}) - E_n(\mathbf{R})$ are finite for some value of $\mathbf{R} = \mathbf{R}_0$. Consider initializing the system with $\mathbf{R} = \mathbf{R}_0$ and in the eigenstate $|n(\mathbf{R}_0)\rangle$ at time $t = 0$:

$$\mathbf{R}(t = 0) = \mathbf{R}_0; \quad (2.11)$$

$$|\psi(t = 0)\rangle = |n(\mathbf{R}_0)\rangle. \quad (2.12)$$

Now assume that during the time $t = 0, \dots, T$ the parameters \mathbf{R} are slowly changed: \mathbf{R} becomes $\mathbf{R}(t)$, the values of $\mathbf{R}(t)$ being along a curve \mathcal{C} . The state of the system evolves according to the time-dependent Schrödinger equation:

$$i \frac{d}{dt} |\psi(t)\rangle = H(\mathbf{R}(t)) |\psi(t)\rangle. \quad (2.13)$$

Further, assume that \mathbf{R} is varied in such a way that at all times the energy gaps around the state $|n(\mathbf{R}(t))\rangle$ remain finite. On the other hand, the rate of variation of $\mathbf{R}(t)$ along path \mathcal{C} has to be slow enough compared to the frequencies corresponding to the energy gap, and then the *adiabatic approximation* holds (for the precise conditions, see [6]). In that case, the system remains in the energy eigenstate $|n(\mathbf{R}(t))\rangle$, only picking up a phase. Using this adiabatic approximation, take as Ansatz

$$|\psi(t)\rangle = e^{i\gamma_n(t)} e^{-i \int_0^t E_n(\mathbf{R}(t')) dt'} |n(\mathbf{R}(t))\rangle. \quad (2.14)$$

Insert this Ansatz into the Schrödinger equation (2.13), we have for the left hand side

$$i \frac{d}{dt} |\psi(t)\rangle = e^{i\gamma_n(t)} e^{-i \int_0^t E_n(\mathbf{R}(t')) dt'} \left(-\frac{d\gamma_n}{dt} |n(\mathbf{R}(t))\rangle + E_n(\mathbf{R}(t)) |n(\mathbf{R}(t))\rangle + i \left| \frac{d}{dt} n(\mathbf{R}(t)) \right\rangle \right). \quad (2.15)$$

To see what we mean by $\left| \frac{d}{dt} n(\mathbf{R}(t)) \right\rangle$, we write it out explicitly in terms of a fixed basis. For better readability, in the following we often drop the t argument of $\mathbf{R}(t)$.

$$|m\rangle_0 \equiv |m(\mathbf{R}_0)\rangle; \quad (2.16)$$

$$|n(\mathbf{R})\rangle = \sum_m c_m(\mathbf{R}) |m\rangle_0; \quad (2.17)$$

$$\left| \frac{d}{dt} n(\mathbf{R}(t)) \right\rangle = \frac{d\mathbf{R}}{dt} \cdot |\nabla_{\mathbf{R}} n(\mathbf{R})\rangle = \frac{d\mathbf{R}}{dt} \sum_m \nabla_{\mathbf{R}} c_m(\mathbf{R}) |m\rangle_0. \quad (2.18)$$

We insert the Ansatz (2.14) into the rhs of the Schrödinger equation (2.13), use

$$H(\mathbf{R}) |n(\mathbf{R})\rangle = E_n(\mathbf{R}) |n(\mathbf{R})\rangle, \quad (2.19)$$

simplify and reorder the Schrödinger equation, we obtain

$$-\left(\frac{d}{dt} \gamma_n \right) |n\rangle + i \left| \frac{d}{dt} n \right\rangle = 0. \quad (2.20)$$

Multiply from the left by $\langle n(\mathbf{R}(t))|$, and obtain

$$\frac{d}{dt} \gamma_n(t) = i \left\langle n(\mathbf{R}(t)) \left| \frac{d}{dt} n(\mathbf{R}(t)) \right\rangle = \frac{d\mathbf{R}}{dt} i \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle. \quad (2.21)$$

For the last equality we used that the only dependence on time is via the parameters \mathbf{R} .

We have found that for a path in parameter space \mathcal{C} , traced out by $\mathbf{R}(t)$, there is an adiabatic phase $\gamma_n(\mathcal{C})$ associated with it,

$$\gamma_n(\mathcal{C}) = \int_{\mathcal{C}} i \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle d\mathbf{R}. \quad (2.22)$$

Where did we use the adiabatic approximation?

On the face of it, our derivation seems to do too much. We have produced an exact solution of the Schrödinger equation. Where did we use the adiabatic approximation?

In fact, Eq. (2.21) does not imply Eq. (2.20). For the more complete derivation, showing how the nonadiabatic terms appear, see [6].

2.1.3 Berry phase

Berry connection

We define the integrand of Eq. (2.22) as the *Berry connection* or *Berry vector potential*:

$$\mathbf{A}^{(n)}(\mathbf{R}) = i \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle = -\text{Im} \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle, \quad (2.23)$$

where the second equality follows from the conservation of the norm, $\nabla_{\mathbf{R}} \langle n(\mathbf{R}) | n(\mathbf{R}) \rangle = 0$.

Gauge dependence

As the name “vector potential” suggests, the Berry connection is not gauge invariant. Consider a gauge transformation:

$$|n(\mathbf{R})\rangle \rightarrow e^{i\alpha(\mathbf{R})} |n(\mathbf{R})\rangle : \quad (2.24)$$

$$\mathbf{A}^{(n)}(\mathbf{R}) \rightarrow \mathbf{A}^{(n)}(\mathbf{R}) - \nabla_{\mathbf{R}} \alpha(\mathbf{R}). \quad (2.25)$$

Therefore, in the generic case, the adiabatic phase cannot be observed.

Adiabatic phase of a closed loop is observable: the Berry phase

To get the adiabatic phase to have physical consequences, we need to have an interferometric setup. This means coherently splitting the wavefunction of the system into two parts, taking them through two adiabatic trips in parameter space, via $\mathbf{R}(t)$ and $\mathbf{R}'(t)$, and bringing the parts back together. The two parts can interfere only if $|n(\mathbf{R}(T))\rangle = |n(\mathbf{R}'(T))\rangle$, which is typically ensured if $\mathbf{R}(T) = \mathbf{R}'(T)$. The difference in the adiabatic phases γ_n and γ'_n is the adiabatic phase associated with the closed loop \mathcal{C} , which is the path of $t \rightarrow \mathbf{R}(t)\Theta(T-t) + \mathbf{R}(2T-t)\Theta(t-T)$.

Although the adiabatic phase of a general path in parameter space is gauge dependent, for a closed loop \mathcal{C} , it is gauge invariant. This is obvious, since a gauge transformation is single valued, but can also be proven via the Stokes theorem. The adiabatic phase of the loop, the integral of \mathbf{A} around the closed loop, is the *Berry phase*.

2.1.4 Berry curvature

We calculated the Berry phase using the gauge dependent Berry connection. However, since the final result was gauge independent, there should be a gauge independent way to calculate it. This is provided by the Berry curvature.

We define the Berry curvature

$$\mathbf{B}^{(n)}(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathbf{A}^{(n)}(\mathbf{R}). \quad (2.26)$$

In the following, we drop the index (n) , and the argument \mathbf{R} for better readability, wherever this leads to no confusion. We also use ∇ for $\nabla_{\mathbf{R}}$.

Then, by virtue of the Stokes theorem, we have for the Berry phase,

$$\gamma_n(\mathcal{C}) = \int_{\mathcal{S}} \mathbf{B}^{(n)}(\mathbf{R}) d\mathcal{S}, \quad (2.27)$$

where \mathcal{S} is any surface whose boundary is the loop \mathcal{C} .

We use 3D notation here, but the above equations can be generalized for any dimensionality of \mathbf{R} .

The Berry curvature \mathbf{B} is very much like a magnetic field. For instance, $\nabla \mathbf{B} = 0$, from definition (2.26).

Berry provided [4] two practical formulas for the Berry curvature. First,

$$B_j = -\text{Im} \epsilon_{jkl} \partial_k \langle n | \partial_l n \rangle = -\text{Im} \epsilon_{jkl} \langle \partial_k n | \partial_l n \rangle + 0, \quad (2.28)$$

where the second term is 0 because $\partial_k \partial_l = \partial_l \partial_k$ but $\epsilon_{jkl} = -\epsilon_{jlk}$.

To obtain Berry's second formula, inserting a resolution of identity in the snapshot basis in the above equation, we obtain

$$\mathbf{B}^{(n)} = -\text{Im} \sum_{n' \neq n} \langle \nabla n | n' \rangle \times \langle n' | \nabla n \rangle. \quad (2.29)$$

The term with $n' = n$ is omitted from the sum, as it is zero, since because of the conservation of the norm of $|n\rangle$, $\langle \nabla n | n \rangle = -\langle n | \nabla n \rangle$. To calculate $\langle n' | \nabla n \rangle$, start from the definition of the eigenstate $|n\rangle$, act on both sides with $\nabla_{\mathbf{R}}$, and then project unto $|n'\rangle$:

$$H(\mathbf{R}) |n\rangle = E_n |n\rangle; \quad (2.30)$$

$$(\nabla H(\mathbf{R})) |n\rangle + H(\mathbf{R}) |\nabla n\rangle = (\nabla E_n) |n\rangle + E_n |\nabla n\rangle; \quad (2.31)$$

$$\langle n' | \nabla H | n \rangle + \langle n' | H | \nabla n \rangle = 0 + E_n \langle n' | \nabla n \rangle. \quad (2.32)$$

Act with H towards the left in Eq. (2.32), rearrange, substitute into (2.29), and you should obtain the second form of the Berry curvature:

$$\mathbf{B}^{(n)} = -\text{Im} \sum_{n' \neq n} \frac{\langle n | \nabla H | n' \rangle \times \langle n' | \nabla H | n \rangle}{(E_n - E_{n'})^2}. \quad (2.33)$$

This shows that the monopole sources of the Berry curvature, if they exist, are the points of degeneracy.

2.2 Electronic polarization and Berry phase in a 1D crystal

We now apply the concept of Berry phase on an insulator by formally treating the wavenumber k as an externally controlled parameter. A lattice model in 1D is specified by giving the bulk Hamiltonian as a function of the wavenumber $H(k)$, with the energy bands $|n(k)\rangle$,

$$H(k) |n(k)\rangle = E_n(k) |n(k)\rangle. \quad (2.34)$$

Formally, we can treat k as a parameter and tune it across the Brillouin Zone: $k = -\pi, \dots, \pi$. Since $H(-\pi) = H(\pi)$, to each nondegenerate band n we can associate a Berry phase:

$$\gamma_n = i \int_{BZ} dk \langle n(k) | \frac{d}{dk} | n(k) \rangle. \quad (2.35)$$

This generalization of the Berry phase is known as Zak phase.

Although the Zak phase is defined above by a completely formal procedure, which does not correspond to an experimental situation, it does have physical significance: it gives the contribution of the band n to the electric polarization. In suitable units, the bulk electric polarization can be defined as the sum of all the Zak phases of the occupied bands,

$$P = \sum_{n<0} \gamma_n. \quad (2.36)$$

There are two simple ways to show this nontrivial statement [12]. One is to consider the change in bulk polarization as some system parameter is tuned. The other way, which we briefly summarize below, shows that the Zak phase of band n gives the expectation value of the position of the electron in the Wannier state coming from band n centered on an atom at the origin.

2.2.1 Bloch functions and Wannier states

To show the physical interpretation of the Zak phase, we need to go beyond the simple lattice model for a solid state. Instead, consider the full wavefunction of an electron in a periodic potential $V(x)$, with x measured in units of the period, $V(x+1) = V(x)$:

$$\left[\frac{1}{2m} p^2 + V(x) \right] \Psi_n(k, x) = E_n(k) \Psi_n(k, x). \quad (2.37)$$

According to the Bloch theorem, this has the form

$$\Psi_n(k, x) = e^{ikx} u_n(k, x), \quad (2.38)$$

where u_n is a cell periodic function:

$$u_n(k, x) = u_n(k, x + 1). \quad (2.39)$$

The Schrodinger equation rewritten for u_n reads

$$\mathcal{H}(k, x) u_n(k, x) = \left[\frac{1}{2m} (p + k)^2 + V(x) \right] u_n(k, x) = E_n(k) u_n(k, x). \quad (2.40)$$

We specify a periodic gauge, by requiring

$$\Psi_n(k + G, x) = \Psi_n(k, x) \quad (2.41)$$

for any reciprocal lattice vector $G = 2\pi l$, with l integer. This entails

$$u_n(k + G, x) = e^{-iGx} u_n(k, x). \quad (2.42)$$

Thereby, even though $u_n(k, x)$ and $u_n(k + G, x)$ are eigenfunctions of different Hamiltonians, they are related by a fixed unitary transformation, which allows us to relate their phases to each other in a well defined way. Details of the definition of this “open-path” geometric phase can be found in Resta’s lecture notes, [12]. In the continuum limit, the phase reads

$$\gamma_n = i \int_{-\pi}^{\pi} dk \int_0^1 dx u_n(k, x)^* \partial_k u_n(k, x). \quad (2.43)$$

The energy eigenstates of electrons in a perfect lattice are given by the Bloch functions that are delocalized over the entire lattice. For energy eigenstates within a band, a unitary transformation can be defined that transforms to an orthonormal set of wavefunctions $\Phi_m^{(n)}(x)$, that are each localized around site m . Of course, these Wannier modes are not energy eigenstates, but they are useful tools in solid state physics. The definition of Wannier states is the following:

$$w_n(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \Psi_n(k, x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk e^{ikx} u_n(k, x); \quad (2.44)$$

$$\Phi_m^{(n)}(x) = w_n(x - m). \quad (2.45)$$

The inverse of the above transformation expresses the Bloch function in terms of the Wannier states:

$$u_n(k, x) = \sum_m e^{-ik(x-m)} w_n(x - m). \quad (2.46)$$

Substituting the above relation into the definition of the Zak phase above, Eq. (2.43), we find

$$\begin{aligned}\gamma_n &= \int_0^1 dx \sum_{m,m'} w_n(x-m)^* (x-m') w_n(x-m') \int_{-\pi}^{\pi} dk e^{ik(m'-m)} \\ &= \sum_m |w_n(x-m)|^2 (x-m) = \int_{-\infty}^{\infty} dx |\phi_n(x)|^2 x. \quad (2.47)\end{aligned}$$

The final result is that the Zak phase of the n th band, is the first moment of the center of the charge in the Wannier state centered on the atom at $x = 0$. This is a quantity which can be identified with the contribution of the band to the bulk electric polarization.

Chapter 3

Chern number

3.1 Reminder – Berry phase in a Two-level system

The simplest application of the Berry phase is a single two-level system, e.g., a single electron at a fixed point whose only degree of freedom is its spin (we could call this a “0-dimensional” system). There are no “position” or “momentum” variables, the Hamiltonian simply reads

$$H(\mathbf{h}) = \mathbf{h}\boldsymbol{\sigma}, \quad (3.1)$$

As long as $\mathbf{h} \neq 0$, the two energy eigenstates have different energy. Its two eigenstates are $|\pm, \mathbf{h}\rangle$, defined by

$$\mathbf{h}\boldsymbol{\sigma} |+, \mathbf{h}\rangle = \sqrt{\mathbf{h}^2} |+, \mathbf{h}\rangle; \quad \mathbf{h}\boldsymbol{\sigma} |-, \mathbf{h}\rangle = -\sqrt{\mathbf{h}^2} |-, \mathbf{h}\rangle. \quad (3.2)$$

Now take a closed curve \mathcal{C} in the parameter space \mathbb{R}^3 . We are going to calculate the Berry phase γ_- of the $|-, \mathbf{h}\rangle$ eigenstate on this curve:

$$\gamma_-(\mathcal{C}) = \oint_{\mathcal{C}} \mathbf{A}(\mathbf{h}) d\mathbf{h}, \quad (3.3)$$

with the Berry vector potential defined as

$$\mathbf{A}(\mathbf{h}) = i \langle -, \mathbf{h} | \nabla_{\mathbf{h}} | -, \mathbf{h} \rangle. \quad (3.4)$$

The calculation becomes straightforward if we use the Berry curvature,

$$\mathbf{B}(\mathbf{h}) = \nabla_{\mathbf{h}} \times \mathbf{A}(\mathbf{h}); \quad (3.5)$$

$$\gamma_-(\mathcal{C}) = \int_{\mathcal{S}} \mathbf{B}(\mathbf{h}) d\mathcal{S}, \quad (3.6)$$

where \mathcal{S} is any surface whose boundary is the loop \mathcal{C} . (Alternatively, it is a worthwhile exercise to calculate the Berry phase directly in a fixed gauge, e.g., one of the three gauges of the previous chapter.)

Specifically, we make use of Berry's gauge invariant formulation of the Berry curvature, derived in the last chapter (2.33):

$$\mathbf{B}^{(n)} = -\text{Im} \sum_{n' \neq n} \frac{\langle n | \nabla_{\mathbf{h}} H | n' \rangle \times \langle n' | \nabla_{\mathbf{h}} H | n \rangle}{(E_n - E_{n'})^2}. \quad (3.7)$$

In the case of the generic 2×2 Hamiltonian (3.1) the above definition gives

$$\mathbf{B}^{\pm}(\mathbf{h}) = -\text{Im} \frac{\langle \pm | \nabla_{\mathbf{h}} H | \mp \rangle \times \langle \mp | \nabla_{\mathbf{h}} H | \pm \rangle}{4\mathbf{h}^2}, \quad (3.8)$$

with

$$\nabla_{\mathbf{h}} H = \boldsymbol{\sigma}. \quad (3.9)$$

To evaluate (3.8), we choose the quantization axis parallel to \mathbf{h} , thus the eigenstates simply read

$$|+, \mathbf{h}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad |-, \mathbf{h}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (3.10)$$

The matrix elements can now be computed as

$$\langle - | \sigma_x | + \rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1, \quad (3.11)$$

and similarly,

$$\langle - | \sigma_y | + \rangle = i; \quad (3.12)$$

$$\langle - | \sigma_z | + \rangle = 0. \quad (3.13)$$

So the cross product of the vectors reads

$$\langle - | \boldsymbol{\sigma} | + \rangle \times \langle + | \boldsymbol{\sigma} | - \rangle = \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix} \times \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 2i \end{pmatrix}. \quad (3.14)$$

This gives us for the Berry curvature,

$$\mathbf{B}^{\pm}(\mathbf{h}) = \pm \frac{\mathbf{h}}{|\mathbf{h}|} \frac{1}{2\mathbf{h}^2}. \quad (3.15)$$

We can recognize in this the field of a pointlike monopole source in the origin. Alluding to the analog between the Berry curvature and the magnetic field of electrodynamics (both are derived from a “vector potential”) we can refer to this field, as a “magnetic monopole”. Note however that this monopole exists in the abstract space of the vectors \mathbf{h} and not in real space.

The Berry phase of the closed loop \mathcal{C} in parameter space, according to Eq. (3.6), is the flux of the monopole field through a surface \mathcal{S} whose boundary is \mathcal{C} . It is easy to convince yourself that this is half of the solid angle subtended by the curve,

$$\gamma_-(\mathcal{C}) = \frac{1}{2}\Omega_{\mathcal{C}}. \quad (3.16)$$

In other words, since the Berry phase is independent of the energies, we can project \mathbf{h} on the surface of a unit sphere, i.e., assume $\mathbf{h}^2 = 1$. This is the Bloch sphere, representing the Hamiltonian $\mathbf{h}\boldsymbol{\sigma}$ as well as the eigenstate $|+\rangle$. The Berry phase is half of the area enclosed by this projected image of \mathcal{C} , as illustrated in Fig. 3.1.

What about the Berry phase of the other energy eigenstate? From Eq. (3.8), the corresponding Berry curvature \mathbf{B}_+ is obtained by inverting the order of the factors in the cross product: this flips the sign of the cross product. Therefore the Berry phase

$$\gamma_+(\mathcal{C}) = -\gamma_-(\mathcal{C}). \quad (3.17)$$

One can see the same result on the Bloch sphere. Since $\langle + | - \rangle = 0$, the point corresponding to $|-\rangle$ is antipodal to the point corresponding to $|+\rangle$. Therefore, the curve traced by the $|-\rangle$ on the Bloch sphere is the inverted image of the curve traced by $|+\rangle$. These two curves have the same orientation, therefore the same area, with opposite signs.

In fact, a more general statement follows directly from Eq. (3.7), for a Hamiltonian H with an arbitrary number of levels. If all the spectrum of $H(\mathbf{R})$ is discrete along a closed curve \mathcal{C} , then one can add up the Berry phases of all the energy eigenstates. This sum has to be 0, because

$$\sum_n \gamma_n(\mathcal{C}) = \sum_n \frac{1}{2\pi} \int_{\mathcal{S}} \mathbf{B}^{(n)}(\mathbf{R}) d\mathcal{S} = \frac{1}{2\pi} \int_{\mathcal{S}} \sum_n \mathbf{B}^{(n)}(\mathbf{R}) d\mathcal{S}; \quad (3.18)$$

$$\sum_n \mathbf{B}^{(n)} = -\text{Im} \sum_n \sum_{n' \neq n} \frac{\langle n | \nabla_{\mathbf{R}} H | n' \rangle \times \langle n' | \nabla_{\mathbf{R}} H | n \rangle}{(E_n - E_{n'})^2} \quad (3.19)$$

$$= -\text{Im} \sum_n \sum_{n' < n} \frac{1}{(E_n - E_{n'})^2} \left(\langle n | \nabla_{\mathbf{R}} H | n' \rangle \times \langle n' | \nabla_{\mathbf{R}} H | n \rangle \right. \quad (3.20)$$

$$\left. + \langle n' | \nabla_{\mathbf{R}} H | n \rangle \times \langle n | \nabla_{\mathbf{R}} H | n' \rangle \right) = 0. \quad (3.21)$$

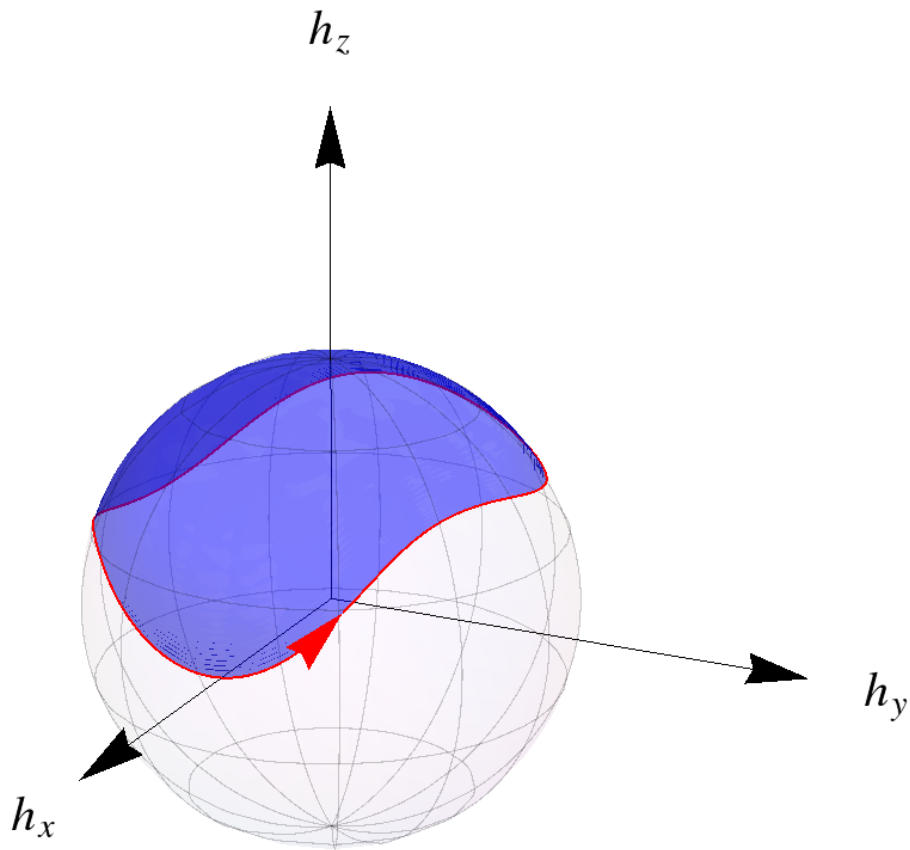


Figure 3.1: The Berry phase of a closed curve \mathcal{C} is half the area enclosed by the curve when it is projected onto the surface of the Bloch sphere.

3.2 Chern number – General Definition

Take a Hamiltonian that depends continuously on some parameters \mathbf{R} . Take a closed surface \mathcal{S} in the parameter space of \mathbf{R} , such that the n th eigenstate of the Hamiltonian is nondegenerate on the surface. The integral of the Berry curvature of the energy eigenstate $|n(k)\rangle$ on that surface is the Chern number,

$$Q^{(n)} = -\frac{1}{2\pi} \oint_{\mathcal{S}} \mathbf{B}^{(n)} d\mathcal{S}. \quad (3.22)$$

We are now going to prove that the Chern number is an integer. Take a simply connected closed loop \mathcal{C} in the surface \mathcal{S} . This cuts the surface into two parts: \mathcal{S}_1 and \mathcal{S}_2 . The Berry phase associated to $|n\rangle$ on the loop can be calculated by integrating the Berry connection on the loop, or by integrating the Berry curvature on either of these surfaces. The resulting Berry phase, modulo 2π , is measurable, and therefore cannot depend on which surface we integrated on,

$$\gamma^{(n)} = \oint_{\mathcal{C}} \mathbf{A}^{(n)} d\mathbf{R} = \int_{\mathcal{S}_1} \mathbf{B}^{(n)} d\mathcal{S} + 2\pi m_1 = \int_{\mathcal{S}_2} \mathbf{B}^{(n)} d\mathcal{S} + 2\pi m_2, \quad (3.23)$$

where $m_1, m_2 \in \mathbb{Z}$. The Chern number of the state $|n\rangle$ on the surface \mathcal{S} is obtained by integrating $\mathbf{B}^{(n)}$ on the surfaces \mathcal{S}_1 and \mathcal{S}_2 , but with opposite orientations of the surface element,

$$Q^{(n)} = -\frac{1}{2\pi} \oint_{\mathcal{S}} \mathbf{B}^{(n)} d\mathcal{S} = -\frac{1}{2\pi} \oint_{\mathcal{S}_1} \mathbf{B}^{(n)} d\mathcal{S} + \frac{1}{2\pi} \oint_{\mathcal{S}_2} \mathbf{B}^{(n)} d\mathcal{S} = m_2 - m_1. \quad (3.24)$$

The Chern number is a topological invariant. Since the Chern number of a state $|n\rangle$ on a closed surface \mathcal{S} is an integer, it cannot change under smooth deformations of either the Hamiltonian H or the surface \mathcal{S} . The only way its value can change is if the gap closes, i.e., the state $|n\rangle$ becomes degenerate with $|n+1\rangle$ or $|n-1\rangle$ at some point on the surface \mathcal{S} .

3.2.1 \mathbb{Z} -invariant: Chern number of a lattice Hamiltonian

As we did with the Berry phase, we are now going to apply the Chern number to a lattice Hamiltonian, treating the wavenumbers (quasimomenta) \mathbf{k} as tunable parameters. Take a lattice Hamiltonian on a 2-dimensional lattice,

$$H(k_x, k_y) |n(\mathbf{k})\rangle = E_n |n(\mathbf{k})\rangle \quad (3.25)$$

Here the two wavenumbers are from the Brillouin Zone, $\mathbf{k} = (k_x, k_y) \in \text{BZ}$, which is a 2-dimensional torus, $\text{BZ} = S_1 \times S_1$, since for any $n_x, n_y \in \mathbb{Z}$,

$$|n(k_x + 2n_x\pi, k_y + 2n_y\pi)\rangle = |n(k_x, k_y)\rangle. \quad (3.26)$$

As with the Berry phase, assume the n th energy eigenstate has an energy gap around it for any (k_x, k_y) . The Berry connection reads

$$A_j^{(n)} = -i \langle n(k_x, k_y) | \partial_{k_j} | n(k_x, k_y) \rangle, \quad \text{for } j = x, y. \quad (3.27)$$

The Chern number of the n 'th energy eigenstate is

$$Q^{(n)} = -\frac{1}{2\pi} \iint_{BZ} dk_x dk_y \left(\frac{\partial A_y^{(n)}}{\partial k_x} - \frac{\partial A_x^{(n)}}{\partial k_y} \right). \quad (3.28)$$

The Chern number of a band of an insulator is a topological invariant. Its value cannot change under smooth deformations of the parameters of the Hamiltonian, as long as at each $\mathbf{k} \in BZ$, the energy of the band is distinct from the neighboring bands, i.e., there are no direct band gap closings.

3.3 Two Level System

The simplest case where a Chern number can arise is a two-band system. Consider a particle with two internal states, hopping on a 2D lattice. The two internal states can be the spin of the conduction electron, but can also be some sublattice index of a spin polarized electron. In the translation invariant bulk, the wavenumbers k_x, k_y are good quantum numbers, and the Hamiltonian reads

$$H(k_x, k_y) = \mathbf{h}(\mathbf{k}) \boldsymbol{\sigma}, \quad (3.29)$$

with the function $\mathbf{h}(\mathbf{k})$ mapping a 2D vector from the Brillouin zone into a 3D vector. Since the Brillouin Zone is a torus, the endpoints of the vectors $\mathbf{h}(\mathbf{k})$ map out a deformed torus in \mathbb{R}^3 . This torus is a directed surface: its inside can be painted red, its outside, blue.

The Chern number of $|-\rangle$ is the flux of $\mathbf{B}_-(\mathbf{h})$ through this torus. We have seen above that $\mathbf{B}_-(\mathbf{h})$ is the magnetic field of a monopole at the origin $\mathbf{h} = 0$. If the origin is on the inside of the torus, this flux is +1. If it is outside of the torus, it is 0. If the torus is turned inside out, and contains the origin, the flux is -1. The torus can also intersect itself, and therefore contain the origin any number of times.

One way to count the number of times is to take any line from the origin to infinity, and count the number of times it intersects the torus, with a +1 for intersecting from the inside, and a -1 for intersecting from the outside. The sum is independent of the shape of the line, as long as it goes all the way from the origin to infinity.

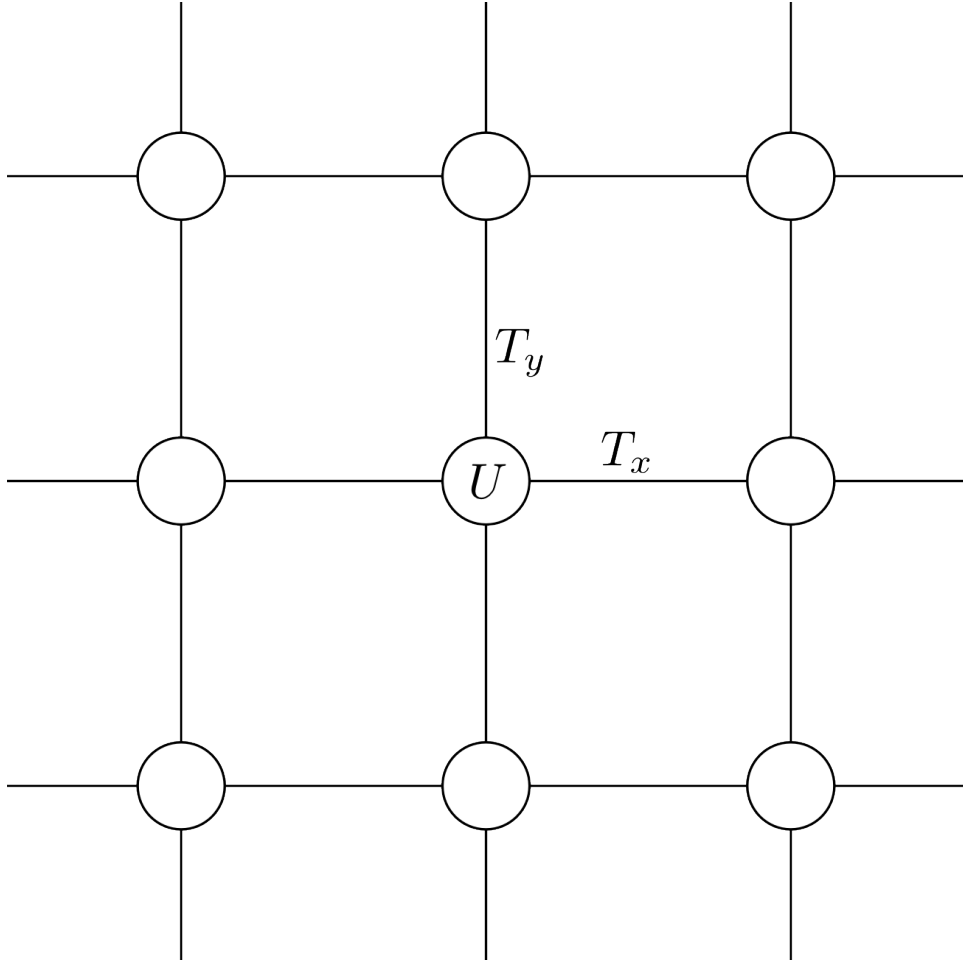


Figure 3.2: Sketch of the half BHZ model: a particle hopping on a square lattice. Each unit cell (circle) has two internal degrees of freedom. This can be rephrased as the particle being a spinor, and the onsite potential U and the hopping amplitudes T_x and T_y are 2×2 matrices.

3.3.1 The “half BHZ” model

To illustrate the concepts of Chern number, we take a simple toy model introduced by Bernevig, Hughes and Zhang, the “half BHZ” model. The attribute “half”, although somewhat ambiguous at the moment, will attain clarity in a following chapter. As sketched in Fig. 3.2, the half BHZ model describes a spinor particle hopping on a lattice (equivalent to a structureless particle hopping on a bipartite lattice), with the following Hamiltonian:

$$H(k) = [\Delta + \cos k_x + \cos k_y]\sigma_z + A(\sin k_x\sigma_x + \sin k_y\sigma_y). \quad (3.30)$$

This Hamiltonian has a Zeeman splitting term, with energy Δ , a spin- z dependent hopping, with unit amplitude, and a spin-orbit coupling type term with amplitude A (which we set to 1 for most of the calculations). This last term corresponds to hopping with associated spin flips: around the x axis for y direction hopping, and vice versa. Introducing a more general notation, we have

$$H(k) = \frac{1}{2}U + T_x e^{ik_x} + T_y e^{ik_y} + h.c.; \quad (3.31)$$

$$U = \Delta\sigma_z; \quad (3.32)$$

$$T_x = \frac{1}{2}\sigma_z - \frac{iA}{2}\sigma_x; \quad (3.33)$$

$$T_y = \frac{1}{2}\sigma_z - \frac{iA}{2}\sigma_y. \quad (3.34)$$

In real space generalization, with possibly site-dependent onsite and hopping terms, can be written using two-component cell indices $\mathbf{n} = (n_x, n_y)$, and unit vectors $\hat{\mathbf{x}} = (1, 0)$ and $\hat{\mathbf{y}} = (0, 1)$,

$$H_{\mathbf{m},\mathbf{n}} = \delta_{\mathbf{m},\mathbf{n}}U(\mathbf{n}) + \delta_{\mathbf{m}-\hat{\mathbf{x}},\mathbf{n}}T_x(\mathbf{n}) + \delta_{\mathbf{m},\mathbf{n}-\hat{\mathbf{x}}}T_x(\mathbf{m})^\dagger + \delta_{\mathbf{m}-\hat{\mathbf{y}},\mathbf{n}}T_y(\mathbf{n}) + \delta_{\mathbf{m},\mathbf{n}-\hat{\mathbf{y}}}T_y(\mathbf{m})^\dagger. \quad (3.35)$$

On a lattice with $N_x \times N_y$ unit cells, this includes periodic boundary conditions, e.g., if T_x and T_y are independent of \mathbf{n} , and open boundary conditions, if $T_x(N_x, n_y) = 0$ and $T_y(n_x, N_y) = 0$ for any n_x, n_y .

3.3.2 Dispersion relation

Making use of the algebraic properties of the Pauli matrices the bulk dispersion relation can be easily calculated. The spectrum is simply given in terms of the magnitude of the vector

$$\mathbf{h}(k_x, k_y) = \begin{pmatrix} A \sin k_x \\ A \sin k_y \\ \Delta + \cos k_x + \cos k_y \end{pmatrix}. \quad (3.36)$$

Thus

$$E_{\pm}(k_x, k_y) = \pm |\mathbf{h}(k_x, k_y)| \quad (3.37)$$

$$= \pm \sqrt{A^2(\sin^2(k_x) + \sin^2(k_y)) + (\Delta + \cos(k_x) + \cos(k_y))^2}. \quad (3.38)$$

This spectrum is depicted for some special parameter values in Fig.3.3. As can be seen from the figure, by tuning of the parameters one can close and reopen gaps in the spectrum. If $\Delta = -2$, the energy gap closes at the center of the Brillouin Zone, i.e., $k_x = k_y = 0$. In the vicinity of this so-called “Dirac point”, the dispersion relation has the shape of a “Dirac cone”. For $\Delta = 2$, we have a similar situation, with a Dirac cone at the corners of the Brillouin Zone, $k_x = k_y = \pm\pi$. Since each corner is equally shared between 4 Brillouin Zones, and we have 4 of them, this still leaves 1 Dirac point, 1 Dirac cone per Brillouin Zone. For $\Delta = 0$, we find two Dirac cones: one at $k_x = 0, k_y = \pm\pi$ and a second one at $k_x = \pm\pi, k_y = 0$. For all other values of Δ the spectrum is gapped, and thus it makes sense to investigate the topological properties of the system.

3.3.3 Torus argument

To calculate the Chern number for the valence band we shall employ the method discussed at the end of the last section. Namely we shall investigate how many times does the torus of the image of the Brillouin zone in the space of \mathbf{h} contain the origin. To get some feeling about the not so trivial geometry of the torus, it is instructive to follow a gradual sweep of the Brillouin zone in Fig. 3.4. The parameter Δ shifts the whole torus along the z-direction, thus as we tune it we also control whether the origin is contained inside it or not. Generally three situations can occur as it is also depicted in Fig. 3.5. The torus either does not contain the origin as in a) and d) and the Chern number is $Q = 0$ for $|\Delta| > 2$, or we can take a straight line to infinity from the origin that pierces the torus first from the blue side (outside) of the surface as in b) with $Q = -1$ for $-2 < \Delta < 0$, or piercing the torus from the red side (inside) as in c) with $Q = 1$ for $0 < \Delta < 2$.

3.4 Chern number as an obstruction

3.4.1 An apparent paradox

One might think that the most straightforward way to calculate the Chern number by just integrating the Berry vector potential around the Brillouin Zone. Applying Stokes’ theorem to Eq. (3.28) we get

$$Q^{(n)} = \oint_C \mathbf{A} d\mathbf{k}. \quad (3.39)$$

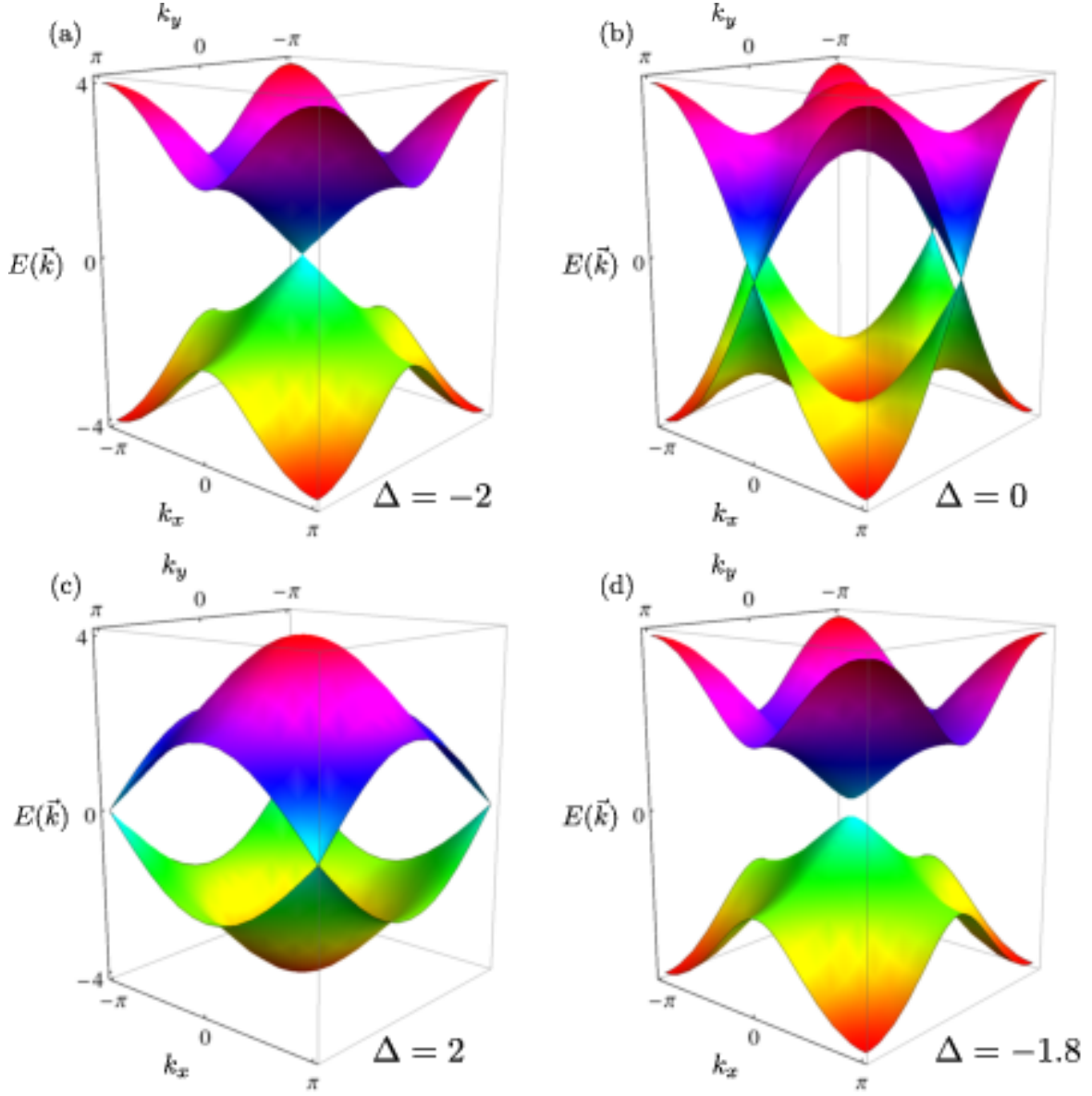


Figure 3.3: The dispersion relation of the “half BHZ” model, with spin-orbit coupling constant $A = 1$, and for various values of Δ , as indicated in the plots. In a-c), the gapless cases are shown, where the bulk gap closes at so-called Dirac points. In d), a generic value $\Delta = -1.8$, the system is insulating.

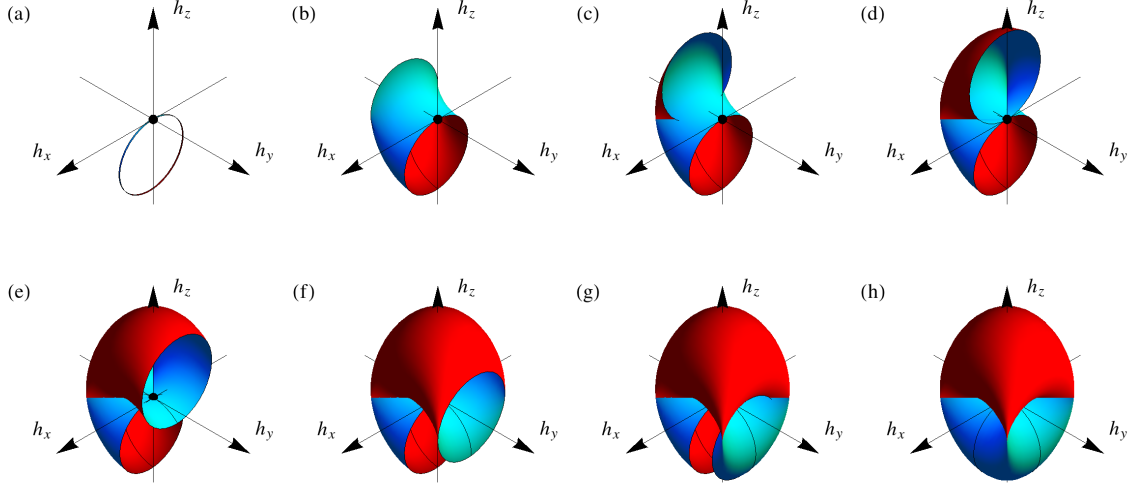


Figure 3.4: The surface $\mathbf{h}(\mathbf{k})$ for the half BHZ model as \mathbf{k} sweeps through the whole Brillouin zone. To illustrate how this surface is a torus the sweeping is done gradually with parameters $A = 1$ and $\Delta = 0$. In a) the image of the $k_y = -\pi$ line is depicted. In b) the image for the region $k_y = -\pi \cdots -0.5\pi$, in c) $k_y = -\pi \cdots -0.25\pi$, in d) $k_y = -\pi \cdots 0$, in e) $k_y = -\pi \cdots 0.25\pi$, in f) $k_y = -\pi \cdots 0.5\pi$, in g) $k_y = -\pi \cdots 0.75\pi$ and finally in h) the image of the whole Brillouin zone is depicted and the torus is closed.

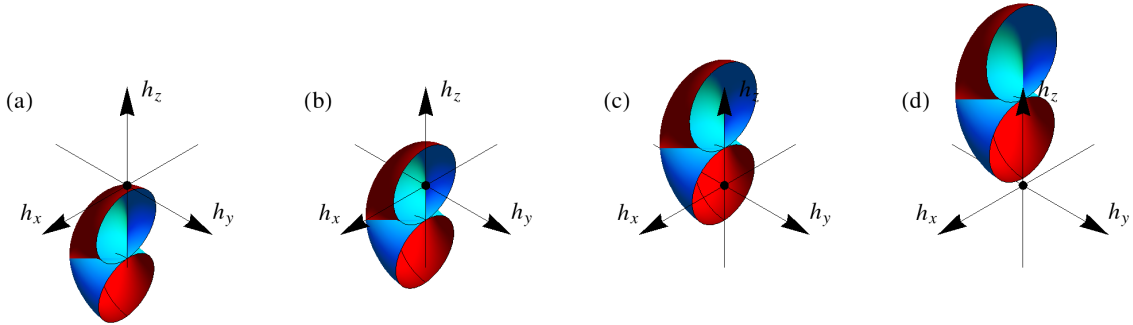


Figure 3.5: The torus $\mathbf{h}(\mathbf{k})$ of the half BHZ model for different values of Δ keeping $A = 1$. For clarity only the image of half of the Brillouin zone is shown. In a) and d) $\Delta = \mp 2.2$ and the torus does not contain the origin hence $Q = 0$. In b) $\Delta = -1$, taking an infinite line from the origin along the positive z axis we hit the blue side of the torus once hence $Q = -1$. In c) $\Delta = 1$, taking the infinite line in the negative z direction we hit the red side of the torus thus $Q = 1$.

The boundary of the Brillouin zone is obtained by cutting the torus open: cutting it along two circles \mathcal{C}_1 and \mathcal{C}_2 . The boundary means traversing along \mathcal{C}_1 , then \mathcal{C}_2 , then \mathcal{C}_1 , but in the opposite direction, then along \mathcal{C}_2 in the opposite direction. The Berry vector potential \mathbf{A} is a single-valued vector field on the torus. Its line integral then has to be 0.

This apparent paradox can be resolved by realizing that there must be a problem when we apply the Stokes' theorem to get from Eq. (3.28) to Eq. (3.39). If \mathbf{A} is smoothly defined everywhere on the surface of the torus, the Chern number must indeed be 0. However, it can happen that \mathbf{A} cannot be smooth over the whole Brillouin Zone. This is the case, if there is no choice of global gauge where the energy eigenstate $|n, k\rangle$ is a smooth function of k everywhere. As an example consider the two-level system.

A nonzero value of the Chern number shows that there is an obstruction towards defining a global, smooth energy eigenstate $|n, k\rangle$. The Chern number measures the number of *vortices*: points in k -space, for which the phase of $|n, k\rangle$ depends on the direction of approach. For an infinitesimal circle around such a point, the phase of $|n, k + dk\rangle$ must wind at least once. If it winds more than once, we can with a gauge transformation take the vortex apart to two singly charged vortices. If it does not wind, we can again with a gauge transformation get rid of the singularity. To read more on this picture of the Chern number, see the paper of Kohmoto [9]. This picture of the Chern number as an obstruction also points towards the efficient way of numerically calculating the Chern number.

3.4.2 Efficient discretization of the Chern number

We follow the paper of Fukui, Hatsugai, and Suzuki [5] in the discussion.

Above, we have seen that the Chern number reads

$$Q = -\frac{1}{2\pi} \int \int_{BZ} dk_x dk_y F(k_x, k_y); \quad (3.40)$$

$$F(k_x, k_y) = \frac{\partial A_y}{\partial k_x} - \frac{\partial A_x}{\partial k_y}, \quad (3.41)$$

using the notation of F for the Berry curvature. For brevity, we drop the index (n) where this leads to no confusion.

We now show how to efficiently discretize this integral on a momentum lattice:

$$\mathbf{k} = \frac{2\pi}{N} \mathbf{j}, \quad (3.42)$$

with \mathbf{j} a 2D vector of integers. Assume we have in some gauge a set of eigenstates

$$|n(\mathbf{j})\rangle. \quad (3.43)$$

Even if there is no globally continuous gauge, these eigenstates only need to be well defined on the lattice points, no problem with that.

Define as link variables the relative phase between eigenstates on neighbouring lattice sites:

$$U_\mu(\mathbf{j}) = \frac{\langle n(\mathbf{j} + \hat{\mu}) | n(\mathbf{j}) \rangle}{|\langle n(\mathbf{j} + \hat{\mu}) | n(\mathbf{j}) \rangle|}, \quad (3.44)$$

for

$$\mu = x, y : \quad \hat{x} \equiv (1, 0); \quad \hat{y} \equiv (0, 1). \quad (3.45)$$

For each plaquette, take the product of the relative phases around its boundary:

$$G(\mathbf{j}) \equiv U_x(\mathbf{j}) U_y(\mathbf{j} + \hat{x}) U_x(\mathbf{j} + \hat{y})^{-1} U_y(\mathbf{j})^{-1}. \quad (3.46)$$

If instead of the vectors $|n(\mathbf{j})\rangle$ we had complex numbers $\alpha(\mathbf{j})$ on the sites, with their relative phases defining the link variables U_μ , this product would have to be 1. However, because of the extra “room” in the Hilbert space, the plaquette variable can have any phase:

$$G(\mathbf{j}) = e^{iF(\mathbf{j})}. \quad (3.47)$$

Multiplying together all of the plaquette variables $G(\mathbf{j})$, we get 1:

$$\Pi_{\mathbf{j}} G(\mathbf{j}) = 1. \quad (3.48)$$

To prove this, consider multiplying the plaquette variables G together for two neighbouring plaquettes. The edge that they share cancels out from the product (See Fig. 3.6):

$$\begin{aligned} G(\mathbf{j})G(\mathbf{j} + \hat{y}) &= U_x(\mathbf{j}) U_y(\mathbf{j} + \hat{x}) U_x(\mathbf{j} + \hat{y})^{-1} U_y(\mathbf{j})^{-1} \\ &\quad U_x(\mathbf{j} + \hat{y}) U_y(\mathbf{j} + \hat{y} + \hat{x}) U_x(\mathbf{j} + 2\hat{y})^{-1} U_y(\mathbf{j} + \hat{y})^{-1} \\ &= U_x(\mathbf{j}) U_y(\mathbf{j} + \hat{x}) U_y(\mathbf{j})^{-1} U_y(\mathbf{j} + \hat{y} + \hat{x}) U_x(\mathbf{j} + 2\hat{y})^{-1} U_y(\mathbf{j} + \hat{y})^{-1}. \end{aligned} \quad (3.49)$$

When we calculate the product of all the plaquette variables on the full lattice all edges are shared by two neighboring plaquettes, taking into account the periodic boundary conditions. Therefore, from the product of the G for all plaquettes all edge contributions cancel: the product is 1.

Now concentrate on the plaquette variables $F(\mathbf{j})$, which are the phases of the $G(\mathbf{j})$. To properly define these phases, we have to select a branch for the logarithm:

$$F(\mathbf{j}) \equiv i \ln (U_x(\mathbf{j}) U_y(\mathbf{j} + \hat{x}) U_x(\mathbf{j} + \hat{y})^{-1} U_y(\mathbf{j})^{-1}); \quad (3.50)$$

$$-\pi < F(\mathbf{j}) \leq \pi. \quad (3.51)$$

If we sum the variables $F(\mathbf{j})$ over all the plaquettes, do we get 0? No, for the above “cancellation of the edges” argument to go through, we would need to consider

$$\tilde{F}(\mathbf{j}) \equiv i \ln U_x(\mathbf{j}) + i \ln U_y(\mathbf{j} + \hat{x}) - i \ln U_x(\mathbf{j} + \hat{y}) - i \ln U_y(\mathbf{j}) \quad (3.52)$$

If $-\pi \leq \tilde{F}(\mathbf{j}) < \pi$, then it is equal to $F(\mathbf{j})$. However, \tilde{F} can be outside that range: then it is taken back into $[-\pi, \pi)$ by adding an integer multiple of 2π . This happens when the relative phase around the loop, $\tilde{F}(\mathbf{j})$, has a magnitude that is too big: i.e., when there is a vortex in plaquette \mathbf{j} .

The discretized version of the Berry curvature counts the vortices by adding up the projected variables $F(\mathbf{j})$,

$$Q \equiv \frac{1}{2\pi} \sum_{\mathbf{j}} F(\mathbf{j}). \quad (3.53)$$

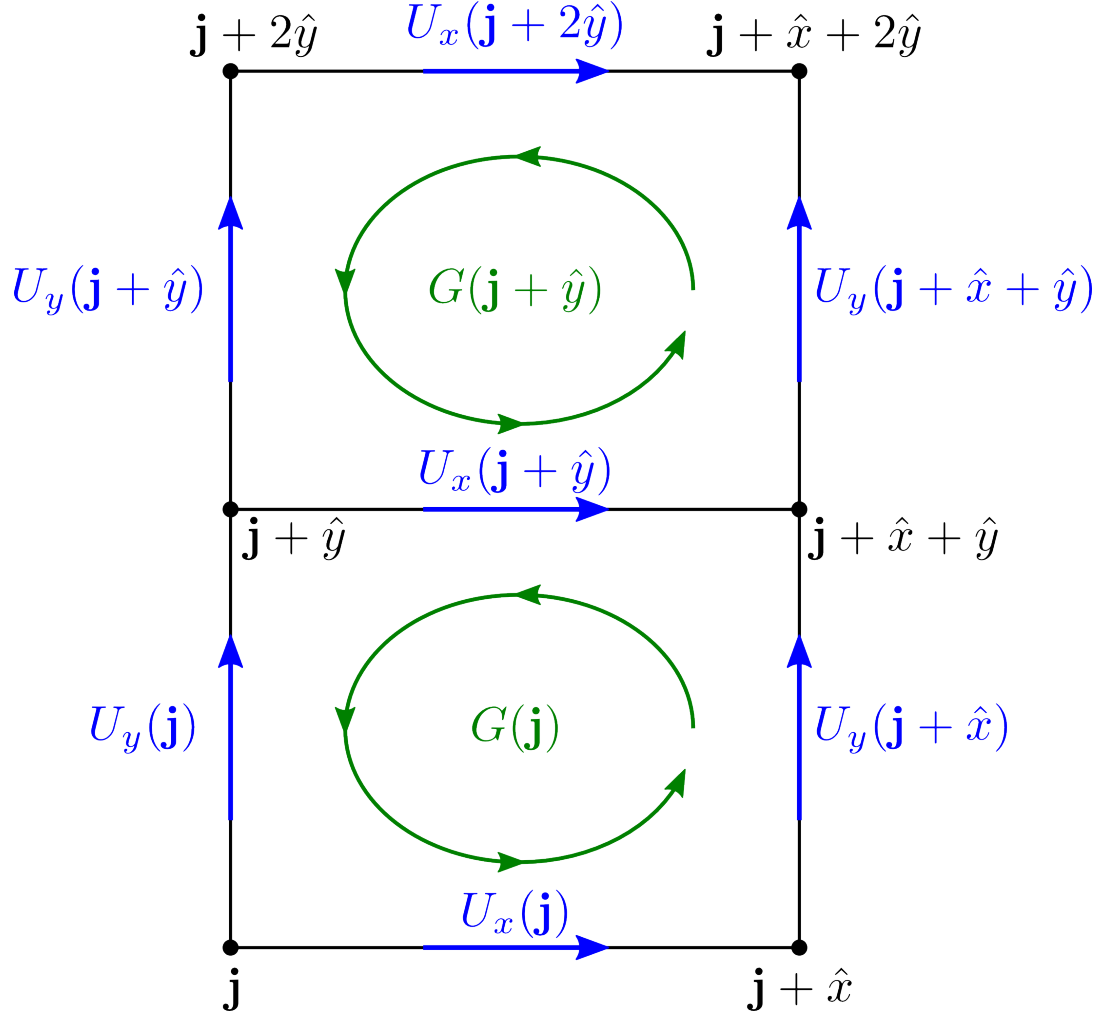


Figure 3.6: Illustration for the numerical plaquette method to calculate the Chern number of an arbitrary lattice model. The link variables $U_{x/y}$ are defined on links of neighboring sites, indexed by the coordinate of the vertex that is more to the left and more to the bottom. Each plaquette is associated a variable G indexed by the position of its left-bottom corner.

Chapter 4

Edge states in half BHZ

The unique physical feature of topological insulators is the guaranteed existence of low-energy states at their boundaries. We have seen an example of this for a 1-dimensional topological insulator, the SSH model: A finite, open, “topologically nontrivial” SSH chain hosts 0 energy bound states at both ends. The “bulk–boundary correspondence” was the way in which the topological invariant of the bulk – in the case of the SSH chain, the winding number of the bulk Hamiltonian – can be used to predict the number of edge states.

For insulators of dimensions 2 and above, the edge states are not simple bound states that live at the edges of a finite sample, but consist of propagating modes. In this chapter we show what these edge states are, how they arise for 2-dimensional insulators with broken time-reversal symmetry. There can be any number N_+ of counterclockwise and N_- of clockwise propagating edge states in a single sample. We show that the difference of these numbers, $N_+ - N_-$, is a topological invariant, i.e., cannot change under adiabatic deformations of the Hamiltonian, including those that introduce disorder at the edges of the sample. Moreover, this difference (or “signed sum”) of edge states is equal to the sum of the Chern numbers of the occupied (valence) bands of the translationally invariant bulk. This is the bulk–boundary correspondence for 2-dimensional “Chern insulators”.

4.1 Edge states

Consider a strip of a clean 2D insulator with a Chern number Q , depicted in Fig. 4.1. The strip is infinite along x , but along y consists of N sites, and is terminated by “open boundaries”, e.g., setting the hopping amplitudes to 0. Translation invariance holds along x , so we can partially Fourier transform – only along x . After the Fourier transformation, the original Hamiltonian has the form of a 1D lattice Hamiltonians with a continuous parameter k_x , which is the wavenumber along x . For a concrete example, we consider a

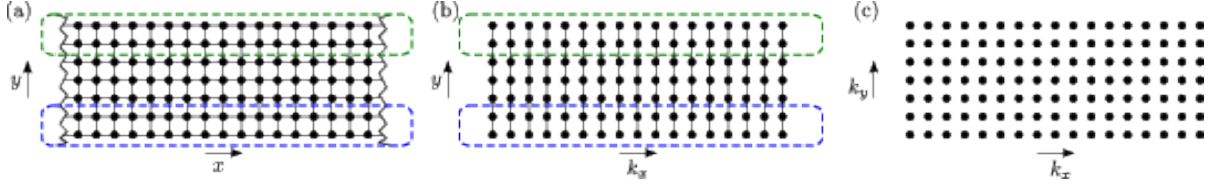


Figure 4.1: A strip of a lattice model for a 2D insulator (a), infinite along x , but terminated along y with open ends (hopping amplitudes set to 0). The end regions are outlined by blue/green rectangles, while the bulk part is not colored. Upon Fourier transformation along the translationally invariant direction x , the Hamiltonian can be written as an ensemble of 1D Hamiltonians (b), indexed by k_x . Each of these 1D chains consists of a lower edge (surrounded by the blue line), upper edge (surrounded by the green line), and a long, bulk part. The central, bulk part of each chain has translational invariance along y . Thus, the bulk part of each chain, upon Fourier transformation along y , can be written as a 0-dimensional Hamiltonian that depends continuously on k_x and k_y (c).

strip of the “half BHZ” model, Eq. (3.30). The k_x -dependent Hamiltonian reads

$$H(k_x) = \sum_{y=1}^N \left[(\Delta + \cos k_x) \sigma_z + A \sin k_x \sigma_x \right] \otimes |y\rangle \langle y| + \frac{1}{2} \sum_{y=1}^{N-1} (\sigma_z - iA\sigma_y) \otimes |y+1\rangle \langle y| + (\sigma_z + iA\sigma_y) \otimes |y\rangle \langle y+1| \quad (4.1)$$

We plot the energy eigenvalues of this Hamiltonian, for strip width $N = 20$, “spin-orbit parameter” $A = 1$ and $\Delta = -1.5$, in Fig. 4.2. Apart from the bulk bands and the energy gap around $E = 0$, characteristic of an insulator, there is a distinctive feature of the spectrum near $k_x \approx 0$. Here, as k_x is swept from roughly $-\pi/4$ to $\pi/4$, the N th (blue) and $N + 1$ th (green) energy eigenstate separate from the other eigenstates, leaving their bulk bands, cross near $k_x = 0$, and then switch places, each going to the bulk band the other departed from. While $-\pi/4 < k < \pi/4$, these eigenstates have energies deep inside the bulk gap, and so they must be at the edges: they are *edge states*. That they indeed are at the edges are confirmed by their wavefunctions, whose absolute values are plotted in Fig. 4.2 b). Roughly for $-\pi/4 < k_x < \pi/4$, these wavefunctions are localized at the edges. Clearly there is a crossing: the state propagating from left to right is localized at the lower edge, while the one propagating from right to left on the upper edge, for both $-\pi/4 < k_x < 0$ and $0 < k_x < \pi/4$. In the rest of the Brillouin Zone, where the N th and the $N + 1$ th eigenstate join the bulk bands, the corresponding energy eigenstates are delocalized over the whole system.

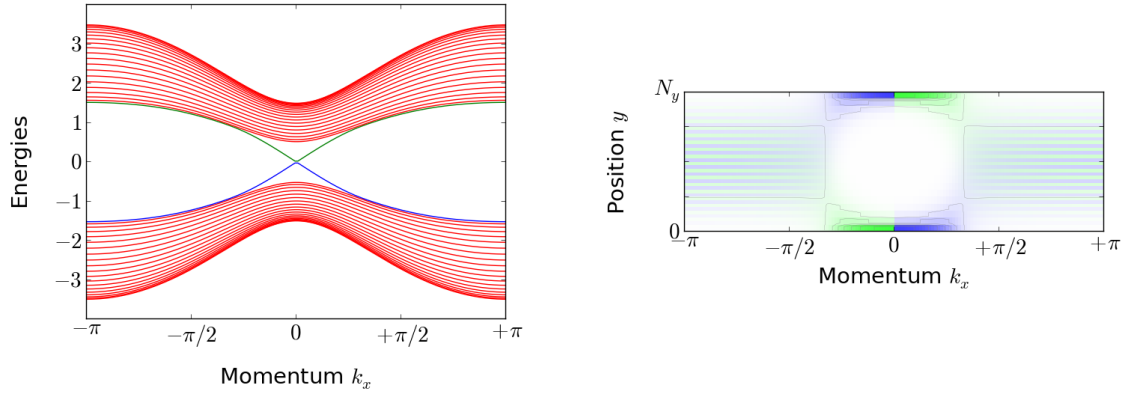


Figure 4.2: Dispersion relation of a strip of half BHZ model, of width $N = 20$, “spin-orbit parameter” $A = 1$ and gap parameter $\Delta = -1.5$. Because the strip is translation invariant along the edge, the wavenumber k_x is a good quantum number, and the energy eigenvalues can be plotted (left figure) as a function of k_x , forming the dispersion relations. The two middle eigenvalues, the N th and $N + 1$ th, are plotted in blue (green), all other energy eigenvalues are in red. These two branches of the dispersion relation are special because they cross near $k_x = 0$. In reality this is an avoided crossing with energy splitting $\propto e^{-N}$. The wavefunctions of the corresponding eigenstates are plotted as functions of k_x and y in the plot to the right. Here blue (green) corresponds to the N th ($N + 1$ th) energy eigenstate, and the intensity at to the absolute value of the wavefunction at the given position. In the vicinity of the crossing, for $-\pi/4 < k < \pi/4$, the two middle eigenstates have energies deep inside the bulk gap, and so their wavefunctions are concentrated at the edges: they are *edge states*. For other momenta they delocalize over the whole chain.

4.2 Number of edge states as a topological invariant

The signed sum, $N_+ - N_-$, of the number of edge states inside the gap on a single edge is a topological invariant. To understand what this statement means we explain the terms and provide illustrations using the half BHZ model. We identify an “edge state” as an energy eigenstate whose wavefunction has over 90% of its weight within 3 unit cells of the edge. In Figs. 4.4–4.7, the energies of such states on the lower (upper) edge are marked by dark blue (green) dots. Since we want to talk about edge states on a single edge, e.g. the lower edge, we have to be careful to count only the blue branches of the dispersion relation.

First, we clarify what we mean by the “number of edge states inside the gap”. The bulk states of a 2D system form 2-dimensional bands. For a system with a “clean” edge, i.e., with translational invariance along the edge direction x , the edge states form 1-dimensional bands (wavenumber k_x is a good quantum number). Pick an energy inside the bulk gap; a convenient choice is $E = 0$, but any other energy value is equally good. This defines a horizontal line in the graph of the dispersion relations. Pick an edge. Identify the number of times this line intersects the edge bands corresponding to this edge (this number can also be 0). At each intersection, the group velocity of the edge band (dE/dk_x) is either positive or negative: use this to assign +1 or −1 to the intersection. The number of intersections with positive group velocity is N_+ ; the number of those with negative group velocity is N_- . The difference of these two numbers is the “net number of edge states inside the gap”.

The “net number of edge states inside the gap”, $N_+ - N_-$, defined above is a topological invariant, i.e., it is invariant under smooth changes of the Hamiltonian. This “topological protection” is straightforward to prove, by considering processes that might change this number.

The number of times edge state bands intersect $E = 0$ can change because new intersection points appear. These can form because an edge state band is deformed, and as a result of an adiabatic deformation of the system gradually develops a “bump”, local maximum, and the local maximum gets displaced from $E < 0$ to $E > 0$. For a schematic example, see Fig. 4.3 (a)-(c). Alternatively, the dispersion relation branch of the edge state can also form a local minimum, gradually displaced from $E > 0$ to $E < 0$. In both cases, the number of intersections of the edge band with the $E = 0$ line grows by 2, but the two new intersections must have opposite group velocities. Therefore, both N_+ and N_- increase by 1, but their signed sum, $N_+ - N_-$, stays the same.

New intersection points can also arise because a new edge state band forms. As long as the bulk gap stays open, though, this new edge state band has to be a deformed version of one of the bulk bands, as shown in Fig. 4.3 (a)-(h)-(i). Because the periodic boundary conditions must hold in the Brillouin Zone, the dispersion relation of the new edge state has to “come from” a bulk band and go back to the same bulk band, or it can be detached from the bulk band, and be entirely inside the gap, but then its average

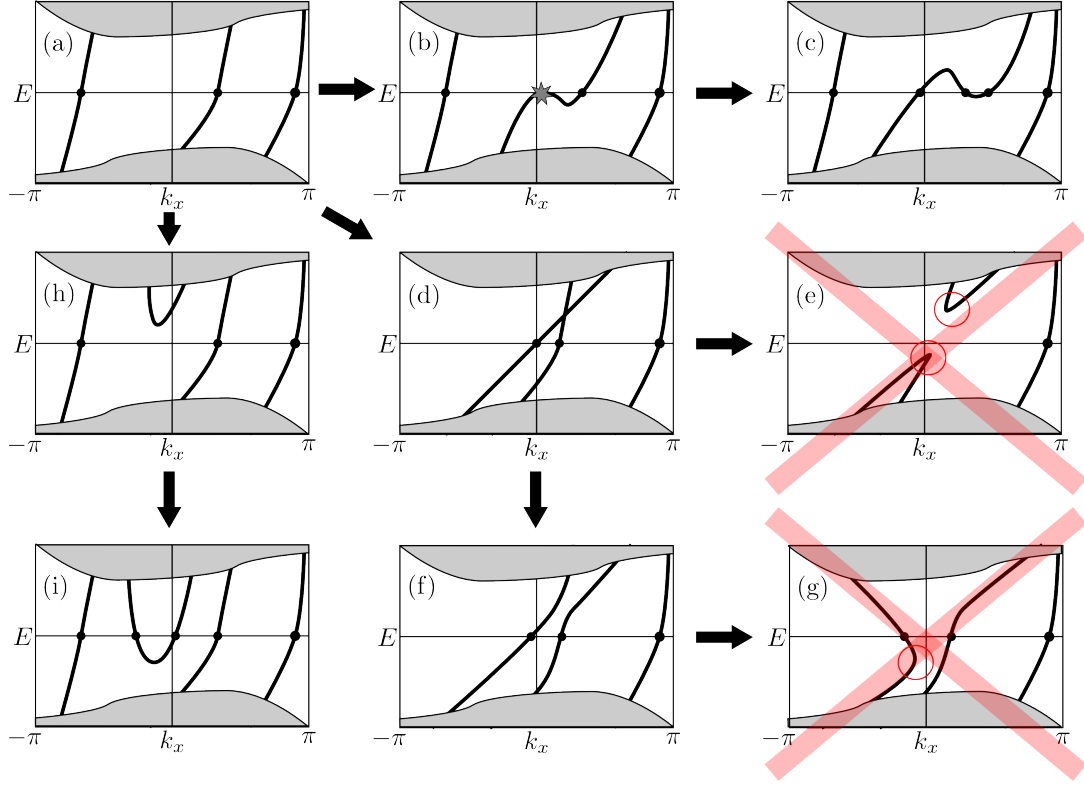


Figure 4.3: Adiabatic deformations of dispersion relations of edge states on one edge, in an energy window that is deep inside the bulk gap. Starting from a system with 3 copropagating edge states (a), an edge state’s dispersion relation can develop a “bump”, (b)-(c). This can change the number of edge states at a given energy (intersections of the branches with the horizontal line corresponding to the energy), but always by introducing new edge states pairwise, with opposite directions of propagation. Thus the signed sum of edge states remains unchanged. Alternatively, two edge states can develop a crossing, that because of possible coupling between the edge states turns into an avoided crossing (d),(f). This cannot open a gap between branches of the dispersion relation (e), as this would mean that the branches become multivalued functions of the wavenumber k_x (indicating a discontinuity in $E(k_x)$, which is not possible for a system with short-range hoppings). Therefore, the signed sum of edge states is also unchanged by this process. One might think the signed sum of edge states can change if an edge state’s direction of propagation changes under the adiabatic deformation, as in (g). However, this is also not possible, as it would also make a branch of the dispersion relation multivalued. Deformation of the Hamiltonian can also form a new edge state dispersion branch, as in (a)-(h)-(i), but because of periodic boundary conditions along k_x , this cannot change the signed sum of the number of edge states.

group velocity is 0. In both cases, the above argument applies, and it has to intersect the $E = 0$ line an even number of times, with 0 signed sum.

The number of times edge state bands intersect $E = 0$ can also decrease if two edge state bands develop a gap. However, to open a gap, the edge states have to propagate in different directions: otherwise a crossing between edge states simply becomes an avoided crossing, but no gap is opened, see Fig. 4.3 d)-f). This same argument show why it is not possible for an edge state to change its direction of propagation under an adiabatic deformation without developing a local maximum or minimum (which cases we already considered above). As shown in Fig. 4.3 (g), this would entail that at some stage during the deformation the edge state band was not single valued.

4.3 Numerical examples: the “half BHZ model”

We illustrate the ways translational invariant disorder (translational invariant along x) can affect edge states in the half BHZ model. First, we take the half BHZ model, Hamiltonian (4.1), and add disorder at the lower edge. The results are shown in Fig. 4.4. Different types of disorder were used to deform the edge state bands, for details, see the figure caption.

To show how disorder can open gaps in the edge state dispersion relations, we need a system with more than one edge state. The most straightforward path to such a system, based, e.g., on the BHZ model, is layering sheets of Chern Insulators onto each other, as illustrated in Fig. 4.5. As an example, the Hamiltonian for a whole system of 3 layers is constructed as

$$H_2(k_x) = \begin{bmatrix} H(\Delta_1, A_1, k_x) & C & 0 \\ C & H(\Delta_2, A_2, k_x - k_2) & C \\ 0 & C & H(\Delta_3, A_3, k_x - k_3) \end{bmatrix} \quad (4.2)$$

The coupling between the layers is taken independent of position, $C_{mn} = C\delta_{mn}$.

Numerical results for two and three coupled layers, with the Chern number of the second layer $+1$ or -1 , are shown in Figs. 4.6, 4.7. The coupling of copropagating edge modes lifts the degeneracies, but cannot open gaps in the spectrum. This is a simple consequence of the fact that an energy eigenstate has to be a single valued function of momentum. To open a gap, counterpropagating edge states have to be coupled. We achieve this by coupling layers of the BHZ model with opposite sign of the gap parameter Δ . For the case of two layers (Fig. 4.6, second row), this opens a gap in the spectrum. If there are three layers, there is a majority direction for the edge states, and so one edge state survives the coupling.

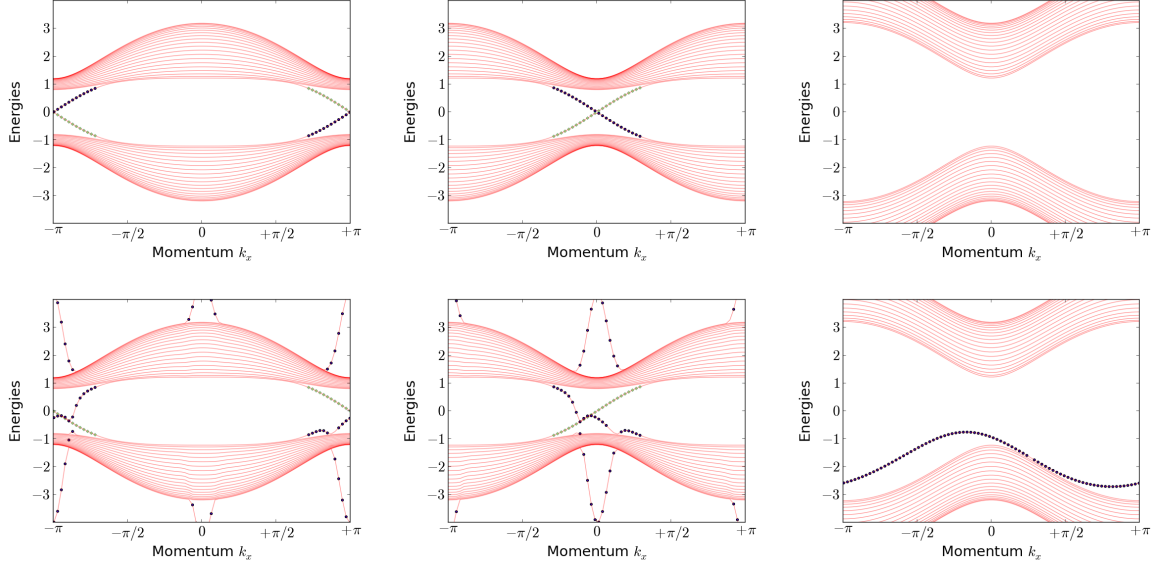


Figure 4.4: Dispersion relation of a strip of half BHZ. Edge states, whose wavefunction has over 90% on the first/last 3 unit cells, are marked in dark blue/green. Top row: a strip with clean terminations, with $\Delta = -1.2$ (left), $\Delta = 1.2$ (middle), $\Delta = 3.2$ (right). Bottom row: with the same parameters above, we added translation invariant deformation to the edge region at $y = 1$. For the Chern insulators, this deformation is a long range hopping term (in this case, a 20th neighbor hopping term, $\propto \cos^{20} k_x$), whereas for a trivial insulator, a simple onsite potential is used. The edge deformations do not affect the edge state at $y \approx N$, nor the bulk states, but distorts the edge mode at $y \approx 1$ and brings in new edge modes at energies that are in the bulk gap or above/below all bulk energies. The deformation can change the number of edge states at a specific energy, but only by adding a pair of edge states with opposite propagation directions. This leaves the topological invariant unchanged.

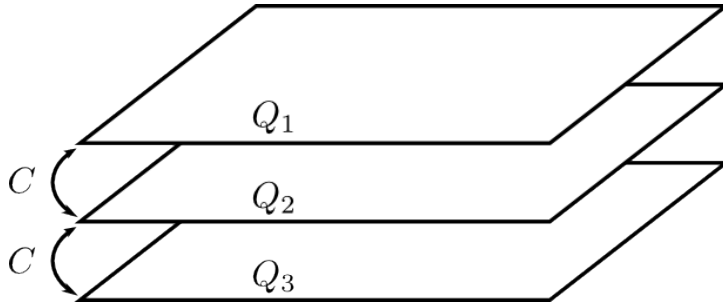


Figure 4.5: Layering sheets of 2-dimensional insulators on top of each other leads to a 2D insulator with possibly higher Chern number. For simplicity, we assume the sheets have the same lattice and the same Hamiltonians, only with different parameters. For uncoupled layers, the Chern numbers can simply be summed to give the total Chern number of the 3-layer structure, $Q_1 + Q_2 + Q_3$. Switching on coupling (hopping terms) between the sheets cannot change the Chern number as long as the bulk gap is not closed.

4.4 Laughlin argument, charge pumping, Chern number, chiral edge states

A large sample of a two-dimensional insulator consists of a bulk part, with Chern number Q the edges, which host a net number $N_+ - N_-$ of edge states. Both of these are topological invariants. We now use an argument due to Laughlin to show that in fact these two topological invariants are equal:

$$Q = N_+ - N_- . \quad (4.3)$$

Consider a strip of a 2D lattice insulator, translationally invariant along x , with Chern number Q , as in the previous section. As we have seen above, upon Fourier transformation along the translational invariant direction x , the 2D strip formally becomes a set of 1D lattice Hamiltonians, indexed by the parameter k_x . Now treat this parameter k_x as the time in a 1D adiabatic charge pumping process: consider initializing the system in the ground state at one specific value of k_x , and then increase k_x adiabatically by 2π . Since the strip was insulating, all of these 1D systems have a bulk gap, and so it is conceivable that the parameter k_x is tuned adiabatically. The Chern number indicates that the sum of the Zak phases of the occupied bulk bands changes during one period, $k_x = -\pi \dots \pi$, by $2\pi Q$. This means that the bulk polarization changes by Qea , where e is the electron charge and a the lattice constant (which we use as the unit of length anyway). Thus, through each unit cell in the bulk, a total of Q electrons must flow during the period $k_x = -\pi \dots \pi$ in the direction of $+y$ ($-y$) if the Chern number is positive (negative). Therefore at the upper (lower) edge Q extra electrons have accumulated during one time period, and Q electrons have left the lower (upper) edge.

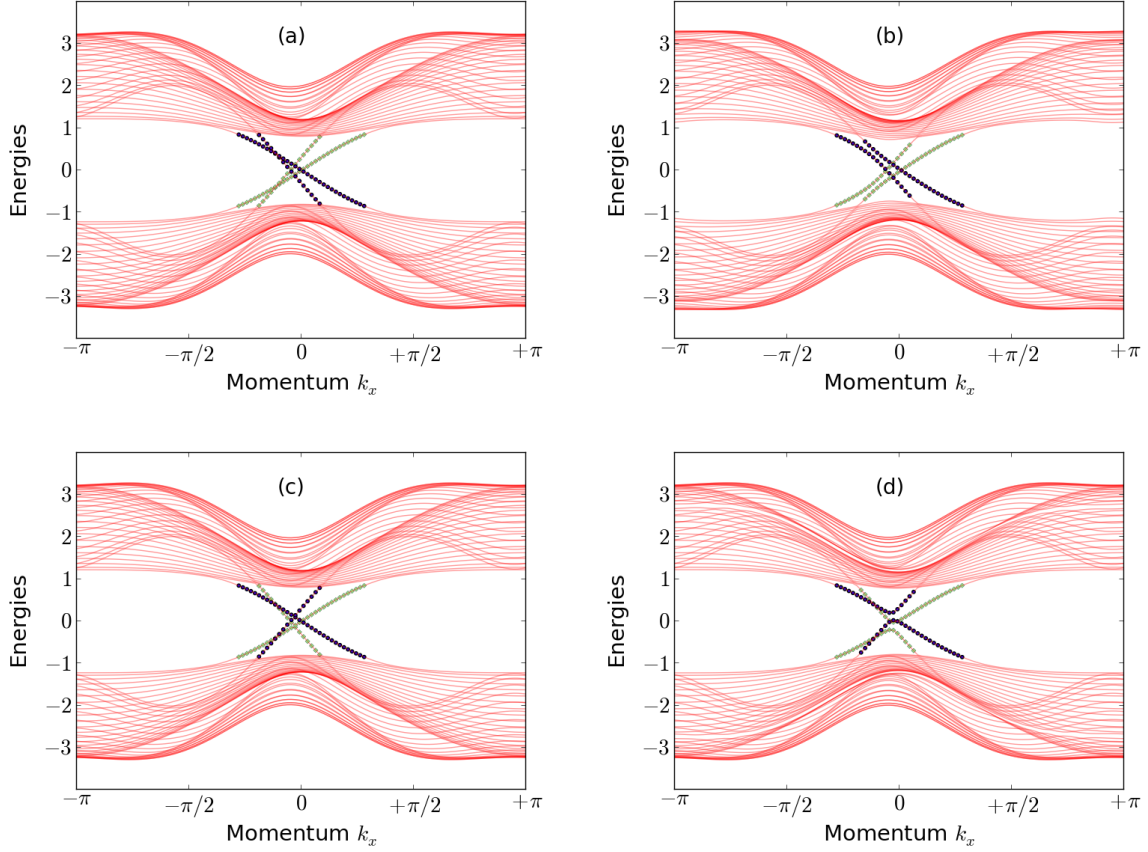


Figure 4.6: Dispersion relations of a strip of two layers the half BHZ model, $N = 20$ unit cells wide, with a clean termination along y . Red lines: energy eigenstates. Blue/Light Green dots: edge states (more than 90% weight on the first/last 3 unit cells). For the first layer, we use $A_1 = 1, \Delta_1 = -1.2$. The second layer, we set $A_2 = 1.8$, which gives faster edge modes, and we use Δ_2 to tune the direction of propagation of the edge mode in the second layer ($\Delta_2 = \Delta_1$ for copropagating, or $\Delta_2 = -\Delta_1$ and $k_2 = \pi$ for counterpropagating edge modes). We also displace k_x slightly in each layer for better visibility of the different edge modes. In each row, we plot uncoupled layers (left, $C = 1$) and coupled ones (right, $C = 1$).

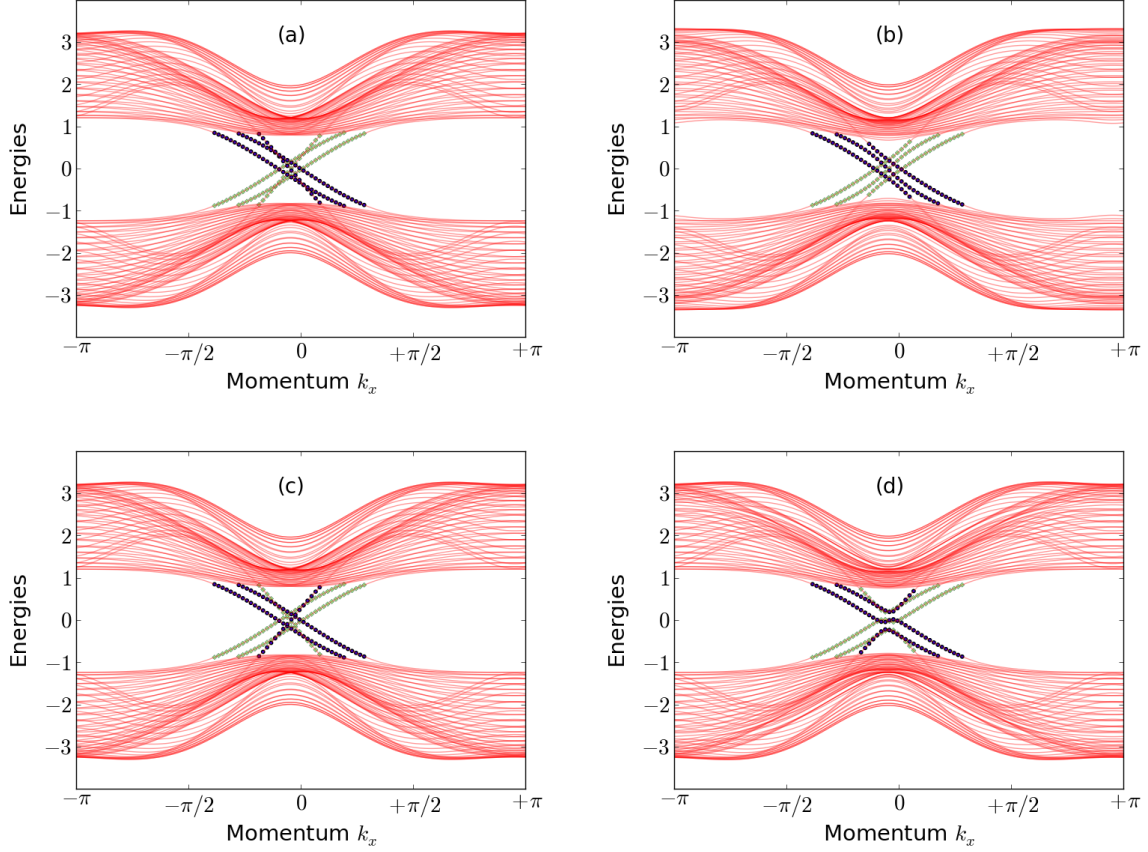


Figure 4.7: Dispersion relations of a strip of three layers of the half BHZ model, $N = 20$ unit cells wide, with a clean termination along y . Red lines: energy eigenstates. Blue/Light Green dots: edge states (more than 90% weight on the first/last 3 unit cells). For the first and third layer, we use $A_1 = 1, \Delta_1 = -1.2$. For the second layer, we set $A_2 = 1.8$, which gives faster edge modes, and we use $\Delta_2 = \Delta_1$ (top row) or $\Delta_2 = -\Delta_1$ and $k_2 = \pi$ (bottom row) We additionally displace k_x slightly in each layer for better visibility. In each row, we plot uncoupled layers (left, $C = 1$) and coupled ones (right, $C = 1$).

The only way this electron pumping can occur is if, at the end of the pumping cycle, the system is not in the ground state any more. At the end of the cycle, a number $|Q|$ of states with negative energy at the lower (upper) edge will be empty, and the same number of states with positive energy at the upper (lower) edge will be occupied. We remark that although these states are assigned to the upper or the lower edge, their energies are not necessarily in the bulk gap, and so their wavefunctions can extend far into the bulk.

Since the pump cycle was adiabatic, the energies of all states change continuously as the parameter k_x is tuned from $-\pi$ to π . Thus, there have to be $|Q|$ branches of the dispersion relation with positive (negative) group velocity inside the gap at the upper edge, and $|Q|$ branches with negative (positive) group velocity inside the gap at the lower edge, if the Chern number Q of the bulk is positive (negative). Each of these branches of the dispersion relation correspond to an edge state.

This completes the proof: the magnitude of the Chern number of the bulk of a 2D lattice system gives the number of edge states at the edges of the system. The sign of the Chern number gives the direction of propagation of these edge states. These are chiral states: at any edge, all of these propagate in the same direction. Since their energy is in the bulk gap, their wavefunctions decay exponentially away from the edge towards the bulk.

4.5 Robustness of edge states

Up to now, we have considered clean edges, i.e., 2D Chern Insulators that were terminated by an edge (at $y = 0$ and $y = N$), but translationally invariant along the edge, along x . This translational invariance, and the resulting fact that the wavenumber k_x is a good quantum number, was used for the definition of the topological invariant $N_+ - N_-$, which was the net number of edge bands propagating along the edge, equal to the bulk Chern number, Q . With disorder in the edge region that breaks translational invariance along x , we no longer have a good quantum number k_x , and edge state bands are not straightforward to define. However, as we show in this section, the edge states must still be there in the presence of disorder, since disorder at the edges cannot close the bulk gap.

Consider a finite, sample of a Chern insulator, with a clean bulk part but disordered edge region, as depicted in Fig. 4.8. The bulk gap of the sample decreases due to disorder, but we suppose that it is not closed completely (just renormalized). Consider now a small part of the sample, containing some of the edge, indicated by the dotted rectangle on the right of Fig. 4.8. Although this is much smaller than the whole sample, it is big enough so that part of it can be considered as translation invariant “bulk”. Now in this small part of the sample, we adiabatically (and smoothly) deform the Hamiltonian in such a way that we set the disorder gradually to 0. This includes straightening the part of the

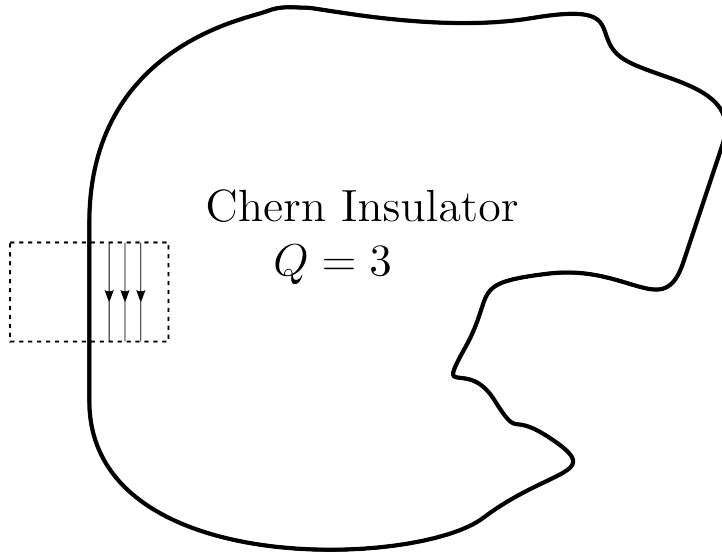


Figure 4.8: A disordered sample of Chern insulator. The dotted lines indicate rectangular parts of the sample, where disorder can be turned off adiabatically to reveal edge states (indicated in black). These describe electrons with energies deep in the bulk gap, propagating unidirectionally along the edge: a charge pump. Since the pumped electrons cannot turn back (unidirectional, or *chiral* channels), and cannot go into the bulk (in the gap), they have to travel all the way on the perimeter of the disordered sample, coming back to the rectangular, clean part. This means that there must be as many open channels for electrons to propagate along the edge, as the number of edge states in the clean part of the sample. The argument rests on charge conservation, and so is also valid in the presence of decoherence.

open boundary of the sample that falls into the dotted rectangle, to a straight line. The deformation is adiabatic in the sense that the bulk gap is not closed in the process. Since this small part is a clean Chern insulator, with a bulk Chern number of Q , it can be deformed in such a way that the only edge states it contains are $|Q|$ states propagating counterclockwise (if $Q > 0$, say).

Consider an electron in an edge state in the small clean part of the sample, with energy deep inside the bulk gap ($E \approx 0$). What can its future be, as its time evolution follows the Schrödinger equation appropriate for this closed system? Since the edge state is a chiral mode, the electron has to propagate along the edge until it leaves the clean region. Because of unitarity, the electron cannot “stop” at the edge: that would mean that at the “stopping point”, the divergence of the particle current in the energy eigenstate is nonzero. In other words, the particle current that flows in the edge state has to flow somewhere. (Put differently, if the mode describing an edge state electron “stopped at the interface”, two electrons, initially orthogonal, following each other in the mode, would after some time arrive to the same final state. This would break unitarity.) After leaving the clean part of the sample, the electron cannot propagate into the bulk, since its energy is deep in the bulk gap. The disorder in the clean part was removed adiabatically, and thus there are no edge states at the interface of the clean part and the disordered part of the sample, along the dashed line. The electron cannot turn back, as there are no edge states running “down” along the edge in the clean part. The only thing the electron can do is propagate along the edge, doing a full loop around the sample until it comes back to the clean part from below again.

The argument of the previous paragraph shows that even though the sample is disordered, there has to be a low energy mode that conducts perfectly (reflectionless) along the edge. Since at 0 energy there are Q orthogonal states an electron can be in at the edge of the clean part of the sample, unitarity of the dynamics of the electrons requires that all along the edge of the disordered sample there are Q orthogonal modes that conduct counterclockwise. There can be additional low energy states, representing trapped electrons, or an equal number of extra edge states for electrons propagating counterclockwise and clockwise. However, the total number of counterclockwise propagating edge modes at any part of the edge always has to be larger by Q than the number of clockwise propagating edge modes. Because the Hamiltonian is short range, our conclusions regarding the number of edge states at any point far from the deformed region have to hold independent of the deformation.

To be precise, in the argument above we have shown the existence of Q edge states all along the edge of the sample, except for the small part that was adiabatically cleaned from disorder. One way to finish the argument is by considering another part of the sample. If we now remove the disorder adiabatically only in this part, we obtain the existence of the edge modes in parts of the sample including the original dotted rectangle, which was not covered by the argument of the previous paragraph.

Chapter 5

Edge states in the 2D Dirac equation

The appearance of edge states in the half BHZ lattice model was discussed in the preceding Chapter. There, the edge states were revealed and analyzed via numerical diagonalization of the Hamiltonian of a terminated lattice. Here, we argue that it is also possible to describe these states in terms of a partial differential equation (PDE) similar to the Schrödinger and the Dirac equation. Working with a PDE instead of a lattice model offers the potential advantage of obtaining analytical results for certain physical properties of the considered material. Here we derive the Schrödinger-type PDE that provides a low-energy continuum description of the half BHZ lattice model, and use it to analytically characterize the edge states appearing at boundaries between regions with different Chern numbers, without the need to numerically diagonalize large tight-binding Hamiltonians. Even though in the entire Chapter we build our discussion on the half BHZ model, the applicability of the technique introduced here, called *envelope function approximation* (EFA), is more general and widely used to describe electronic states in various crystalline solids [1].

5.1 Reminder: the half BHZ model

The k -space Hamiltonian of the half BHZ model was defined in Eq. (3.30):

$$H(k_x, k_y) = (\Delta + \cos k_x + \cos k_y) \sigma_z + A(\sin k_x \sigma_x + \sin k_y \sigma_y) = \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \quad (5.1)$$

with

$$\mathbf{h}(\mathbf{k}) = \begin{pmatrix} A \sin k_x & \\ & A \sin k_y \\ \Delta + \cos k_x + \cos k_y & \end{pmatrix}. \quad (5.2)$$

The corresponding dispersion relation is

$$E_{\pm}(\mathbf{k}) = \pm h(\mathbf{k}) \equiv \pm |\mathbf{h}(\mathbf{k})|. \quad (5.3)$$

The half BHZ model describes an insulator if Δ is not equal to -2, 0 or 2. The Chern number Q of the half BHZ insulator can take on three different values, determined by the single parameter Δ :

$$Q = \begin{cases} 0, & \text{if } 2 < \Delta, \\ +1 & \text{if } 0 < \Delta < 2, \\ -1 & \text{if } -2 < \Delta < 0, \\ 0 & \text{if } \Delta < -2 \end{cases} \quad (5.4)$$

The number and propagation direction of topologically protected edge states at a domain wall is determined by the magnitude and difference of the Chern numbers of the two domains, respectively.

5.2 2D Dirac equation as a low-energy effective model

5.2.1 Gapless spectrum in the half BHZ model

First, consider the cases when the half BHZ model is metallic, ie, when its spectrum has no energy gap. This is the case if and only if Δ equals -2, 0 or 2. The corresponding band structures with $A = 1$ are shown in Fig. 3.3a, b and c. For $\Delta = -2$, the two bands touch at $\mathbf{k} = (0, 0)$, and form a conically shaped dispersion relation in the vicinity of that point, see Fig. 3.3a. For $\Delta = 0$ there are two inequivalent touching points at $\mathbf{k} = (0, \pi)$ and $\mathbf{k} = (\pi, 0)$. Fig. 3.3 shows four of them, though note that $\mathbf{k} = (-\pi, 0)$ is equivalent to $(\pi, 0)$ and $\mathbf{k} = (0, -\pi)$ is equivalent to $\mathbf{k} = (0, \pi)$. For $\Delta = 2$ there is a single touching point at $\mathbf{k} = (\pi, \pi)$. The other three touching points seen in Fig. 3.3c are equivalent with (π, π) .

The points where the bands touch are called Dirac points, and the conically shaped parts of the bands are called Dirac cones. The Dirac points and the Dirac cones are also referred to as valleys, or as Dirac valleys.

To describe low-energy excitations just above the filled valence band in such a conductor, it is sufficient to use a linearized approximation of the half BHZ Hamiltonian $H(\mathbf{k})$ that is obtained via a Taylor expansion of $H(\mathbf{k})$ up to first order in the k -space location $\mathbf{q} = \mathbf{k} - \mathbf{k}_D$ measured from the Dirac point \mathbf{k}_D . For example, in the case $\Delta = -2$ and correspondingly, $\mathbf{k}_D = (0, 0)$, the linearized Hamiltonian reads

$$H(\mathbf{k}_D + \mathbf{q}) \approx A(q_x \sigma_x + q_y \sigma_y) \quad (5.5)$$

The dispersion relation is $E_{\pm}(\mathbf{q}) = \pm Aq$, which equals the dispersion relation obtained after linearizing Eq. (5.3) around \mathbf{k}_D . Note that the dispersion relation of the Dirac equation of fermions with zero mass is

$$E_{\pm}(\mathbf{k}) = \pm \hbar k c, \quad (5.6)$$

where \hbar is the reduced Planck's constant and c is the speed of light. Therefore, the parameter A of the half BHZ model plays the role of $\hbar c$ of the relativistic dispersion relation (5.6). The eigenstates of the linearized Hamiltonian are

$$\psi_{\pm}(\mathbf{q}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{i\varphi} \end{pmatrix}, \quad (5.7)$$

where φ is the azimuthal angle of the wave vector \mathbf{q} . i.e., $\varphi = \arctan \frac{q_y}{q_x}$.

Note that at this point, the linearization of the Hamiltonian does not seem to be a particularly fruitful simplification: to obtain the dispersion relation and the eigenstates, a 2×2 matrix has to be diagonalized, no matter if the linearization has been done or not. However, linearizing the Hamiltonian is the first step towards a simple continuum description of inhomogeneous lattices, as shown below.

5.2.2 Opening a gap

Now consider a half BHZ insulator that is close to being metallic, ie, $\Delta \approx \Delta_0$ where Δ_0 is either -2, 0 or 2. To be specific, we consider the example where $\Delta_0 = -2$ and the corresponding Dirac point is at the Brillouin zone center, $\mathbf{k}_D = (0, 0)$. The dispersion relation for $\Delta = -1.8$ is shown in Fig. 3.3d. In the vicinity of the metallic state, as seen in the figure, a small gap equal to the energy splitting of the two states at the Dirac point $\mathbf{k}_D = (0, 0)$, opens in the spectrum.

The states and the dispersion relation around \mathbf{k}_D can again be described by a linearized approximation of the half BHZ Hamiltonian $H(\mathbf{k})$ that is obtained via a Taylor expansion of $H(\mathbf{k})$ up to first order in the k -space location $\mathbf{q} = \mathbf{k} - \mathbf{k}_D$ measured from the Dirac point \mathbf{k}_D . For example, in the case of $\Delta_0 = -2$ and $\mathbf{k}_D = (0, 0)$, the linearization yields

$$H(\mathbf{k}_D + \mathbf{q}) \approx M\sigma_z + A(q_x\sigma_x + q_y\sigma_y), \quad (5.8)$$

where we defined $M = \Delta - \Delta_0$. The dispersion relation reads

$$E_{\pm}(\mathbf{q}) = \pm \sqrt{M^2 + A^2 q^2}. \quad (5.9)$$

Note that the dispersion relation of the Dirac equation for fermions with finite mass $\mu \neq 0$ reads

$$E_{\pm}(\mathbf{k}) = \pm \sqrt{\mu^2 c^4 + \hbar^2 k^2 c^2}. \quad (5.10)$$

Therefore, the parameter M of the half BHZ model plays the role of μc^2 of the relativistic dispersion relation (5.10). The (unnormalized) eigenstates of the linearized Hamiltonian (5.8) have the form

$$\psi_{\pm}(\mathbf{q}) = \begin{pmatrix} q_x - iq_y \\ E_{\pm} - M \end{pmatrix}. \quad (5.11)$$

5.2.3 Inhomogeneous systems

A half BHZ lattice with inhomogeneous Δ parameter might support topologically protected bound states at boundaries separating locally homogeneous regions with different Chern numbers. Under certain conditions, as shown below, these bound states can be described analytically using the envelope function approximation (EFA) that results in a low-energy continuum description, i.e., a partial differential equation similar to the Dirac equation, of the states of the lattice. EFA is based on the assumption that the low-energy eigenstates of the inhomogeneous system are localized in Fourier space to the close neighborhood of a given wave vector. In the rest of this Chapter, we focus on the case where the inhomogeneous Δ is in the vicinity of -2 (e.g., $|\Delta + 2| \ll 1$), in which case the low-energy excitations are expected to localize in Fourier space around the band extremum point $\mathbf{k}_D = (0, 0)$ (see Figs. 3.3a and d). Here we derive the Schrödinger-type PDE, in fact resembling the two-dimensional Dirac equation, relevant for this case, and in the next Section we solve that for simple domain-wall arrangements.

The considered lattice is inhomogeneous due to the spatial dependence of the parameter Δ . In the tight-binding lattice model, we denote the value of Δ on site $\mathbf{m} = (m_x, m_y)$ as $\Delta_{\mathbf{m}}$, and correspondingly, we introduce the *local mass parameter* on site \mathbf{m} as $M_{\mathbf{m}} = \Delta_{\mathbf{m}} - (-2) = \Delta_{\mathbf{m}} + 2$. The main result of the EFA in our case is that the eigenstates and eigenvalues of the continuum Hamiltonian

$$\hat{H}_{\text{EFA}} = M(\mathbf{r})\sigma_z + A(\hat{q}_x\sigma_x + \hat{q}_y\sigma_y), \quad (5.12)$$

which we will refer to as the EFA Hamiltonian, correspond to and determine the low-energy eigenstates and eigenvalues of the tight-binding Hamiltonian of the inhomogeneous lattice model. In (5.12), $M(\mathbf{r})$ is a smooth extension of $M_{\mathbf{m}}$ such that $M(\mathbf{r}_{\mathbf{m}}) = M_{\mathbf{m}}$, and \hat{q}_α is the differential operator $-i\partial_\alpha$. Note that \hat{H}_{EFA} is related to the linearized k -space Hamiltonian (5.8) by the relations $M \leftrightarrow M(\mathbf{r})$ and $q_\alpha \leftrightarrow \hat{q}_\alpha$. The eigenvalue equation

$$\hat{H}_{\text{EFA}}\psi(\mathbf{r}) = E\psi(\mathbf{r}). \quad (5.13)$$

will be referred to as the *EFA Schrödinger equation* and we call $\psi(\mathbf{r})$ the envelope function. Note that in the case considered here, the EFA Schrödinger equation (5.13) takes the form of a 2D Dirac equation with inhomogeneous mass.

Before specifying the connection between \hat{H}_{EFA} and the inhomogeneous tight-binding model, a rather informal definition of spatially slowly varying functions is in order. We will call the envelope function $\psi(\mathbf{r})$ *spatially slowly varying* on the scale of the lattice constant (‘ssv’ for short), if its Fourier-transform $\psi^F(\mathbf{q})$ is localized to the $|\mathbf{q}| \ll \pi$ region, i.e., to the vicinity of the center of the first Brillouin zone of the lattice.

With this definition at hand, we can formulate the EFA proposition. Consider an inhomogeneous half-BHZ lattice with spatially varying mass parameter $M_{\mathbf{m}}$, with $|M_{\mathbf{m}}| \ll 1$ as discussed above. The Hamiltonian of the lattice is $\hat{H} = \sum_{\ell, \ell'} H_{\ell, \ell'} a_\ell^\dagger a_{\ell'}$,

where $\ell = (\mathbf{m}, j) \equiv (m_x, m_y, j)$ is a composite index of the two-component unit cell index $\mathbf{m} = (m_x, m_y)$ and internal (spin) quantum number $j \in \{\uparrow, \downarrow\}$, and a_ℓ^\dagger creates an electron on site \mathbf{m} with spin quantum number j . The matrix elements $H_{\ell, \ell'}$ are given in Eq. (3.35). Assume that the pair $(\psi(\mathbf{r}), E)$ solves the EFA Schrödinger equation corresponding to this lattice and $\psi(\mathbf{r})$ is ssv. Define the tight-binding state $|\Psi\rangle = \sum_{\ell=(\mathbf{m}, j)} \psi_j(\mathbf{r}_\mathbf{m}) a_\ell^\dagger |0\rangle$. It is claimed that the tight-binding state $|\Psi\rangle$ is approximately an eigenstate of the inhomogeneous lattice Hamiltonian with the eigenvalue E : $\hat{H} |\Psi\rangle = E |\Psi\rangle$.

To prove this, we calculate $\hat{H} |\Psi\rangle$:

$$\hat{H} |\Psi\rangle = \left(\sum_{\ell, \ell'} H_{\ell, \ell'} \hat{a}_\ell^\dagger \hat{a}_{\ell'} \right) \left(\sum_{\ell''} \psi_{j''}(\mathbf{r}_{\mathbf{m}''}) \hat{a}_{\ell''}^\dagger |0\rangle \right) = \sum_{\ell, \ell'} H_{\ell, \ell'} \psi_{j''}(\mathbf{r}_{\mathbf{m}''}) \hat{a}_\ell^\dagger |0\rangle, \quad (5.14)$$

which, after separating H to a spatially dependent on-site part $U_{\ell, \ell'} = \Delta_\mathbf{m} \delta_{\mathbf{m}, \mathbf{m}'} (\sigma_z)_{j, j'}$ and a spatially homogeneous hopping part $T_{\ell, \ell'} = H_{\ell, \ell'} - U_{\ell, \ell'}$ reads

$$\hat{H} |\Psi\rangle = \sum_{\ell, \ell'} (U_{\ell, \ell'} + T_{\ell, \ell'}) \psi_{j'}(\mathbf{r}_{\mathbf{m}'}) |\ell\rangle. \quad (5.15)$$

Here we introduced the notation $|\ell\rangle = a_\ell^\dagger |0\rangle$.

Consider the hopping part of (5.15) first:

$$\sum_{\ell, \ell'} T_{\ell, \ell'} \psi_{j'}(\mathbf{r}_{\mathbf{m}'}) |\ell\rangle = \sum_{\ell, \ell'} T_{\ell, \ell'} \left(\int d\mathbf{q} \psi_{j'}^F(\mathbf{q}) e^{i\mathbf{q}\mathbf{r}_{\mathbf{m}'}} \right) |\ell\rangle = \sum_{\ell, j'} \int d\mathbf{q} T_{j, j'}(\mathbf{q}) \psi_{j'}^F(\mathbf{q}) e^{i\mathbf{q}\mathbf{r}_\mathbf{m}} |\ell\rangle. \quad (5.16)$$

In the first step we inserted the Fourier transform $\psi^F(\mathbf{q})$ of the envelope function $\psi(\mathbf{r})$, and in the second we utilized the fact that T is representing a homogeneous lattice Hamiltonian and therefore $\sum_{\ell'} T_{\ell, \ell'} \psi_{j'}(\mathbf{q}) e^{i\mathbf{q}\mathbf{r}_{\mathbf{m}'}} = e^{i\mathbf{q}\mathbf{r}_\mathbf{m}} \sum_{j'} T_{j, j'}(\mathbf{q}) \psi_{j'}(\mathbf{q})$. Note that the explicit form of $T(\mathbf{q})$ is $T(\mathbf{q}) = (\cos q_x + \cos q_y) \sigma_z + A(\sin q_x \sigma_x + \sin q_y \sigma_y)$ in our case, see Eq. (5.1).

We now make use of the assumption that $\psi(\mathbf{r})$ is ssv, which implies that the integrand of the \mathbf{q} -integral in the last formula of (5.16) is significant only around $\mathbf{q} = 0$. Therefore we can expand $T(\mathbf{q})$ around $\mathbf{q} = 0$, yielding the following approximation:

$$\sum_{\ell, \ell'} T_{\ell, \ell'} \psi_{j'}(\mathbf{r}_{\mathbf{m}'}) |\ell\rangle \approx \sum_{\ell, j'} \int d\mathbf{q} \left[T_{j, j'}(\mathbf{q} = 0) + (\nabla_\mathbf{q} T_{j, j'})_{\mathbf{q}=0} \cdot \mathbf{q} \right] \psi_{j'}^F(\mathbf{q}) e^{i\mathbf{q}\mathbf{r}_\mathbf{m}} |\ell\rangle. \quad (5.17)$$

As the next step, we use $q_\alpha e^{i\mathbf{q}\mathbf{r}_\mathbf{m}} = (-i\partial_\alpha e^{i\mathbf{q}\mathbf{r}})_{\mathbf{r}=\mathbf{r}_\mathbf{m}} = (\hat{q}_\alpha e^{i\mathbf{q}\mathbf{r}})_{\mathbf{r}=\mathbf{r}_\mathbf{m}}$, which implies that the second factor (\mathbf{q}) of the second term in the square bracket of Eq. (5.17) can be substituted with $\hat{\mathbf{q}}$. Therefore

$$\begin{aligned} \sum_{\ell, \ell'} T_{\ell, \ell'} \psi_{j'}(\mathbf{r}_{\mathbf{m}'}) |\ell\rangle &\approx \sum_{\ell} \left[\int d\mathbf{q} A(\hat{q}_x \sigma_x + \hat{q}_y \sigma_y) \psi^F(\mathbf{q}) e^{i\mathbf{q}\mathbf{r}} \right]_{j, \mathbf{r}=\mathbf{r}_\mathbf{m}} |\ell\rangle \\ &= \sum_{\ell} [A(\hat{q}_x \sigma_x + \hat{q}_y \sigma_y) \psi(\mathbf{r})]_{j, \mathbf{r}=\mathbf{r}_\mathbf{m}} |\ell\rangle. \end{aligned} \quad (5.18)$$

Together with the on-site U terms of Eq. (5.15) we have

$$\hat{H} |\Psi\rangle \approx \sum_{\ell} \{[M(\mathbf{r})\sigma_z + A(\hat{q}_x\sigma_x + \hat{q}_y\sigma_y)] \psi(\mathbf{r})\}_{j,\mathbf{r}=\mathbf{r}_m} |\ell\rangle, \quad (5.19)$$

which, as $\psi(\mathbf{r})$ solves the EFA Schrödinger equation with energy E , equals

$$\hat{H} |\Psi\rangle \approx \sum_{\ell} E \psi_j(\mathbf{r}_m) |\ell\rangle = E |\Psi\rangle. \quad (5.20)$$

With this the proof is concluded.

Even though this proposition was stated for the special case of the half BHZ model with $\Delta(\mathbf{r}_m) \approx -2$, it can be straightforwardly generalized to the other two nearly metallic states of the half BHZ model ($\Delta(\mathbf{r}_m) \approx 0$ and $\Delta(\mathbf{r}_m) \approx 2$), as well as to describe electronic states in the vicinity of a band extremum in a generic crystalline solid. In fact, EFA is a widely used method to describe such electronic states in the presence of a spatially slowly varying electromagnetic field.

Finally, let us highlight a limitation of the EFA that perhaps is not obvious from the above statement. Even though there was no explicit condition on the characteristics of the mass inhomogeneity in the EFA proposition above, the ssv condition on the envelope function $\psi(\mathbf{r})$ is actually an implicit condition for the inhomogeneous mass $M(\mathbf{r}_m)$. Namely, if the Fourier components of the spatial mass inhomogeneity that correspond to wave vectors outside the central part of the Brillouin zone are strong enough, then the low-energy solutions of the EFA Schrödinger equation acquire large- \mathbf{q} Fourier components, and therefore cannot fulfill the ssv criterion. Therefore, the applicability of the EFA scheme is limited to inhomogeneities that are also, in a certain sense, spatially slowly varying.

5.3 Edge states

Having the EFA Hamiltonian (5.12) at hand, we can now use it to describe low-energy states in the inhomogeneous half BHZ model, provided $|M(x, y)| \ll 1$ everywhere in the x-y plane. From now on, we measure the prefactors in the EFA Hamiltonian in units of A , hence the Dirac-type EFA Schrödinger equation reads:

$$[M(x, y)\sigma_z + \sigma_x\hat{q}_x + \sigma_y\hat{q}_y] \psi(x, y) = E\psi(x, y). \quad (5.21)$$

Consider the homogeneous case first: $M(x, y) = M_0$, where M_0 might be positive or negative. What is the dispersion relation for propagating waves? What are the energy eigenstates? The answers follow from the plane-wave Ansatz

$$\psi(x, y) = \begin{pmatrix} a \\ b \end{pmatrix} e^{iq_x x} e^{iq_y y} \quad (5.22)$$

with $q_x, q_y \in \mathbb{R}$ and $a, b \in \mathbb{C}$. With this trial wave function, Eq. (5.21) yields two solutions:

$$E_{\pm} = \pm \sqrt{M_0^2 + q_x^2 + q_y^2}, \quad (5.23)$$

and

$$\frac{a_{\pm}}{b_{\pm}} = \frac{q_x - iq_y}{E_{\pm} - M_0}. \quad (5.24)$$

Now let us turn to our main focus and establish the edge states at a domain wall between two locally homogeneous regions where the sign of the mass parameter is different. Remember that the sign of the mass parameter in the EFA Hamiltonian is related to the Chern number of the corresponding homogeneous half-BHZ lattice: in our case, a positive (negative) mass implies a Chern number -1 (0).

To be specific, we will consider the case when the two domains are defined as the $y < 0$ and the $y > 0$ half-planes, i.e., the mass profiles in Eq. (5.21) are

$$M(x, y) = \begin{cases} M_0 & \text{if } y > 0, \\ -M_0 & \text{if } y < 0 \end{cases}. \quad (5.25)$$

Let M_0 be positive; the corresponding mass profile is illustrated in Fig. 5.1a.

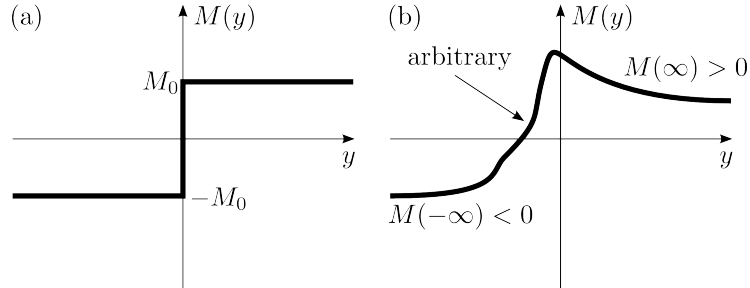


Figure 5.1: (a) Step-like and (b) irregular spatial dependence of the mass parameter of the 2D Dirac equation.

Now we look for edge-state solutions of Eq. (5.21), i.e., for states that reside in the energy range $-M_0 < E < M_0$, i.e., in the bulk gap of the two domains and which propagate along but decay perpendicular to the domain wall at $y = 0$. Our wave-function Ansatz for the upper half plane $y > 0$ is

$$\psi_u(x, y) = \begin{pmatrix} a_u \\ b_u \end{pmatrix} e^{iq_x x} e^{iq_y^{(u)} y} \quad (5.26)$$

with $q_x \in \mathbb{R}$, $q_y^{(u)} \in i\mathbb{R}^+$ and $a, b \in \mathbb{C}$. For the lower half plane, $\psi_l(x, y)$ is defined as $\psi_u(x, l)$ but with $u \leftrightarrow l$ interchanged and $q_y^{(l)} \in i\mathbb{R}^-$. The wave function $\psi_u(x, y)$ does

solve the 2D Dirac equation defined by Eqs. (5.21) and (5.25) in the upper half plane $y > 0$ provided

$$q_y^{(u)} = i\kappa \equiv i\sqrt{M_0^2 + q_x^2 - E^2} \quad (5.27)$$

and

$$\frac{a_u}{b_u} = \frac{q_x + \kappa}{E - M_0} \quad (5.28)$$

Similar conditions apply for the ansatz $\psi_l(x, y)$ for the lower half plane, with the substitutions $u \mapsto l$, $\kappa \mapsto -\kappa$ and $M_0 \mapsto -M_0$. The complete (unnormalized) wave function has the form

$$\psi(x, y) = \psi_u(x, y)\Theta(y) + c\psi_l(x, y)\Theta(-y), \quad (5.29)$$

where c is a yet unknown complex parameter to be determined from the boundary conditions at the domain wall.

The wave function (5.29) is an eigenstate of the EFA Hamiltonian with energy E if the boundary condition that the wave function is continuous on the line $y = 0$, that is,

$$\psi_u(x, 0) = \psi_l(x, 0), \quad (5.30)$$

is fulfilled for every x . Note that in our case, the Dirac equation is a first-order differential equation and therefore there is no boundary condition imposed on the derivative of the wave function.

The boundary condition (5.30) determines the value of the parameter c as well as the dispersion relation $E(q_x)$ of the edge states. First, (5.30) implies

$$q_x - \kappa = c(q_x + \kappa) \Rightarrow c = \frac{q_x - \kappa}{q_x + \kappa}, \quad (5.31)$$

$$E + M_0 = c(E - M_0) \Rightarrow -q_x M_0 = \kappa E. \quad (5.32)$$

Note that κ depends on E according to Eq. (5.27). It is straightforward to find the dispersion relation of the edge states by solving $-q_x M_0 = \kappa(E)E$ for E with the condition $-M_0 < E < M_0$:

$$E = -q_x. \quad (5.33)$$

This simple dispersion relation is shown in Fig. 5.2a. Together with Eq. (5.27), this dispersion implies that the localization length of edge states is governed by M_0 only, i.e., is independent of q_x . The squared wave function of an edge state is shown in Fig. 5.2b.

A remarkable consequence of this simple dispersion relation is that the spinor components of the envelope function also have a simple form:

$$\begin{pmatrix} a_u \\ b_u \end{pmatrix} = \begin{pmatrix} a_l \\ b_l \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (5.34)$$

Edge states at similar mass domain walls at $\Delta(y) \approx 0$ and $\Delta(y) \approx 2$ can be derived analogously. Note that at $\Delta(y) \approx 0$, the low-energy states can reside in two different

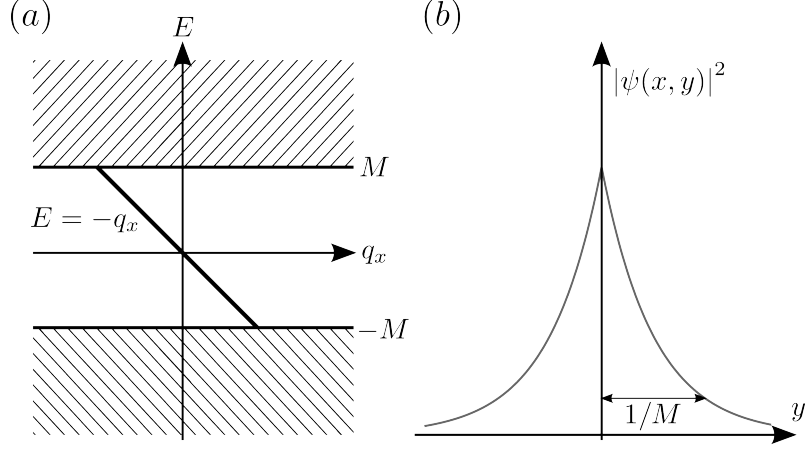


Figure 5.2: Edge state obtained from the 2D Dirac equation. (a) Dispersion relation and (b) squared wave function of an edge state localized at the mass domain wall illustrated in Fig. 5.1a.

Dirac valleys, around $\mathbf{k}_D = (0, \pi)$ or $\mathbf{k}_D = (\pi, 0)$, and there is one edge state in each valley. The number of edge states obtained in the continuum model, as well as their directions of propagation, are in correspondence with those obtained in the lattice model; as we have seen for the latter case, the number and direction are given by the magnitude and the sign of Chern-number difference across the domain wall, respectively.

An interesting fact is that the existence of the edge state is not constrained to case of a sharp, step-like domain wall described above. Moreover, the simple dispersion relation and spinor structure found above generalize for more irregular domain walls. To see this, consider an almost arbitrary 1D spatial dependence of the mass, illustrated in Fig. 5.1b: $M(x, y) = M(y)$ with the only condition that M changes sign between the half-planes $y < 0$ and $y > 0$, i.e., $M(y \rightarrow -\infty) < 0$ and $M(y \rightarrow \infty) > 0$. We claim that there exists a solution of the corresponding 2D Dirac equation that propagates along the domain wall, has the dispersion relation $E = -q_x$, is confined in the direction perpendicular to the domain wall, and has the wave function

$$\psi(x, y) = \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{iq_x x} f(y). \quad (5.35)$$

To prove this proposition, insert this wave function $\psi(x, y)$ to the 2D Dirac equation and substitute E with $-q_x$ therein. This procedure results in two equivalent equations that are fulfilled if $\partial_y f(y) = -M(y)f(y)$, implying that Eq. (5.35) is indeed a normalizable solution with $E = -q_x$ provided that the function f has the form

$$f(y) = e^{-\int_0^y dy' M(y')}. \quad (5.36)$$

In the preceding Chapters, we introduced the topological characterization of lattice models and the corresponding edge states, with the Brillouin zone of the lattice playing a central role in the formulation. In this Chapter, we demonstrated that under certain conditions, a low-energy continuum description (the EFA Schrödinger equation) can be derived from a lattice model, and can be used to describe edge states at domain walls between regions of differing topological character. Besides being a convenient analytical tool to describe inhomogeneous lattices, the envelope-function approximation also demonstrates that the emergence of protected edge states is not restricted to lattice models.

Chapter 6

2-dimensional time-reversal invariant topological insulators

In the previous chapters, we have understood how 2-dimensional insulators can host chiral (i.e., one-way propagating) edge states. The existence of chiral edge states precludes time-reversal symmetry. Indeed, time-reversed edge states would describe particles propagating backwards along the edge. In “Chern insulators”, the fact that these states are not present in the spectrum is what ensures the reflectionless propagation of particles at the edges.

What about time-reversal symmetric (or time-reversal invariant, TRI) two-dimensional insulators? According to the above, they cannot be Chern insulators. Interestingly though, the same time-reversal symmetry that ensures that for every edge state there is a “backward-propagating” partner, can also ensure that no scattering between these two modes occurs. This means that it is possible for time-reversal invariant 2D insulators to host edge states that show reflectionless propagation, in both directions, at both edges. The details of why and how this happens are discussed in this and the following chapters.

We will find that all two-dimensional time-reversal invariant insulators fall into two classes: the trivial class, with an even number of pairs of edge states at a single edge, and the topological class, with an odd number of pairs of edge states at a single edge. We then subsequently show that disorder that breaks translational invariance along the edge can destroy edge state conduction in the trivial class, but not in the topological class.

For Chern Insulators, we had a simple way to relate the topological invariant characterizing the properties of the edge of a finite sample, the net number of edge states on the edge, $N_+ - N_-$, to a topological invariant characterizing the translation invariant bulk, the Chern number Q . We showed that $Q = N_+ - N_-$ using the Laughlin argument, which mapped the 2-dimensional system to a periodically, adiabatically pumped 1-dimensional chain. After the mapping, the unit of charge pumped through the chain during a period could be identified with the net number of chiral edge states. This is the bulk–boundary

correspondence for Chern insulators.

Unfortunately, identifying and calculating the bulk topological invariant of a time-reversal invariant two-dimensional insulator is much more cumbersome than for a Chern insulator. There is extensive mathematical work on how to formulate the bulk invariant, but there is no general and simple recipe for actually calculating it for a lattice model. Therefore, in this chapter we only give some of the theoretical elements used in the constructions, and the numerical recipe for the special (but rather common) case of systems with inversion symmetry.

6.1 Time-Reversal Symmetry

Before we discuss Time-reversal symmetric topological insulators, we first need to understand what we mean by time reversal symmetry, and how it leads to Kramers' degeneracy.

6.1.1 Time Reversal in continuous variable quantum mechanics

Take a single particle with time independent Hamiltonian $\hat{H} = (\hat{p} - e\mathbf{A}(\hat{r}))^2 + V(\hat{r})$, where \mathbf{A} and V are the vector and scalar potentials, real valued functions of \hat{r} , respectively, and e is the charge of the particle. The corresponding Schrödinger equation for the wavefunction $\Psi(\mathbf{r}, t)$ reads

$$i\partial_t \Psi(\mathbf{r}, t) = \{(-i\partial_{\mathbf{r}} - e\mathbf{A}(\mathbf{r}))^2 + V(\mathbf{r})\} \Psi(\mathbf{r}, t). \quad (6.1)$$

Any solution Ψ of the above equation can be complex conjugated, and gives a solution of the complex conjugate of the Schrödinger equation,

$$-i\partial_t \Psi(\mathbf{r}, t)^* = \{(-i\partial_{\mathbf{r}} + e\mathbf{A}(\mathbf{r}))^2 + V(\mathbf{r})\} \Psi(\mathbf{r}, t)^*. \quad (6.2)$$

We use K to denote the operator that complex conjugates everything to its right in real space basis. Note that $K^2 = 1$, and therefore, $KAK = A^*$, where A is any operator or vector, and $*$ denotes complex conjugation in real space basis. The Schrödinger equation above can thus be written succinctly as

$$Ki\partial_t \Psi = Ki\partial_t K K \Psi = -i\partial_t \Psi^* = K\hat{H} K K \Psi = \hat{H}^* \Psi^*. \quad (6.3)$$

The above relation shows that for any closed quantum mechanical system, there is a simple way to implement time reversal. This requires to change both the wavefunction Ψ to Ψ^* and the Hamiltonian \hat{H} to \hat{H}^* .

In the special case where the Hamiltonian in real space basis is real, $\hat{H}^* = \hat{H}$, we can implement time reversal by only acting on the wavefunction. In that case, we say that the system has time reversal symmetry. For the scalar Schrödinger equation above, this happens if there is no vector potential, $\mathbf{A} = 0$. To see this more explicitly, consider time

evolution for a time t , then applying the antiunitary operator K , then continuing time evolution for time t , then applying K once more:

$$\hat{U} = K e^{-i\hat{H}t} K e^{-i\hat{H}t} = e^{-K i\hat{H}t K} e^{-i\hat{H}t} = e^{i\hat{H}^* t} e^{-i\hat{H}t} \quad (6.4)$$

If $\hat{H}^* = \hat{H}$, then $\hat{U} = 1$, which means that K acts like time reversal.

Time reversal is an operation that is local in space, that takes $\hat{x} \rightarrow \hat{x}$ and $\hat{p} \rightarrow -\hat{p}$.

6.1.2 Two types of time reversal

For a particle with an internal degree of freedom, time reversal \mathcal{T} can also include a unitary rotation of this internal degree of freedom:

$$\mathcal{T} = \tau K, \quad (6.5)$$

where τ is a unitary operator. For complex conjugation K to be well defined we also have to fix the internal basis on which it acts. For example, for a spin-1/2 particle, time reversal should also flip the spin, which is achieved by $\mathcal{T} = -i\sigma_y K$, if K is defined on the basis of the eigenstates of σ_z . The fact that this works can be checked by $\mathcal{T}\sigma_j\mathcal{T}^{-1} = -\sigma_j$ for $j = x, y, z$.

A simple requirement for a time reversal operator is that if squared, it should give at most a phase, $e^{i\phi}$:

$$\tau K \tau K = \tau \tau^* = e^{i\phi}. \quad (6.6)$$

This phase turns out to have only two possible values: 0 or π . Multiplying Eq. (6.6) from the left by τ^\dagger , we get $\tau^* = e^{i\phi} \tau^\dagger = e^{i\phi} (\tau^*)^T$, where T denotes transposition. Iterating this last relation once more, we obtain $\tau^* = e^{2i\phi} \tau^*$, which means $e^{i\phi} = \pm 1$, wherefore

$$\mathcal{T}^2 = \pm 1. \quad (6.7)$$

6.1.3 $\mathcal{T}^2 = -1$ gives Kramers' degeneracy

Time reversal \mathcal{T} is an antiunitary operator, i.e., the product of a unitary operator τ and complex conjugation operator K . Therefore, for any pair of states $|\Psi\rangle$ and $|\Phi\rangle$, we have

$$\langle \mathcal{T}\Phi | \mathcal{T}\Psi \rangle = (\tau |\Phi^*\rangle)^\dagger \tau |\Psi^*\rangle = |\Phi^*\rangle^\dagger \tau^\dagger \tau |\Psi^*\rangle = \langle \Phi^* | \Psi^* \rangle = \langle \Phi | \Psi \rangle^*. \quad (6.8)$$

Consider now this relation with $\Phi = \mathcal{T}\Psi$:

$$\langle \mathcal{T}\Psi | \Psi \rangle^* = \langle \mathcal{T}^2 \Psi | \mathcal{T}\Psi \rangle = \langle \pm \Psi | \mathcal{T}\Psi \rangle = \pm \langle \mathcal{T}\Psi | \Psi \rangle^*, \quad (6.9)$$

where the \pm stands for the square of the time reversal operator \mathcal{T} , which is ± 1 . If $\mathcal{T}^2 = +1$, the above line gives no information, but if $\mathcal{T}^2 = -1$, it leads immediately to $\langle \mathcal{T}\Psi | \Psi \rangle = 0$, which means that for every energy eigenstate, its time-reversed partner, which is also an energy eigenstate with the same energy, is orthogonal. This is known as Kramers degeneracy.

6.1.4 Time-Reversal Symmetry of a Bulk Hamiltonian

Solid-state systems are represented by lattice Hamiltonians, which have a bulk, translationally invariant part. Translational invariance implies that the total bulk Hamiltonian H is block diagonal in the momentum (wavevector) eigenbasis:

$$H = e^{i\mathbf{k}\mathbf{r}} H(\mathbf{k}) e^{-i\mathbf{k}\mathbf{r}}, \quad (6.10)$$

where \mathbf{k} are the wavevectors.

The time-reversal symmetry operator is antiunitary, and local, and therefore $\mathcal{T} e^{i\mathbf{k}\mathbf{r}} = e^{-i\mathbf{k}\mathbf{r}} \mathcal{T}$. This implies that the requirement for time reversal symmetry, $\mathcal{T} H \mathcal{T}^{-1} = H$, reads for the bulk Hamiltonian,

$$H(\mathbf{k}) = \mathcal{T} H(-\mathbf{k}) \mathcal{T}^{-1} \quad (6.11)$$

for every k .

A direct consequence is that the dispersion relation of a time-reversal symmetric Hamiltonian has to be symmetric with respect to inversion in the Brillouin Zone, $k \rightarrow -k$. Note however, that this is only a one-way implication: symmetry of the dispersion relation can suggest time-reversal symmetry, but by itself is not enough to ensure it.

It is especially interesting to look at points in the Brillouin Zone which map unto themselves under inversion: the Time-reversal invariant momenta (TRIM). In d dimensions there are 2^d such points, one of which is at the center of the Brillouin Zone (so-called Γ point), and others at the edges. In light of Eq. (6.11), the Hamiltonian of a TRS system at a TRIM has

$$\mathcal{T} H(\mathbf{k}_{\text{TRIM}}) \mathcal{T}^{-1} = H(\mathbf{k}_{\text{TRIM}}). \quad (6.12)$$

6.2 Doubling the Hilbert Space for Time-Reversal Symmetry

There is a simple way to construct lattice systems with Time-Reversal Symmetry. Take as a starting point a lattice model of a d dimensional insulator, with a Hamiltonian $H(k)$. We define a time-reversal invariant new system by giving the Hamiltonian,

$$H_2(\mathbf{k}) = \begin{bmatrix} H(\mathbf{k}) & 0 \\ 0 & H^*(-\mathbf{k}) \end{bmatrix} = \frac{1 + \tau_z}{2} H(\mathbf{k}) + \frac{1 - \tau_z}{2} H^*(-\mathbf{k}). \quad (6.13)$$

Here H^* denotes the complex conjugate of the matrix, an operation that is basis dependent (and H^* is equal to H^T , the basis-dependent transpose of H). Furthermore, $K H(\mathbf{k}) K = H^*(-\mathbf{k})$, with the basis-dependent antilinear operator K of complex conjugation in the real space and in the given basis. We also used the Pauli operators τ_j for $j = x, y, z$, which shuffle the submatrices, as above.

The Hamiltonian $H_2(\mathbf{k})$ has time-reversal symmetry (TRS), represented by $\mathcal{T} = i\tau_y K$. The factor of i is included for convenience, so that $i\tau_y$ is real - but now its inverse is $-i\tau_y$. A quick proof of time-reversal symmetry:

$$(i\tau_y K)H_2(\mathbf{k})(i\tau_y K)^{-1} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \cdot \begin{bmatrix} H^*(-\mathbf{k}) & 0 \\ 0 & H(\mathbf{k}) \end{bmatrix} \cdot \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \quad (6.14)$$

$$= \begin{bmatrix} 0 & H(\mathbf{k}) \\ -H^*(-\mathbf{k}) & 0 \end{bmatrix} \cdot \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = H_2(\mathbf{k}) \quad (6.15)$$

The TRS operator \mathcal{T} squares to -1 , and therefore implies Kramers degeneracy.

6.2.1 A concrete example: the BHZ model

To be concrete, we can build a simple model for a time-reversal invariant topological insulator starting from the “half BHZ” model of Eq. (3.30),

$$H_1(\mathbf{k}) = [\Delta + \cos k_x + \cos k_y]\sigma_z + A(\sin k_x \sigma_x + \sin k_y \sigma_y), \quad (6.16)$$

and doubling the Hilbert space as in the recipe (6.13). Following the recipe

$$H_{BHZ}(\mathbf{k}) = [(\Delta + \cos k_x + \cos k_y)\sigma_z + A \sin k_y \sigma_y]\tau_0 + A \sin k_x \sigma_x \tau_z. \quad (6.17)$$

which is a simple 4-band model for HgTe, introduced by Bernevig, Hughes and Zhang [3], known as “BHZ model”. We introduced the name “half BHZ” for the original Chern insulator $H(k)$ to indicate that it forms the basis of the full BHZ model.

6.3 Edge States in 2-dimensional $\mathcal{T}^2 = -1$ insulators

After the general considerations of the previous sections, we now focus on 2D time-reversal invariant (TRI) lattice models with a time-reversal symmetry \mathcal{T} which squares to $\mathcal{T}^2 = -1$. We explore edge states of these TRI topological insulators, much in the same way as we did for the Chern insulators of Chapter 4. We separate a 2D sample into a translational invariant bulk, with a finite energy gap around $E = 0$, and an edge. Because the bulk is insulating, when we consider the low energy physics, we can restrict our attention to the vicinity of an edge. Edge states are eigenstates with energies that lie in the gap of the bulk of the sample, and whose wavefunction therefore has most of its weight at the edge.

As with Chern insulators, we first consider clean samples, i.e., translational invariant along the edge direction x . Then, the wavenumber k_x is a good quantum number. The states form 1-dimensional edge state bands in the 1D Brillouin Zone $k_x = -\pi, \dots, \pi$, shown schematically in Fig. 6.1. In general, an edge will host edge states propagating

in both directions. However, due to time-reversal symmetry, the dispersion relations must be left-right symmetric when plotted against the wavenumber k_x along the edge direction. This means that the number N_+ of right-moving edge states (these are plotted with solid lines in Fig. 6.1), and N_- , the number of left-moving edge states (dashed lines) have to be equal at any energy,

$$N_+(E) = N_-(E). \quad (6.18)$$

As with Chern insulators, we next consider the effect of adiabatic deformations of the clean Hamiltonian on edge states. We consider terms in the Hamiltonian that conserve translational invariance along the edge, and respect Time Reversal Symmetry. The whole discussion of section 4.5 applies, and therefore adiabatic deformations cannot change the signed sum of the left- and right-propagating edge states in the gap. However, time-reversal symmetry restricts this sum to zero anyway.

Time reversal symmetry that squares to $\mathcal{T}^2 = -1$, however, provides a further restriction: adiabatic deformations can only change the number of edge states by integer multiples of four (pairs of pairs). To understand why, consider the adiabatic deformation corresponding to Fig. 6.1 (a)-(d). Degeneracies in the dispersion relation can be lifted by coupling the edge states, as it happens in (b), and this can lead to certain edge states disappearing at certain energies, as in (c). This can be visualized by plotting the k_x values at $E = 0$ of the branches of the edge state dispersion as functions of the deformation parameter (which is some combination of the parameters of the Hamiltonian) a , as in Fig. 6.1 (e). Due to the deformation, two counterpropagating edge states can “annihilate”, when the corresponding modes form an avoided crossing. If this happens at a generic momentum value k , as in (c), then, due to the time reversal invariance, it also has to happen at $-k$, and so the number of edge states decreases by 4, not by 2. The special momentum values of k_x are the TRIM, which in this case are $k_x = 0, \pm\pi$. If the edge state momenta meet at a TRIM, as in (b) at $k_x = 0$, their “annihilation” would change the number of edge states by 2 and not by 4. However, this cannot happen, as it would create a situation that violates the Kramers degeneracy: at the TRIM, energy eigenstates have to be doubly degenerate. The deformations in Fig. 6.1 can be also read from (d) to (a), and therefore apply to the introduction of new edge states as well.

6.3.1 \mathbb{Z}_2 invariant: parity of edge state pairs

At any energy inside the bulk gap, the parity of the number of edge-states Kramers pairs for a given dispersion relation is well defined. In Fig. 6.1(a), there are 3 edge-state Kramers pairs for any energy in the bulk gap, i.e., the parity is odd. In Fig. 6.1(c), there are 3 of them for every energy except for energies in the mini-gap of the bands on the left and right for which the number of edge-state Kramers pairs is 1, and for the upper and lower boundaries of the mini-gap [the former depicted by the horizontal line

in Fig. 6.1(c)], where the number of Kramers pairs is 2. The parity is odd at almost every energy, except the two isolated energy values at the mini-gap boundaries.

The general proposition is that the parity of the number of edge-state Kramers pairs at a given edge for a given Hamiltonian at a given energy is independent of the choice of energy, as long as this energy is inside the bulk gap. Since in a time-reversal invariant system, all edge states have counter-propagating partners, we can express this number as

$$D = \frac{N(E)}{2} \bmod 2 = \frac{N_+(E) + N_-(E)}{2} \bmod 2, \quad (6.19)$$

where $N(E) = N_+(E) + N_-(E)$ is the total number of edge states at an edge. A caveat is that there are a few isolated energy values where this quantity is not well defined, e.g., the boundaries of mini-gaps in the above example, but these energies form a set of zero measure.

Since D is a topological invariant, we can classify 2D time-reversal invariant lattice models according to it, i.e., the parity of the number of edge-state Kramers pairs supported by a single edge of the terminated lattice. Because it can take on two values, this ‘label’ D is called the \mathbb{Z}_2 invariant, and is represented by a bit taking on the value 1 (0) if the parity is odd (even).

As a final step, we should next consider disorder that breaks translational invariance along the edge, in the same way as we did for Chern insulators. Due to the presence of edge states propagating in both directions along the edge, the treatment of disorder is a bit trickier than it was for Chern states, and we therefore relegate it to the next chapter.

6.3.2 Two Time-Reversal Symmetries

A time reversal invariant lattice model constructed by “doubling the Hilbert space”, as in Eq. (6.13), has not one, but two different time reversal symmetries. Not only $\mathcal{T} = \tau_y K$, but also $\mathcal{T}' = \tau_x K$ fulfils the requirements of being antiunitary and commuting with the Hamiltonian of the model, H_2 . This second time reversal symmetry, \mathcal{T}' , squares to $\mathcal{T}'^2 = +1$, and so it belongs to the class of time reversal symmetries that does not imply Kramers degeneracy, and so provides no protection for edge states. Which of these time reversal symmetries is really present depends on which symmetry is respected by extra terms in our Hamiltonian or by the disorder in our system: $\tau_y K$, $\tau_x K$, or perhaps both.

On the one hand, the presence of the extra symmetry should not worry us: we already have a TRS which squares to -1 , and so we already have topological protection for our edge state pairs.

On the other hand, the fact that our model has two different antiunitary time reversal symmetry operations means it must have a conventional unitary symmetry: the

composition of these two. Consider

$$\mathcal{T}_1 \hat{H} \mathcal{T}_1 = \mathcal{T}_2 \hat{H} \mathcal{T}_2 = H; \quad (6.20)$$

$$\mathcal{T}_1 \mathcal{T}_2 \hat{H} \mathcal{T}_2^{-1} \mathcal{T}_1^{-1} = \mathcal{T}_1 \hat{H} \mathcal{T}_1^{-1} = \hat{H}; \quad (6.21)$$

$$A \equiv \mathcal{T}_1 \mathcal{T}_2; \implies A \hat{H} A^\dagger = \hat{H}. \quad (6.22)$$

The extra unitary symmetry of our time-reversal symmetric lattice model H_2 is $i\tau_y K \tau_x K = \tau_z$. This should be no surprise: of course τ_z is a symmetry, this follows from the block diagonal structure of the Hamiltonian. The presence of this unitary symmetry implies that we can factor it out: consider each sector of the symmetry separately. In our case, these sectors correspond to the various blocks, which, on their own, do not have time-reversal symmetry.

6.4 The bulk–boundary correspondence: \mathbb{Z}_2 invariant from the bulk

We defined the \mathbb{Z}_2 invariant D as the parity of the number of edge state pairs at an edge. However, this number does not depend on the type of edge: it is a topological invariant that is set by the bulk Hamiltonian. Suppose we are given a two-dimensional time-reversal invariant lattice model with periodic boundary conditions, so there are no edges. To read off the topological invariant D , there is a surefire way: we have to create an edge by selecting a closed loop \mathcal{C} on the lattice, and setting all hopping amplitudes that hop across this loop to 0. The parity of the number of edge states that propagate along the loop is independent not only of the position along the closed loop \mathcal{C} , but also on the shape and position of the loop itself (as long as the loop is big enough).

Since the \mathbb{Z}_2 invariant is the property of the Hamiltonian independent of the edges, there should be a topological invariant of the bulk Hamiltonian $H(k)$ that corresponds to it. For 2D insulators we already have such a bulk invariant: the Chern number Q , which also gives the net number of edge states at an edge, $N_+(E) - N_-(E)$. This Chern number is 0 for all time-reversal invariant 2-dimensional insulators. For 2-dimensional lattice systems with time reversal that squares to $\mathcal{T}^2 = -1$, there must be another bulk topological invariant equal to D . Finding this other invariant would amount to completing the bulk–boundary correspondence for time-reversal invariant 2-dimensional insulators.

If the time-reversal invariant Hamiltonian was constructed by “doubling the Hilbert space” of an insulator with Chern number Q , via the recipe (6.13), the topological invariant D can easily be calculated as

$$D = Q \bmod 2. \quad (6.23)$$

This is straightforward to show. The “doubling of the Hilbert space” can be understood as taking two layers with Hamiltonians H and H^* . As we saw in chapter 4, the number of counterclockwise (clockwise) propagating edge states in the layer with Hamiltonian H is N_+ (N_-), with $N_+ - N_- = Q$. The total number of edge states in the layer is $|Q| + 2n$, with $|Q|$ of these topologically protected. Each edge state has a time-reversed partner on the other layer which propagates in the opposite direction. Therefore, the total number of edge states in both layers is $N = |2Q| + 4n$. If we substitute this into Eq. (6.19), we obtain Eq. (6.23).

For the BHZ model, Eq. (6.17), this shows that the \mathbb{Z}_2 topological invariant D is:

$$D = 0 \text{ if } |\Delta| > 2; \quad (6.24)$$

$$D = 1 \text{ if } |\Delta| < 2; \quad (6.25)$$

$$D \text{ undefined if } \Delta = 0 \text{ (not an insulator)}. \quad (6.26)$$

If the time-reversal invariant Hamiltonian can be brought to a block diagonal form as in Eq. (6.13) adiabatically, the topological invariant D is again easy to calculate. Since D is a topological invariant, its value is not affected by the adiabatic deformation, i.e., by the switching off of the couplings between the blocks. However, with the couplings between the layer and its time-reversed partner set to 0, we can plug in Eq. (6.23).

In the general case, it can happen that it is not possible to find a way to adiabatically deform the Hamiltonian to the block diagonal form of Eq. (6.13). Although there are mathematical constructions of the \mathbb{Z}_2 invariant in this most general case as well, these are much more difficult to calculate than the discretized Chern number of Section 3.4.2. Therefore we do not detail these constructions in these notes. However, there is an important special case where a simple numerical algorithm exists, which we discuss in the next Section.

6.4.1 The \mathbb{Z}_2 invariant for systems with inversion symmetry

By its standard definition, inversion around the origin is $r \leftrightarrow -r$. When we apply inversion to the wavefunction of a particle with spin, it should not change the spin, but should flip the momentum. If the particle has some other “pseudospin” degrees of freedom, the action of inversion on these is represented by a unitary matrix P . Inversion should commute with time reversal.

Applying the concept of inversion to a lattice system, we say that it has inversion symmetry, if there exists a unitary P independent of k such that

$$P^\dagger P = 1; \quad (6.27)$$

$$P^2 = 1; \quad (6.28)$$

$$PH(\mathbf{k})P^{-1} = H(-\mathbf{k}); \quad (6.29)$$

$$PT = TP. \quad (6.30)$$

A concrete example for inversion symmetry is given by the BHZ model, Eq. (6.17). It can be checked directly that this has inversion symmetry represented by $P = \sigma_z \tau_0$.

Consider the Time-Reversal Invariant Momenta (TRIM), Γ_j . There are 2^d such momenta in a d -dimensional lattice model. Each eigenstate $|\Psi\rangle$ at these momenta has an orthogonal Kramers pair $\mathcal{T}|\Psi\rangle$,

$$H(\Gamma_j)|\Psi\rangle = E|\Psi\rangle; \quad (6.31)$$

$$H(\Gamma_j)\mathcal{T}|\Psi\rangle = E\mathcal{T}|\Psi\rangle. \quad (6.32)$$

If H is inversion symmetric, $|\Psi\rangle$ can be chosen to be an eigenstate of P as well, since

$$PH(\Gamma_j)P = H(-\Gamma_j) = H(\Gamma_j). \quad (6.33)$$

Therefore,

$$P|\Psi\rangle = \pm|\Psi\rangle. \quad (6.34)$$

The Kramers pair of Ψ has to have the same parity eigenvalue:

$$P\mathcal{T}|\Psi\rangle = \mathcal{T}P|\Psi\rangle = \mathcal{T}(\pm)|\Psi\rangle = \pm\mathcal{T}|\Psi\rangle. \quad (6.35)$$

Therefore, in a system with both time-reversal and inversion symmetry, we get 2^d topological invariants. These are the products of the parity eigenvalues $\xi_m(\Gamma_j)$ of the occupied Kramers pairs at Γ_j , for $j = 1, \dots, 2^d$.

Parity breaking disorder can mix the Kramers pairs at the edges, and so these invariants not robust. However, their product is. Without proof, we quote the statement, that this product turns out to be the same as the \mathbb{Z}_2 invariant.

$$(-1)^D = \prod_j \prod_m \xi_m(\Gamma_j). \quad (6.36)$$

We can check the above construction for the BHZ model. It has a simple square lattice, and the four TRIM $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4$, are the combinations of k_x, k_y with $k_x = 0, \pi$ and $k_y = 0, \pi$. The Hamiltonian $H_{BHZ}(k_x, k_y)$ at these momenta reads:

$$H_{BHZ}(\mathbf{k}_1 = 0, 0) = (\Delta + 2) \sigma_z \tau_0; \quad (6.37)$$

$$H_{BHZ}(\mathbf{k}_2 = 0, \pi) = \Delta \sigma_z \tau_0; \quad (6.38)$$

$$H_{BHZ}(\mathbf{k}_4 = \pi, \pi) = (\Delta - 2) \sigma_z \tau_0; \quad (6.39)$$

$$H_{BHZ}(\mathbf{k}_4 = \pi, 0) = \Delta \sigma_z \tau_0. \quad (6.40)$$

At each TRIM, the Hamiltonian is proportional to the parity operator $P = \sigma_z \tau_0$, so they obviously have the same eigenstates. At each TRIM, two of these states form one occupied Kramers pair and the two others one empty Kramers pair. If $\Delta > 2$, at all

four TRIM, the occupied Kramers pair is the one with $\sigma_z\tau_0$ eigenvalue of -1 , and so Eq. (6.36) gives $D = 0$. Likewise, if $\Delta < -2$, the eigenvalues are all $+1$, and we again obtain $D = 0$. For $0 < \Delta < 2$, we have P eigenvalues $-1, -1, +1, -1$ at the four TRIM $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4$, respectively, whereas if $-2 < \Delta < 0$, we have $-1, +1, +1, +1$. In both cases, Eq. (6.36) gives $D = 1$. This indeed is the correct result, Eqs. (6.24), (6.25), (6.26), that we obtained via the Chern numbers earlier.

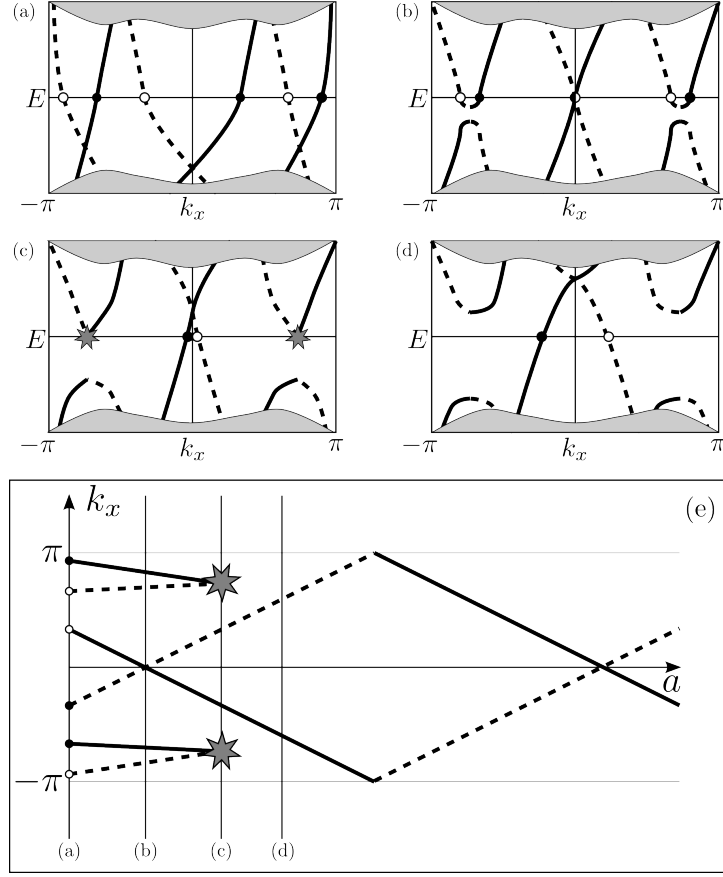


Figure 6.1: Edge states on a single edge of a 2-dimensional time-reversal invariant topological insulator with $\mathcal{T}^2 = -1$. From (a) to (d), the edge region of the sample undergoes a continuous deformation, summarized by an arbitrary parameter a , respecting the symmetry and the translational invariance along the edge. In (a)–(d), the edge state dispersion relations are shown, in the full edge Brillouin zone $k_x = -\pi, \dots, \pi$, and in the energy window corresponding to the bulk gap. For clarity, right- (left-) propagating edge states are denoted by continuous (dashed) lines. Due to the deformation of the Hamiltonian, the edge state dispersion relations can move in the Brillouin zone, bend, and couple, while the bulk energies remain unchanged. From (a) to (b), the crossing points between counterpropagating edge states become anticrossings, i.e., gaps open in these pairs of dispersion relation branches as a usual consequence of any parameter coupling them. Notice that the crossings at $k_x = 0$ and $k_x = \pi$ cannot become avoided crossings, as these degeneracies are protected by the Kramers theorem. From (b) to (d), as a result of the deformation, these gaps become so large that at energy $E = 0$, the number of edge states drops from 6 (3 Kramers pairs) to 2 (1 Kramers pair). The k_x values of the edge states at 0 energy are plotted in (e), where this change in the number of edge states shows up as an “annihilation” of right-propagating and left-propagating edge states.

Chapter 7

Absence of backscattering

A remarkable property of Chern insulators is that they support chiral edge states, i.e., edge states that have no counter-propagating counterparts. A simple fact implied by the chiral nature of these edge states is that impurities are unable to backscatter a particle that occupies them. As we argue below, absence of backscattering is also characteristic of disordered $D = 1$ insulators (that is, 2D TRI topological insulators with $\mathcal{T}^2 = -1$), although the robustness is guaranteed only against time-reversal symmetric scatterers.

In this Chapter we introduce the scattering matrix, a simple concept that allows for a formal analysis of scattering at impurities, and discuss the characteristic properties of edge state scattering in 2D TRI topological insulators. The scattering matrix will also serve as a basic tool in the subsequent Chapter, where we give a simple theoretical description of electronic transport of phase-coherent electrons, and discuss observable consequences of the existence and robustness of edge states.

7.1 The scattering matrix

Consider a phase-coherent 2D conductor with a finite width in the y direction, and perfect translational symmetry along the x axis. The electronic energy eigenstates propagating along the x axis at energy E have a product structure:

$$\psi_{n,\pm}(x, y) = \Phi_{n,\pm}(y)e^{\pm ik_{n,\pm}x} \quad (7.1)$$

The integer $n = 1, 2, \dots, N$ labels the propagating modes, also referred to as scattering channels. The $+$ and $-$ signs correspond to right-moving and left-moving states, respectively. The transverse wave function of mode n, \pm is $\Phi_{n,\pm}(y)$, and its wave number is $k_{n,\pm}$.

Now consider the situation when the electrons are obstructed by a disordered region in the conductor, as shown in Fig. 7.1. A monoenergetic wave incident on the scattering

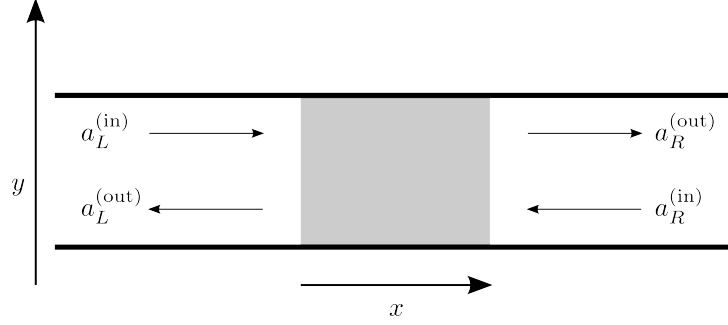


Figure 7.1: Disordered region (gray) obstructing electrons in a 2D phase-coherent conductor. The scattering matrix S relates the amplitudes $a_L^{(\text{in})}$ and $a_R^{(\text{in})}$ of incoming waves to the amplitudes $a_L^{(\text{out})}$ and $a_R^{(\text{out})}$ of outgoing waves.

region is characterized by a vector of coefficients

$$a^{\text{in}} = \left(a_{L,1}^{(\text{in})}, a_{L,2}^{(\text{in})}, \dots, a_{L,N}^{(\text{in})}, a_{R,1}^{(\text{in})}, a_{R,2}^{(\text{in})}, \dots, a_{R,N}^{(\text{in})} \right). \quad (7.2)$$

The first (second) set of N coefficients correspond to propagating waves (7.1) of the clean region on the left (right) side of the disordered part. The reflected and transmitted parts of the wave are described by the vector

$$a^{\text{out}} = \left(a_{L,1}^{(\text{out})}, a_{L,2}^{(\text{out})}, \dots, a_{L,N}^{(\text{out})}, a_{R,1}^{(\text{out})}, a_{R,2}^{(\text{out})}, \dots, a_{R,N}^{(\text{out})} \right). \quad (7.3)$$

The scattering matrix S relates these two vectors,

$$a^{\text{out}} = S a^{\text{in}}. \quad (7.4)$$

The size of the scattering matrix is $2N \times 2N$, and it has the following block structure:

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \quad (7.5)$$

where r and r' are $N \times N$ reflection matrices describing reflection from left to left and from right to right, and t and t' are transmission matrices describing transmission from left to right and right to left.

Particle conservation implies the unitarity of the scattering matrix S . In turn, its unitary character implies that the Hermitian matrices tt^\dagger , $t't'^\dagger$, $1 - rr^\dagger$, and $1 - r'r'^\dagger$ all have the same set of real eigenvalues T_1, T_2, \dots, T_N , called transmission eigenvalues.

7.2 A single Kramers pair of edge states

Now we use the scattering matrix S to characterize defect-induced scattering of an electron occupying an edge state of a 2D TRI topological insulator with $\mathcal{T} = -1$. Consider a half-plane of a homogeneous lattice that is in the $D = 1$ class, and supports exactly one Kramers pair of edge states at a given energy E in the bulk gap, as shown in Fig. 7.2. Consider the scattering of the electron incident on the defect from the left side in Fig. 7.2. The scatterer is characterized by the Hamiltonian V . We show that the impurity cannot backscatter the electron as long as V is time-reversal symmetric.

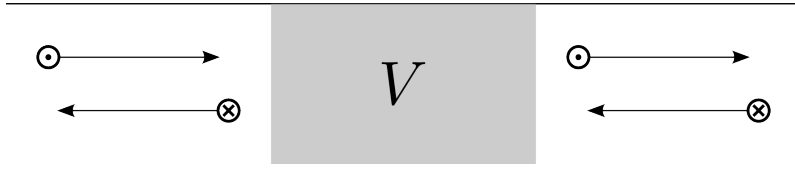


Figure 7.2: Scattering of an edge state on a time-reversal symmetric defect V . In a 2D TRI topological insulator with a single Kramers pair of edge states, the incoming electron is transmitted through such a defect region with unit probability.

We choose our propagating modes such that the incoming and outgoing states are related by time-reversal symmetry, i.e., $\psi_L^{(out)} = T\psi_L^{(in)}$ and $\psi_R^{(out)} = T\psi_R^{(in)}$. In the presence of the perturbation V , the edge states of the disorder-free system are no longer energy eigenstates of the system. A general scattering state ψ at energy E is characterized by the vector $a^{(in)}$ of incoming amplitudes. According to the above definition of the scattering matrix S , the energy eigenstates outside the scattering region can be expressed as:

$$\psi = \sum_{s \in (L,R)} a_s^{(in)} \psi_s^{(in)} + \sum_{s \in (L,R)} (S a^{(in)})_s \psi_s^{(out)}. \quad (7.6)$$

Due to time reversal symmetry,

$$\begin{aligned} -T\psi &= - \sum_{s \in (L,R)} a_s^{(in)*} \psi_s^{(out)} + \sum_{s \in (L,R)} (S^* a^{(in)*})_s \psi_s^{(in)} \\ &= \sum_{s \in (L,R)} (S^* a^{(in)*})_s \psi_s^{(in)} + \sum_{s \in (L,R)} (-S^T S^* a^{(in)*})_s \psi_s^{(out)}, \end{aligned} \quad (7.7)$$

where S^T denotes the transpose of S , is also an energy eigenstate having the same energy as ψ . A direct consequence of Eqs. (7.6) and (7.7) is that $S = -S^T$, that is

$$\begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = S = -S^T = \begin{pmatrix} -r & -t \\ -t' & -r' \end{pmatrix} \quad (7.8)$$

implying

$$r = r' = 0, \quad (7.9)$$

and hence perfect transmission of each of the two incoming waves.

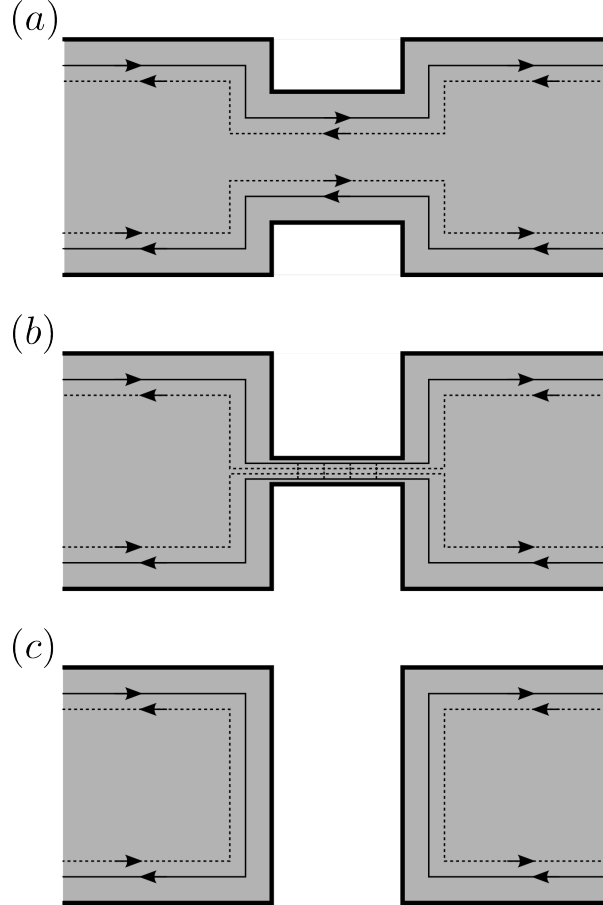


Figure 7.3: Backscattering of edge states at a constriction. The states forming the edge-state Kramers pairs are depicted as solid and dashed lines. (a) A time-reversal symmetric defect localized to the edges, such as a small constriction shown here, is unable to backscatter the incoming electron. (b) Backscattering is possible between different edges, if the width of the constriction is of the order of the decay length of the edge states. (c) A finite spatial gap between the left and right part of the wire implies zero transmission.

If the $D = 1$ lattice has the geometry of a ribbon, and the TRS scatterer extends to both edges, then the absence of backscattering is not guaranteed. This is illustrated in Fig. 7.3, where we compare three examples. In (a), the defect is formed as a wide

constriction on both edges, with a width much larger than the characteristic length of the penetration of the edge states to the bulk region of the ribbon. Backscattering between states at the same edge is forbidden due to TRS, and backscattering between states at different edges is forbidden due to a large spatial separation of their corresponding wave functions. In (b), a similar but narrower constriction with a width comparable to the penetration length of the edge states does allow for scattering between states on the lower and upper edges. In this case, backscattering from a right-moving state on one edge to a left-moving state at the other edge is not forbidden. In (c), the constriction divides the ribbon to two unconnected parts, resulting in zero transmission through the constriction.

Naturally, backscattering is also allowed if the scatterer is not time-reversal symmetric, or if the scattering process is inelastic. Backscattering is not forbidden for the ‘unprotected’ edge states of topologically trivial ($D = 0$) 2D TRI insulators.

7.3 An odd number of Kramers pairs of edge states

The above statement (7.9) implying unit transmission, albeit in a somewhat weakened form, can be generalized for arbitrary $D = 1$ lattice models, including those where the number of edge-state Kramers pairs N is odd but not necessarily one. The proposition is that in such a system, given a time-reversal symmetric scatterer V and an arbitrary energy E in the bulk gap, there exists at least one linear combination of the incoming states of energy E from each side of the defect that is perfectly transmitted through the defect.

The proof follows that in the preceding Section, with the difference that the quantities r and t describing reflection and transmission are $N \times N$ matrices, and that the anti-symmetric nature of the S -matrix $S = -S^T$ implies the antisymmetry of the reflection matrices $r = -r^T$. Every antisymmetric matrix has a vanishing determinant, therefore $\det(r) = 0$ and hence $\det(r^\dagger r) = \det(r^\dagger) \det(r) = 0$, therefore at least one eigenvalue of $r^\dagger r$ is zero, which implies that at least one transmission eigenvalue T_n is unity.

7.4 Robustness against disorder

The absence-of-backscattering result (7.9) implies a remarkable statement regarding the existence of (at least) one perfectly transmitting ‘edge state’ in a finite-size disordered sample of a 2D TRI topological ($D = 1$) insulator. (See also the discussion about Fig. 4.8 in the context of Chern Insulators). Such a sample with an arbitrarily chosen geometry is shown in Fig. 7.4. Assume that the disorder is TRS and localized to the edge of the sample. We claim that any chosen segment of the edge of this disordered sample supports, at any energy that is deep inside the bulk gap, (at least) one counterpropagating Kramers

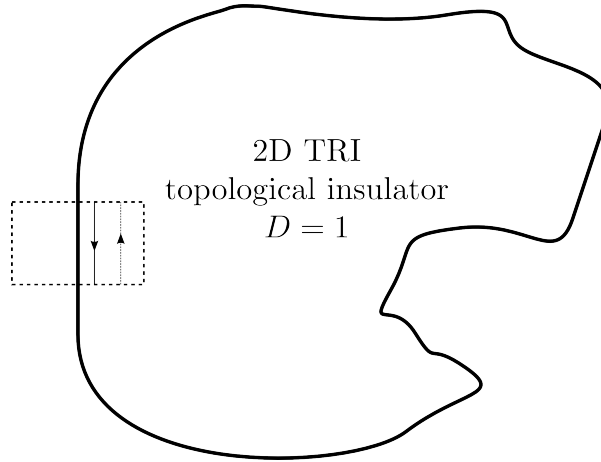


Figure 7.4: A disordered 2D TRI topological insulator contacted with two electrodes. Disorder is ‘switched off’ and the edge is ‘straightened out’ within the dashed box, hence the edge modes there resemble those of the disorder-free lattice.

pair of edge states that are delocalized along the edge and able to transmit electrons with unit probability. This is a rather surprising feature in light of the fact that in truly one-dimensional lattices, a small disorder is enough to induce Anderson localization of the energy eigenstates, and hence render the system an electronic insulator.

To demonstrate the above statement, let us choose an edge segment of the disordered sample for consideration, e.g., the edge segment running outside the dashed box in Fig. 7.4. Now imagine that we ‘switch off’ disorder in the complementer part of the edge of the sample, and ‘straighten out’ the geometry of that complementer part, the latter being shown within the dashed box of Fig. 7.4. Furthermore, via an appropriate spatial adiabatic deformation of the Hamiltonian of the system in the vicinity of the complementer part of the edge (i.e., within the dashed box in Fig. 7.4), we make sure that only a single edge-state Kramers pair is present within this complementer part. The existence of such an adiabatic deformation is guaranteed by the $D = 1$ property of the sample, see the discussion of Fig. 6.1. The disordered edge segment, outside the dashed box in Fig. 7.4, now functions as a scattering region for the electrons in the straightened part of the edge. From the result (7.9) we know that such a TRS scatterer is unable to induce backscattering between the edge modes of the straightened part of the edge, hence we must conclude that the disordered segment must indeed support a perfectly transmitting edge state in each of the two propagation directions.

In the next Chapter, we show that the electrical conductance of such a disordered sample is finite and ‘quantized’, if it is measured through a source and a drain contact that couple effectively to the edge states.

Chapter 8

Electrical conduction of edge states

8.1 Electrical conduction in a clean quantum wire

It is well known that the electrical conduction of ordinary metallic samples at room temperature shows the following two characteristics. First, there is a linear relation between the electric current I that flows through the sample and the voltage V that drops between the two ends of the sample: $I/V = G \equiv R^{-1}$, where G (R) is the conductance (resistance) of the sample. Second, the conductances G_i of different samples made of the same metal but with different geometries show the regularity $G_i L_i / A_i = \sigma$ for $\forall i$, where L_i is the length of the sample and A_i is the area of its cross section. The material-specific quantity σ is called the conductivity. Conductors obeying both of these relations are referred to as Ohmic.

Microscopic theories describing the above behavior (e.g., Drude model, Boltzmann equation) rely on models involving impurities, lattice vibrations, and electron scattering within the material. Electrical conduction in clean (impurity-free) nanostructures at low-temperature might therefore qualitatively deviate from the ordinary case. We demonstrate such deviations on a simple zero-temperature model of a two-dimensional, perfectly clean, constant-cross-section metallic wire, depicted in Fig. 8.1a. In the subsequent Section 8.2, we describe how scattering at static impurities affects the conduction in general, and in Section 8.3 we discuss the influence of edge modes of 2D topological insulators on their phase-coherent electrical conduction.

Assume that the wire lies along the x axis and has a finite width in the y direction, which might be defined by an electric confinement potential or the termination of the crystal lattice. Each electronic energy eigenfunction ψ_{nk} in such a wire is a product of a standing wave along y , labeled by a positive integer n , and a plane wave propagating along x , labeled by a real wave number k (see Eq. (7.1)). A typical set of dispersion relations E_{nk} ('subbands') for different n indices is shown in Fig. 8.1b.

We also make assumptions on the two metallic contacts that serve as source and drain

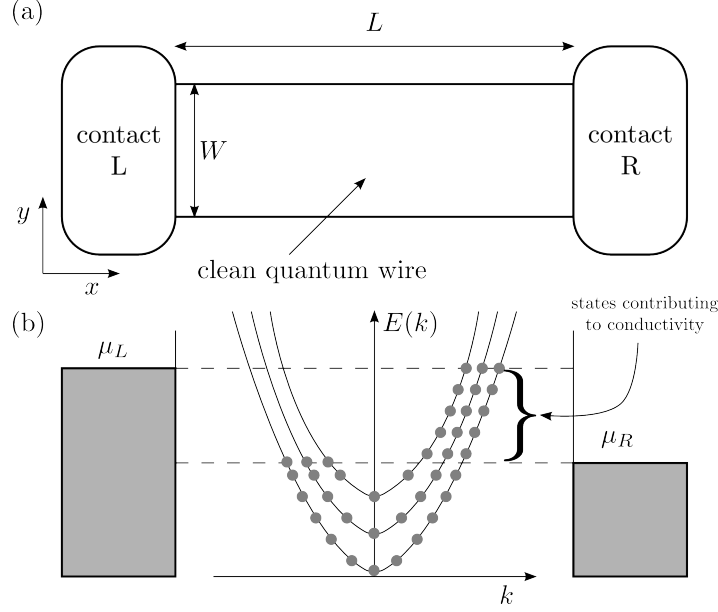


Figure 8.1: (a) Schematic representation of a clean quantum wire contacted to two electron reservoirs (contacts). (b) Occupations of electronic states in the contacts and the quantum wire in the nonequilibrium situation when a finite voltage V is applied between the left and right reservoirs.

of electrons. We assume that the electrons in each contact are in thermal equilibrium, but the Fermi energies in the contacts differ by $\mu_L - \mu_R = |e|V > 0$. We consider the *linear conductance*, that is, the case of an infinitesimal voltage $|e|V \rightarrow 0$. We further assume that both contacts absorb every incident electron with unit probability, and that the energy distribution of the electrons they emit is the thermal distribution with the respective Fermi energy.

These assumptions guarantee that the right-moving (left-moving) electronic states in the wire are occupied according to the thermal distribution of the left (right) contact, as illustrated in Fig. 8.1b. We work with electron states normalized to the area of the channel. It is a simple fact that with this normalization convention, a single occupied state in the n th channel, with wave number k carries an electric current of $\frac{-|e|v_{nk}}{L}$, where L is the length of the wire, and $v_{nk} = \frac{1}{\hbar} \frac{dE_{nk}}{dk}$ is the group velocity of the considered state. Therefore, the current flowing through the wire is

$$I = -|e| \frac{1}{L} \sum_{nk} v_{nk} [f(E_{nk} - \mu_L) - f(E_{nk} - \mu_R)], \quad (8.1)$$

where $f(\epsilon) = \left(\exp \frac{\epsilon}{k_B T} + 1 \right)^{-1}$ is the Fermi-Dirac distribution. Converting the k sum to

an integral via $\frac{1}{L} \sum_k \dots \mapsto \int \frac{dk}{2\pi} \dots$ yields

$$I = -|e| \sum_n \int \frac{dk}{2\pi} \frac{1}{\hbar} \frac{dE_{nk}}{dk} [f(E_{nk} - \mu_L) - f(E_{nk} - \mu_R)]. \quad (8.2)$$

The Fermi-Dirac distribution has a sharp edge at zero temperature, implying

$$I = -\frac{|e|}{h} M \int_{\mu_R}^{\mu_L} dE = -\frac{|e|}{h} (\mu_L - \mu_R) M = M \frac{e^2}{h} V \quad (8.3)$$

Note that the first equality in (8.3) holds only if the number of subbands intersected by μ_L and μ_R are the same, which is indeed the case if the voltage V is small enough. The number of these subbands, also called ‘open channels’, is denoted by the integer M . From (8.3) it follows that the conductance of the wire is an integer multiple of e^2/h (commonly referred to as ‘quantized conductance’):

$$G = \frac{e^2}{h} M. \quad (8.4)$$

The numerical value of e^2/h is approximately $40 \mu\text{S}$ (microsiemens), which corresponds to a resistance of approximately $26 \text{ k}\Omega$. Note the the conductance quantum is defined as $G_0 = 2e^2/h$, i.e., as the conductance of a single open channel with twofold spin degeneracy.

It is instructive to compare the conduction in our clean quantum wire to the ordinary Ohmic conduction summarized above. According to (8.3), the proportionality between voltage and current holds for a clean quantum wire as well as for an ordinary metal. However, the dependence of the conductance on the length of the sample differs qualitatively in the two cases: in an ordinary metal, a twofold increase in the length of the wire halves the conductance, whereas the conductance of a clean quantum wire is insensitive to length variations.

Whether the conductance of the clean quantum wire is sensitive to variations of the wire width depends on the nature of the transversal modes. Conventional quantum wires that are created by a transverse confinement potential have a subband dispersion similar to that in Fig. 8.1b. There, the energy separation between the subbands decreases as the width of the wire is increased, therefore the number of subbands available for conduction increases. This leads to an increased conductance for an increased width, similarly to the case of ordinary metals. If, however, we consider a topological insulator, where the current is carried by states localized to the edges of the wire, the conductance of the wire will be insensitive to the width of the wire.

8.2 Phase-coherent electrical conduction in the presence of scatterers

Having calculated the conductance (8.4) of a clean quantum wire, we now describe how this conductance is changed by the presence of impurities. We analyze the model shown in Fig. 8.2, where the disordered region, described by a scattering matrix S , is connected to the two contacts by two identical clean quantum wires, also called ‘leads’ in this context.

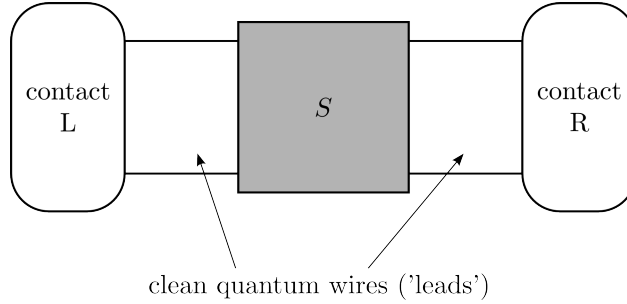


Figure 8.2: Simple model of a phase-coherent conductor in the presence of scatterers. The ideal contacts L and R are connected via ideal leads to the disordered region represented by the scattering matrix S .

First, we consider the case when each lead supports a single open channel. The current in the lead connecting contact L and the scattering region consists of a contribution from right-moving states arriving from contact L and partially backscattered with probability $R = |r|^2$, and from left-moving states arriving from contact R and partially transmitted with probability $T' = |t'|^2$:

$$I = -|e| \frac{1}{L} \sum_k v_k [(1 - R(E_k)) f_L(E_k) - T'(E_k) f_R(E_k)] \quad (8.5)$$

Converting the k sum to an integral, assuming that the transmission and reflection probabilities are independent of energy in the small energy window between μ_R and μ_L , and using $1 - R = T = T'$, we arrive at

$$I = -\frac{|e|}{h} T \int_{\mu_R}^{\mu_L} dE [f_L(E) - f_R(E)] = \frac{e^2}{h} TV, \quad (8.6)$$

which implies that the conductance can be expressed through the transmission coefficient T :

$$G = \frac{e^2}{h} T. \quad (8.7)$$

The result (8.7) can be straightforwardly generalized to the case when the leads support more than one open channel. The generalized result for the conductance, also known as the Landauer formula, reads:

$$G = \frac{e^2}{h} \sum_{n=1}^M T_n, \quad (8.8)$$

where T_n are the transmission eigenvalues of the scattering matrix i.e., the real eigenvalues of the Hermitian matrix tt^\dagger , as defined in the preceding Chapter.

8.3 Electrical conduction in 2D topological insulators

8.3.1 Chern Insulators

In Section 4.4, we have seen that an impurity-free straight strip of a topologically nontrivial Chern Insulator supports edge states. The relation between the Chern number Q of the Chern Insulator and the numbers of edge states at a single edge at a given energy E , propagating ‘clockwise’ ($N_+(E)$) and ‘anticlockwise’ ($N_-(E)$), is $Q = N_+(E) - N_-(E)$. In addition, in Section 4.5 it was shown that any segment of the edge of a disordered Chern Insulator with Chern number Q and an arbitrary geometry supports $|Q|$ chiral edge modes. Here we show that existence of these edge modes leads to experimentally detectable effects in the electrical transport through Chern Insulator samples.

We consider a transport setup where the Chern Insulator is contacted with two metallic electrodes, as shown in Fig. 8.3. In this discussion, we rely on the usual assumptions behind the Landauer formula: phase-coherence of the electrons, good contact between contacts and sample, and large spatial separation of the two electrodes ensuring the absence of tunneling contributions to the conductance.

In the following list, we summarize how the phase-coherent electrical conductance of a Chern Insulator varies with the sample geometry, absence or presence of disorder, and the value of the electronic Fermi energy.

1. Disorder-free sample with a strip geometry (see Fig. 8.1a)
 - (a) *Fermi energy lies in a band.* In this case, the sample is a clean quantum wire (see Section 8.1) with an integer number of open channels. The corresponding transversal wave functions might or might not be localized to the sample edges, and therefore the number of channels might be different from any combination of Q , N_+ or N_- . According to Eq. 8.4, the conductance of such a clean quantum wire is quantized and insensitive to the length of the sample. Furthermore, the conductance grows in a step-like fashion if the width of the sample is increased.

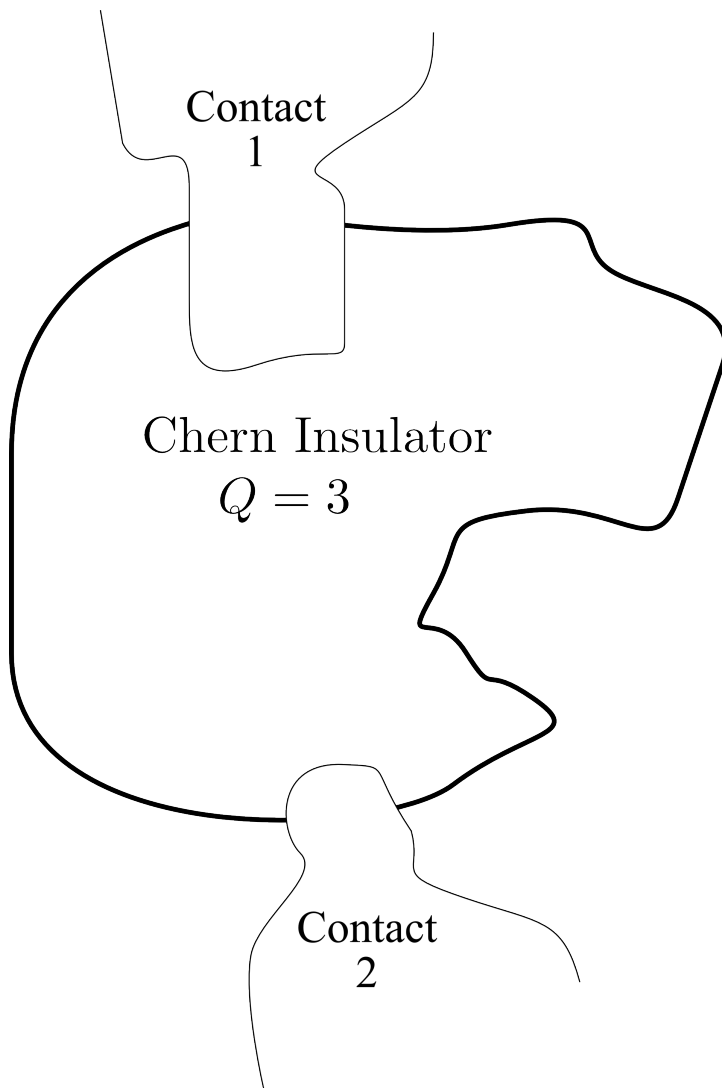


Figure 8.3: A disordered sample of Chern insulator, with contacts 1 and 2, that can be used to pass current through the sample in order to detect edge states.

- (b) *Fermi energy lies in the gap.* The sample is a clean quantum wire with open channels that are all localized to the sample edges. The number of those channels is $N_+(E) + N_-(E)$, where E is the Fermi energy: in each of the two possible direction of current flow, there are N_+ channels on one edge and N_- on the other edge that contribute to conduction. Conductance is finite and quantized, a behavior rather unexpected from an insulator. The conduction is not Ohmic, as the conductance is insensitive to both the length and the width of the sample.

2. Disordered sample with an irregular shape (see Fig. 8.3):

- (a) *Fermi energy lies in a band.* Because of the presence of disorder, the electrical conduction of such a sample is typically Ohmic. There are no protected edge states at the Fermi energy.
- (b) *Fermi energy lies well within the gap.* According to Section 4.5, any edge segment of such a sample supports Q reflectionless chiral edge modes at the Fermi energy. Therefore, conductance is typically quantized, $G = |Q|e^2/h$, although, disorder permitting, it might in principle be larger than this value. The quantized conductance is insensitive to changes in the geometry or the disorder configuration. This transport property, unexpected for an insulator, let alone for one with disorder, is a hallmark of Chern Insulators.

In the case of 2D samples there is often an experimental possibility of tuning the electronic Fermi energy *in situ* by controlling the voltage applied between the sample and a nearby metallic plate, as discussed in Section 8.4. This allows, in principle, to observe the changes in the electrical conduction of the sample as the Fermi energy is tuned across the gap.

8.3.2 2D TRI topological insulators with $\mathcal{T}^2 = -1$

In the following list, we summarize the predictions of the Landauer formalism for the conductance of 2D TRI topological insulators with $\mathcal{T}^2 = -1$ ($D = 1$ insulators' for short).

1. Disorder-free sample with a strip geometry:

- (a) *Fermi energy lies in a band.* A simple consequence of the Landauer formula is that phase-coherent conductance of an impurity-free $D = 1$ topological insulator of the strip geometry shown in Fig. 8.1a is quantized. The conductance grows if the width of the strip is increased, but insensitive to change in the length.

- (b) *Fermi energy lies in the gap.* Only edge channels are open in this case. These also provide conductance quantization. As the number of edge-state Kramers pair per edge is odd, the conductance might be $2e^2/h$, $6e^2/h$, $10e^2/h$, etc. Conductance is insensitive to width or length changes of the sample.

2. Disordered sample with an irregular shape and TRS disorder:

- (a) *Fermi energy lies in a band.* The electrical conduction is Ohmic.
- (b) *Fermi energy lies in the gap.* We have shown in Chapter 7 that a $D = 1$ insulator supports one protected edge-state Kramers pair per edge, which allows for reflectionless electronic transmission if only TRS defects are present. The Landauer formula (8.8) implies, for typical cases, $G = 2e^2/h$ for such a sample, as one edge state per edge contributes to conduction. The conductance might also be larger, provided that the number of edge-state Kramers pairs is larger than 1 and disorder is ineffective in reducing the transmission of the topologically unprotected pairs.

We note that in real materials with \mathbb{Z}_2 invariant $D = 1$, various mechanisms might lead to backscattering and, in turn, to $G < 2e^2/h$. Examples include TRS-breaking impurities, TRS impurities that bridge the spatial distance between the edges (see Chapter 7), hybridization of edge states from opposite edges in narrow samples, and inelastic scattering on phonons or spinful impurities.

8.4 An experiment with HgTe quantum wells

Electrical transport measurements [11] on appropriately designed layers of the semiconductor material mercury-telluride (HgTe) show signatures of edge-state conduction in the absence of magnetic field. These measurements are in line with the theoretical prediction that a HgTe layer with a carefully chosen thickness can realize a topologically nontrivial ($D = 1$) 2D TRI insulator with $\mathcal{T}^2_{\text{nov}} = -1$. In this Section, we outline the main findings of this experiment, as well as its relation to the BHZ model introduced and discussed in Chapter 6.

The experiments are performed on sandwich-like structures formed by a few-nanometer thick HgTe layer (*quantum well*) embedded between two similar layers of the alloy $\text{Hg}_x\text{Cd}_{1-x}\text{Te}$, as shown in Fig. 8.4. (In the experiment reported in [11], the alloy composition $x = 0.3$ was used.) In this structure, the electronic states with energies close the Fermi energy are confined to the HgTe layer that is parallel to the x - y plane in Fig. 8.4. The energy corresponding to the confinement direction z is quantized. The carriers are free to move along the HgTe layer, i.e., parallel to the x - y plane, therefore 2D subbands are formed in the HgTe quantum well. Detailed band-structure calculations of Ref. [3] show that as the thickness d of the HgTe layer is decreased, the lowermost conduction

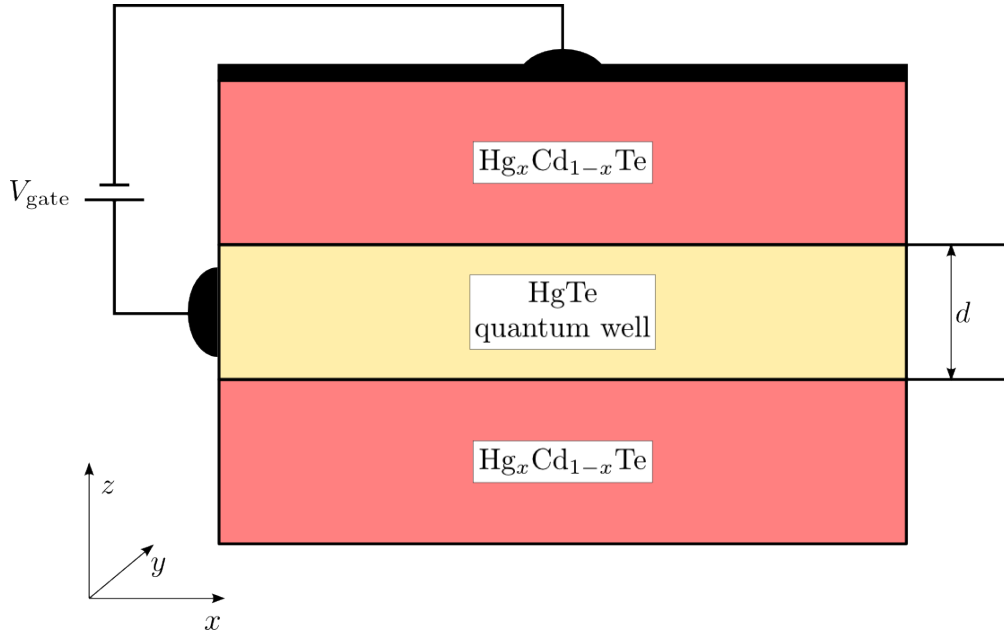


Figure 8.4: Schematic representation of a HgTe quantum well of width d , sandwiched between two $\text{Hg}_x\text{Cd}_{1-x}\text{Te}$ layers. Electrons are confined to the HgTe layer, and their Fermi energy can be tuned *in situ* by adjusting the voltage V_{gate} of the metallic electrode on the top of the sample (black). For a more accurate description of the experimental arrangement, see [10].

subband and the uppermost valence subband touch at a critical thickness $d = d_c$, and the gap is reopened for even thinner HgTe layers. (For the alloy composition $x = 0.3$ used in the experiment, the critical thickness is $d \approx 6.35$ nm.) This behavior is illustrated schematically in Fig. 8.5, where (a) shows, as a function of the quantum well thickness d , the energy of the lowermost conduction subband and the uppermost valence subband at the center of the Brillouin zone (i.e., the energy distance between the two lines at a certain thickness d is the energy gap), whereas (b) illustrates the dispersion relations of these two bands in the vicinity of the Brillouin zone center, for three different quantum well thicknesses.

Band-structure calculations have also revealed a connection between the subbands depicted in Fig. 8.5b and the BHZ model introduced and discussed in Chapter 6. The 4×4 effective Hamiltonian describing the two spinful 2D subbands around their extremum point at the centre of the HgTe Brillouin zone resembles the low-energy continuum Hamiltonian derived from the BHZ lattice model in the vicinity of the $\Delta \approx -2$ value. Changing the thickness d of the HgTe layer corresponds to a change in the parameter Δ of the BHZ model, and the critical thickness $d = d_c$ corresponds to $\Delta = -2$

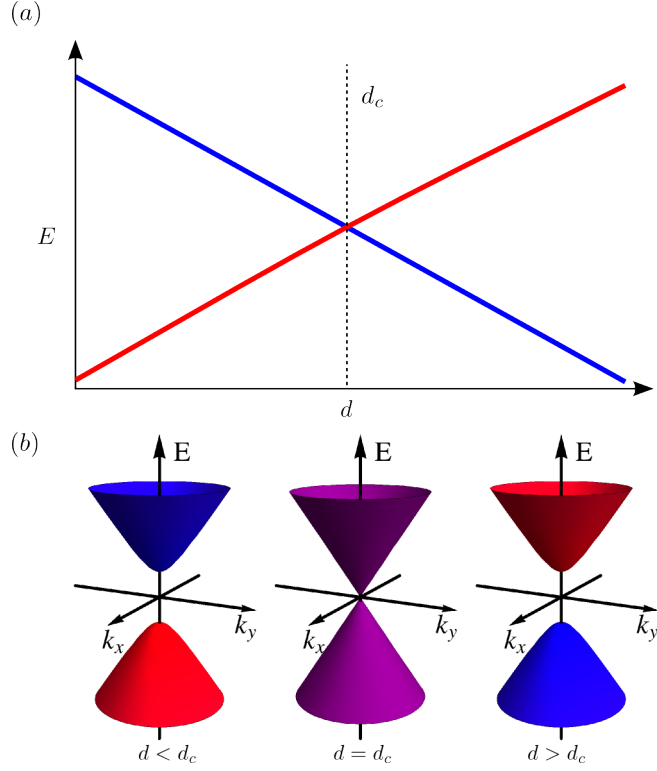


Figure 8.5: Illustration of the evolution of the 2D band structure of a HgTe slab as a function of its thickness d . (a) Energies of the lowermost conduction subband and the uppermost valence subband at the center of the 2D Brillouin zone, as a function of quantum well thickness d . (b) Schematic dispersion relation of the two bands for a HgTe quantum well for three different thicknesses.

and, consequently, a zero mass in the corresponding 2D Dirac equation.

As a consequence of the strong analogy of the band structure of the HgTe quantum well and that of the BHZ model, it is expected that either for $d < d_c$ or for $d > d_c$ the material is a $D = 1$ insulator with a single Kramers pair of edge states. Arguments presented in [3] suggest that the thick quantum wells with $d > d_c$ are topologically nontrivial.

Electrical transport measurements were carried out in HgTe quantum wells patterned in the Hall bar geometry shown in Fig. 8.6. The quantity that has been used in this experiment to reveal edge-state transport is the four-terminal resistance $R_{14,23} = V_{23}/I_{14}$, where V_{23} is the voltage between contacts 2 and 3, and I_{14} is the current flowing between contacts 1 and 4. This quantity $R_{14,23}$ was measured for various devices with different thicknesses d , below and above the critical thickness d_c , of the HgTe layer, and for different values of the Fermi energy. The latter can be tuned *in situ* by controlling the

voltage between the HgTe layer and a metallic ‘gate’ electrode on the top of the layered semiconductor structure, as shown in Fig. 8.4.

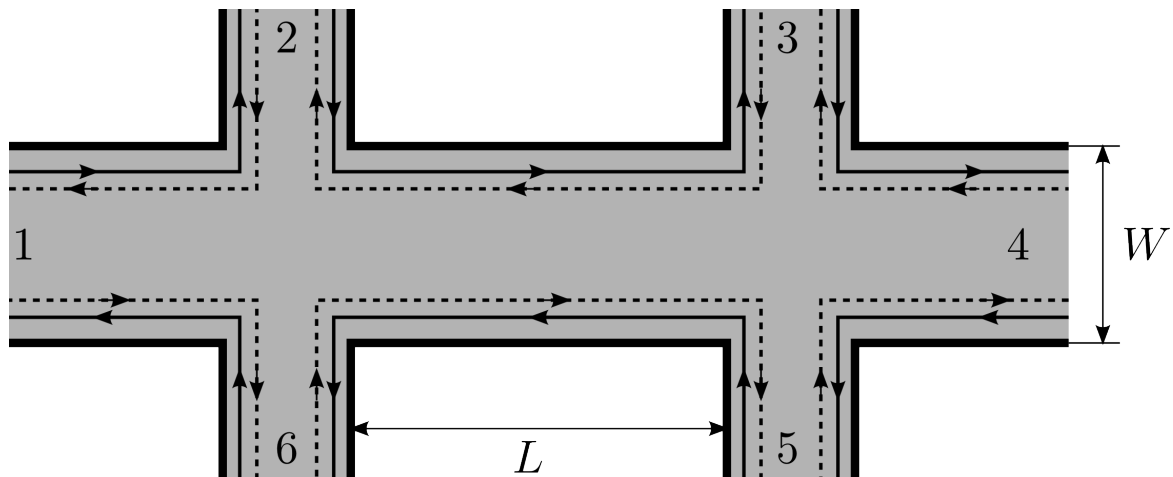


Figure 8.6: HgTe quantum well patterned in the Hall-bar geometry (gray area). Numbered terminals lead to metallic contacts. Solid and dashed lines depict counterpropagating edge states.

To appreciate the experimental result, let us first derive the four-terminal resistance $R_{14,23}$ for such a device. To this end, we express V_{23} with I_{14} . Ohm’s law implies $V_{23} = I_{23}/G_{23}$, where I_{23} is the current flowing through the edge segment between contacts 2 and 3, whereas G_{23} is the conductance of that edge segment. Furthermore, as the current I_{14} flowing through terminals 1 and 4 is equally divided between the upper and lower edges, the relation $I_{23} = I_{14}/2$ holds, implying the result $R_{14,23} = 1/(2G_{23})$.

If the Fermi energy lies in the bands neighboring the gap, then irrespective of the topological invariant of the system, the HgTe quantum well behaves as a good conductor with $G_{23} \gg e^2/h$, implying $R_{14,23} \ll h/e^2$. If the Fermi energy is tuned to the gap in the topologically nontrivial case $d > d_c$, then $G_{23} = e^2/h$ and therefore $R_{14,23} = h/(2e^2)$. This holds, of course, only at a temperature low enough and a sample size small enough such that phase coherence is guaranteed. The presence of static TRI defects is included. If the system is topologically trivial ($d < d_c$), then there is no edge transport, and the quantum well is a good insulator with $R_{14,23} \gg h/e^2$.

The findings of the experiments are consistent with the above expectations. Furthermore, the four-terminal resistance of topologically nontrivial HgTe layers with different widths were measured, with the resistance found to be an approximately constant function of the width W of the Hall bar. This is a further indication that the current in these samples is carried by edge states.

To wrap up this Chapter, we finally note that HgTe quantum wells provide the only

experimental realization of $D = 1$ topological insulators to date. Graphene is believed to be a $D = 1$ topological insulator as well, even though its energy gap between the valence and conduction band, induced by spin-orbit interaction and estimated to be of the order of μeV , seems to be too small to allow for the detection of edge-state transport even at the lowest available temperatures. The concept of a TRI topological insulator can be extended to 3D crystals as well, where the role of the edge states is played by states localized to the 2D surface of the 3D material. The description of such systems is out of the scope of the present course; the interested reader might consult, e.g., Refs. [7, 2].

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