Chapter 4

Chern insulators

Learning goals

- We know Dirac fermions.
- We know what a Chern insulator is.
- We are acquainted with the Chern insulator of Haldane's '88 paper.

- G. Jotzu, M. Messer, R. Desbuquois, M. Lebrat, T. Uehlinger, D. Greif, and T. Esslinger, Nature **515**, 237 (2014)

So far we have been dealing with systems subject to a magnetic field $\mathbf{B}$. We could show how their ground state can be described with a topological invariant, the Chern number. In the present chapter we try to extend these ideas. The main question we are trying to answer is the following: Can there be lattice systems with Bloch bands that are characterized by a non-zero Chern number even in the absence of a net magnetic field? Such an insulator would be termed a *Chern insulator*. Before we embark on this question, we need to understand a simple continuum problem called the Dirac model.

4.1 Dirac fermions

Dirac fermions in two dimensions are described by the Hamiltonian

$$H(\mathbf{k}) = \sum_i d_i(\mathbf{k})\sigma_i \qquad \text{with} \qquad d_1(\mathbf{k}) = k_x, \;\; d_2(\mathbf{k}) = k_y, \;\; d_3(\mathbf{k}) = m. \tag{4.1}$$

The energies and eigenstates are given by

$$\epsilon(\mathbf{k})_\pm = d_\pm(\mathbf{k}) = \pm\sqrt{k^2+m^2} \qquad \text{and} \qquad \psi_\pm(\mathbf{k}) = \frac{1}{\sqrt{2d(\mathbf{k})[d(\mathbf{k})-d_3(\mathbf{k})]}}\begin{pmatrix} d_3(\mathbf{k}) \pm d(\mathbf{k}) \\ d_1(\mathbf{k}) - id_2(\mathbf{k})\end{pmatrix}.$$

It is straight forward to show (exercise!) that the Berry connection of the lower band can be written as

$$\mathcal{A}_\mu(\mathbf{k}) = i\langle\psi_-(\mathbf{k})|\partial_{k_\mu}\psi_-(\mathbf{k})\rangle = -\frac{1}{2d(\mathbf{k})[d(\mathbf{k})+d_3(\mathbf{k})]}\left[d_2(\mathbf{k})\partial_{k_\mu}d_1(\mathbf{k}) - d_1(\mathbf{k})\partial_{k_\mu}d_2(\mathbf{k})\right] \tag{4.2}$$

And the corresponding Berry curvature is given by

$$F_{\mu\nu}(\mathbf{k}) = \frac{1}{2}\epsilon_{\alpha\beta\gamma}\hat{d}_\alpha(\mathbf{k})\partial_{k_\mu}\hat{d}_\beta(\mathbf{k})\partial_{k_\nu}\hat{d}_\gamma(\mathbf{k}) \qquad \text{with} \qquad \hat{\mathbf{d}}(\mathbf{k}) = \frac{\mathbf{d}(\mathbf{k})}{d(\mathbf{k})}. \tag{4.3}$$

Using our concrete d-vector we find

$$\mathcal{A}_x = \frac{-k_y}{2\sqrt{k^2+m^2}(\sqrt{k^2+m^2}+m)} \qquad \text{and} \qquad \mathcal{A}_y = \frac{k_x}{2\sqrt{k^2+m^2}(\sqrt{k^2+m^2}+m)}, \tag{4.4}$$

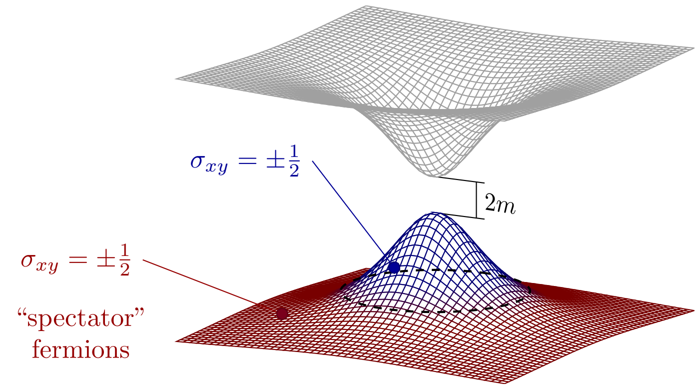


Figure 4.1: Regularization of the Dirac spectrum due to a lattice.

and therefore

$$\mathcal{F}_{\alpha\beta} = \frac{m}{2(k^2+m^2)^{3/2}}. \tag{4.5}$$

Let us plug that into the formula for the Hall conductance

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi}\int d\mathbf{k}\,\mathcal{F}_{\alpha\beta} = \frac{e^2}{h}\int_0^\infty dkk\frac{1}{2}\frac{m}{(k^2+m^2)^{3/2}} = \frac{e^2}{h}\frac{\operatorname{sign}(m)}{2}. \tag{4.6}$$

We can draw several important insights from this results:

1. $\sigma_{xy} \neq 0 \quad \Rightarrow$ we must have broken time-reversal invariance. How did this happen?
2. $\sigma_{xy} \neq \frac{e^2}{h}\nu$ with $\nu \in \mathbb{Z}$. How can this be?

Let us start with the first question. We have to make the distinction between two cases. (i) If the σ-matrices encode a real spin-1/2 degree of freedom the time reversal operator is given by

$$\mathcal{T} = i\sigma_y K,$$

where K denotes complex conjugation. Therefore

$$\mathcal{T}H(\mathbf{k})\mathcal{T}^{-1} = \sum_i -d_i(\mathbf{k})\sigma_i = -k_x\sigma_x - k_y\sigma_y - m\sigma_z.$$

If we want to above Hamiltonian to be time reversal invariant we need this to be

$$\mathcal{T}H(\mathbf{k})\mathcal{T}^{-1} \overset{!}{=} H(-\mathbf{k}) = -k_x\sigma_x - k_y\sigma_y + m\sigma_z.$$

From this we conclude that the Dirac fermions are only time reversal invariant for $d_3(\mathbf{k}) = m = 0$. However, in this case, there is no gap in the spectrum at $\mathbf{k} = 0$ and the calculation of σ_{xy} does

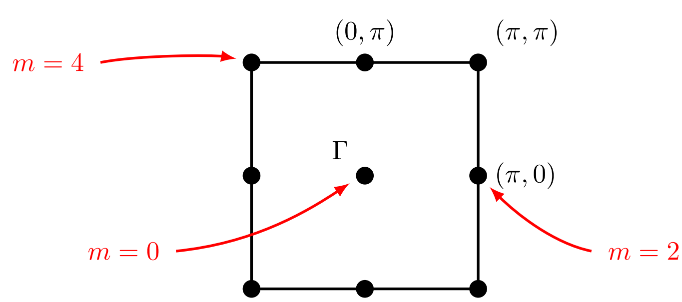
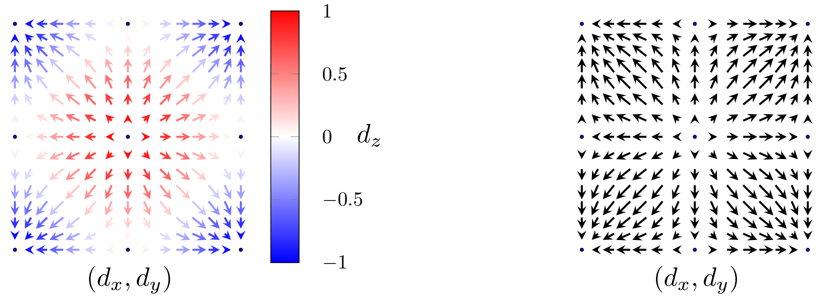


Figure 4.2: Band touching for a simple Chern insulator.



a skyrmion in-plane d-vector

Figure 4.3: Left: spin-configuration of a skyrmion. Right: in-plane d-vector of H.

not make sense. (ii) For the case that the Pauli matrices describe some iso-spin where $\mathcal{T} = K$, we need to have $H(\mathbf{k}) = H(-\mathbf{k})$. Or in other words

$$d_1(\mathbf{k}) = d_1(-\mathbf{k}), \;\; d_2(\mathbf{k}) = -d_2(-\mathbf{k}), \;\; d_3(\mathbf{k}) = d_3(-\mathbf{k}).$$

From these considerations we conclude that our Hamiltonian breaks time reversal invariance in either case and we can indeed expect a non-vanishing Hall conductance.

Let us now address the non-quantized nature of σ_{xy}. The quantization of σ_{xy} arises from the quantized value of the Chern number. We have seen in our derivation, however, that it was crucial that the domain over which we integrated the Berry curvature was closed and orientable. Here we are in a continuum model where the integral over all momenta extends over the whole $\mathbb{R}^2$. We have therefore no reason to expect σ_{xy} to be quantized.

There is value to formula (4.6), however. Imagine that the Dirac Hamiltonian arises from some low-energy expansion ($\mathbf{k}\cdot\mathbf{p}$) around a special point in the Brillouin zone of a lattice model. For the full lattice, the $k \to \infty$ integral would be regularized due to the Brillouin zone boundary. The whole system has a quantized Hall conductivity. However, the region close to the “Dirac-point” contributes $\pm 1/2$ to the Chern number, see Fig. 4.1. Moreover, imagine a gap closing and re-opening transition described by the Dirac Hamiltonian where m changes its value. In such a situation the change in Chern number $\Delta\mathcal{C} = \pm 2\pi$. Therefore, the Dirac model is an excellent way to study *changes in the Chern number*.

Before we continue to the simplest possible Chern insulator we state the following formula without proof (exercise!)

$$H(\mathbf{k}) = \sum_{i,j=1}^{2} A_{ij} k_i \sigma_j + m\sigma_3 \qquad \Rightarrow \qquad \sigma_{xy} = \frac{e^2}{h}\frac{\mathrm{sign}(m)}{2}\mathrm{sign}(\det A). \tag{4.7}$$

4.2 The simplest Chern insulator

We obtain the simplest conceivable Chern insulator by elevating the Dirac model to a lattice problem

$$d_1 = k_x \to \sin(k_x), \;\; d_2 = k_y \to \sin(k_y). \tag{4.8}$$

The σ matrices now act in a space of orbitals. The fact that the coupling between them is odd in $\mathbf{k}$ means that they need to differ by one quantum of angular momentum, e.g., an s-type and a p-type orbital. By symmetry, there can be an even in $\mathbf{k}$ term within each orbital, so we add it to our model

$$d_3 = m \to 2 - m - \cos(k_x) - \cos(k_y).$$

The Hamiltonian is gapped ($d(\mathbf{k}) \neq 0 \; \forall \mathbf{k}$) except at the special points in the Brillouin zone shown in Fig. 4.2.

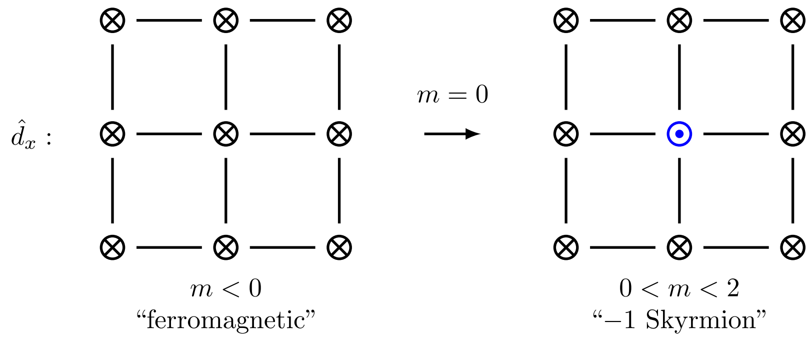


Figure 4.4: Change of the d_3 component at the first critical point.

We begin analyzing the Hamiltonian for $m \ll 0$ and $m \gg 4$. For $m = \pm\infty$, the eigenstates of the Hamiltonian are fully localized to single sites and the system certainly shows no Hall conductance. Another way to see this is to observe that

$$\frac{1}{2\pi}\int_{\mathrm{BZ}} d\mathbf{k}\, \epsilon_{\alpha\beta\gamma}\hat{d}_\alpha \partial_{k_x}\hat{d}_\beta \partial_{k_y}\hat{d}_\gamma$$

counts the winding of $\hat{\mathbf{d}}(\mathbf{k})$ throughout the Brillouin zone, i.e., it provides us what we know as the *skyrmion number*. In Fig. 4.3(a) we show a spin-configuration corresponding to a skyrmion. When we now look at the planar part of the d-vector, we see that we have all laid out for a skyrmion. The only addition we need is a sign change of d_3 at the right places in the Brillouin zone. This does not happen for $m < 0$ or $m > 4$. Note that exactly this sign change closes the gap in a fashion describable by Dirac fermions. Hence we appreciate the importance of the above discussion. It is now trivial to draw the phase diagram.

The case $0 \leq m < 2$: We start from $m = -\infty$ where $\sigma_{xy} = 0$ and go through the gap-closing at $\mathbf{k} = 0$ for $m = 0$. Around $\mathbf{k} = 0$ we find

$$H = k_x\sigma_x + k_y\sigma_y - m\sigma_x.$$

Therefore

$$\Delta\sigma_{xy} = \frac{e^2}{h}\left[\frac{1}{2}\mathrm{sign}(-m)\Big|_{m>0} - \frac{1}{2}\mathrm{sign}(-m)\Big|_{m<0}\right] = -\frac{e^2}{h} = \sigma_{xy}.$$

The correspoding change in $d_3(\mathbf{k})$ is shown in Fig. 4.4.

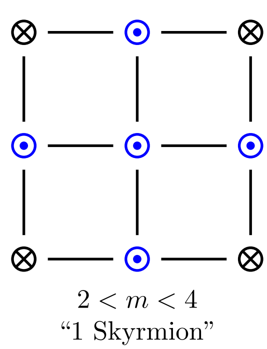


Figure 4.5: d_3 component after the second gap closing.

The case $2 \le m < 4$**:** At $m = 2$ the gap closes at $(\pi, 0)$ and $(0, \pi)$. Let us expand the Hamiltonian around these points

$$\begin{aligned} H_{(\pi,0)} &= \quad k_x\sigma_x - k_y\sigma_y + (2-m)\sigma_z, && (4.9)\\ H_{(0,\pi)} &= -k_x\sigma_x + k_y\sigma_y + (2-m)\sigma_z. && (4.10) \end{aligned}$$

From this we read out the change in σ_{xy}:

$$\Delta\sigma_{xy} = -2\frac{e^2}{h}\left[\frac{1}{2}\text{sign}(2-m)\Big|_{m>2} - \frac{1}{2}\text{sign}(2-m)\Big|_{m<2}\right] = 2\frac{e^2}{h}. \tag{4.11}$$

Note that the 2 in front stems from the two gap closings and the overall $-$ sign arises from the odd sign of the determinant A, cf. Eq. (4.7). Together with the value of σ_{xy} for $0 < m < 2$ we obtain

$$\sigma_{xy} = +\frac{e^2}{h}.$$

The corresponding $d_3(\mathbf{k})$ is shown in Fig. 4.5.

The case $4 \le m$**:** The last gap-closing happens at (π, π) for $m = 4$. At this point

$$H_{(\pi,\pi)} = -k_x\sigma_x - k_y\sigma_y + (4-m)\sigma_z.$$

As before the change in σ_{xy} is given by

$$\Delta\sigma_{xy} = \frac{e^2}{h}\left[\frac{1}{2}\text{sign}(4-m)\Big|_{m>0} - \frac{1}{2}\text{sign}(4-m)\Big|_{m<0}\right] = -\frac{e^2}{h}.$$

And we arrive again at $\sigma_{xy} = 0$ as expected for a phase connected to the $m = \infty$ limit. Again, $d_3(\mathbf{k})$ is shown in Fig. 4.6.

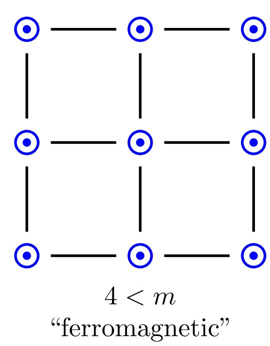


Figure 4.6: Trivial insulator.

We can now summarize our analysis in Fig. 4.7.

We started from a Hamiltonian that breaks time-reversal invariance $\mathcal{T}$ and found a non-vanishing σ_{xy}. We did so not by calculating $\mathcal{F}_{\mu\nu}$ and performing complicated $\mathbf{k}$-space integrals but via a simple analysis of gap closings.

The Chern insulator presented here is the simplest one, but not the first discovered. We now discuss the first Chern insulator due to Haldane [1] as it motivated the first time-reversal invariant topological insulators which we will embark on next.

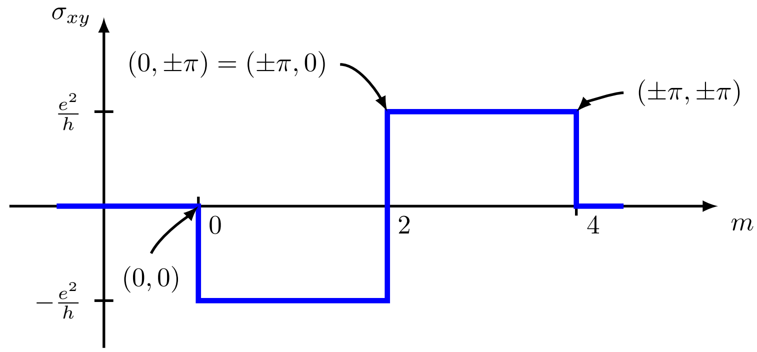


Figure 4.7: Evolution of the topological index as a function of m.

4.3 The Haldane Chern insulator

In his seminal paper [1], Haldane considered a honeycomb model with no net magnetic flux but with complex phases $e^{\pm i\varphi}$ on the next-to-nearest neighbor hoppings. A possible *staggered* flux pattern giving rise to such a situation is shown in Fig. 4.8. In Fig. 4.8 we also indicate the sign structure of the phases. The model can be written as

$$H = \sum_{\langle i,j\rangle} c_i^\dagger c_j + t \sum_{\langle\langle i,j\rangle\rangle} e^{\pm i\varphi} c_i^\dagger c_j + m \sum_i \epsilon_i c_i^\dagger c_i, \tag{4.12}$$

where $\epsilon_i = \pm 1$ for the two sub-lattices of the honeycomb lattice. Written in $\mathbf{k}$-space we find $H = \epsilon(\mathbf{k}) + \sum_i d_i(\mathbf{k})\sigma_i$ with

$$d_1(\mathbf{k}) = \cos(\mathbf{k}\cdot\mathbf{a}_1) + \cos(\mathbf{k}\cdot\mathbf{a}_2) + 1, \tag{4.13}$$

$$d_2(\mathbf{k}) = \sin(\mathbf{k}\cdot\mathbf{a}_1) + \sin(\mathbf{k}\cdot\mathbf{a}_2), \tag{4.14}$$

$$d_3(\mathbf{k}) = m + 2t\sin(\varphi)\left[\sin(\mathbf{k}\cdot\mathbf{a}_1) - \sin(\mathbf{k}\cdot\mathbf{a}_2) - \sin(\mathbf{k}\cdot(\mathbf{a}_1 - \mathbf{a}_2))\right], \tag{4.15}$$

with $\mathbf{a}_1 = a(1,0)$ and $\mathbf{a}_2 = a(1/2, \sqrt{3}/2)$. We ignore the shift $\epsilon(\mathbf{k})$ in the following. What are the symmetries of this Hamiltonian? First, d_1 and d_2 are compatible with the time-reversal $\mathcal{T}$. However, $d_3(\mathbf{k}) = d_3(-\mathbf{k})$ holds only for $\varphi = 0, \pi$. We can therefore expect a non-vanishing Chern number for a general φ. The Hamiltonian has C_3 symmetry. Hence, the gap closings have to happen at the K or K' point, see Fig. 4.9 (Prove!),

$$K = \frac{2\pi}{a}\left(1, \frac{1}{\sqrt{3}}\right), \qquad K' = \frac{2\pi}{a}\left(1, -\frac{1}{\sqrt{3}}\right),$$

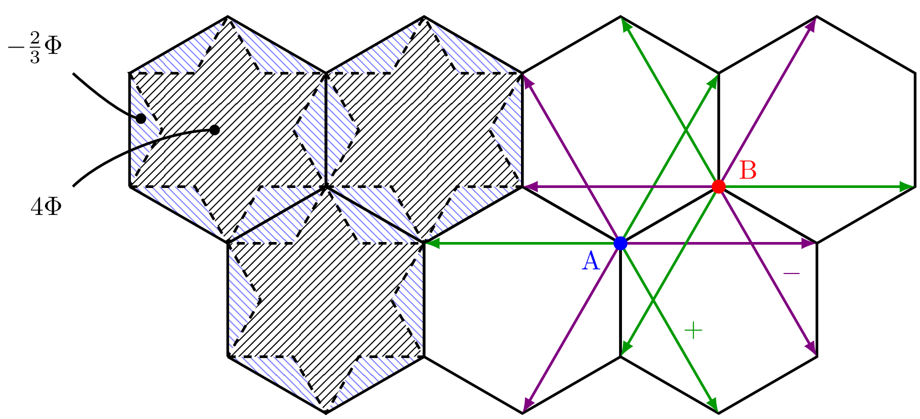


Figure 4.8: The Haldane Chern insulator model.

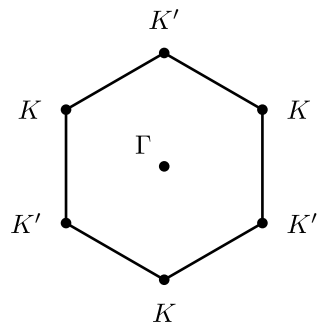


Figure 4.9: Gap closings for the Haldane Chern insulator.

where a denotes the lattice constant. To calculate the Chern number we follow the same logic as in the last chapter. We start from the limit $m \to \infty$ and track the gap-closings at the Dirac points at K and K'. The low energy expansion at these two points read

$$H_K = \frac{3}{2}\left(k_y\sigma_x - k_x\sigma_y\right) + \left(m - 3\sqrt{3}t\sin(\varphi)\right)\sigma_z, \tag{4.16}$$

$$H_{K'} = -\frac{3}{2}\left(k_y\sigma_x + k_x\sigma_y\right) + \left(m + 3\sqrt{3}t\sin(\varphi)\right)\sigma_z. \tag{4.17}$$

Note that the gap-closings at K and K' happen at different values of m (for $\varphi \neq 0, \pi$). Moreover, the two Dirac points give rise to a change in σ_{xy} of opposite sign has $\det(A)$ as a different sign. We can now construct the phase diagram

- $m > 3\sqrt{2}t\sin(\varphi)$: $\sigma_{xy} = 0$
- $-3\sqrt{2}t\sin(\varphi) < m \geq 3\sqrt{2}t\sin(\varphi)$ for $\varphi > 0$: At $m = 3\sqrt{2}t\sin(\varphi)$ the gap closes at K and we have a $\Delta\sigma_{xy} = -\frac{e^2}{h}$. The gap at K' stays open.
- $m \leq -3\sqrt{2}t\sin(\varphi)$ for $\varphi > 0$: The gap at K' closes at $m - 3\sqrt{2}t\sin(\varphi)$ and hence the Chern number changes back to 0.

For $\varphi < 0$ the signs of the Chern numbers are inverted. The resulting phase diagram is summarized in Fig. 4.10.

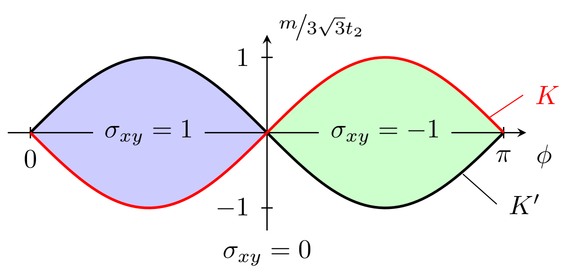


Figure 4.10: Phase diagram of the Haldane model.

The model of Haldane breaks time-reversal invariance $\mathcal{T}$. How can we build a model which is $\mathcal{T}$-symmetric? The easiest way is by doubling the degrees of freedom:

$$\mathcal{T}H\mathcal{T}^{-1} = H' \neq H \Rightarrow H_{\text{doubled}} = \begin{pmatrix} H & \\ & H' \end{pmatrix}.$$

We will see in the next chapter how Kane and Mele [2] took this step.

References

1. Haldane, F. D. M. "Model for a Quantum Hall Effect without Landau Levels". *Phys. Rev. Lett.* **61,** 2015 (1988).
2. Kane, C. L. & Mele, E. J. "Quantum Spin Hall Effect in Graphene". *Phys. Rev. Lett.* **95,** 226801 (2005).