GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Advanced Solid State Theory
Swap Lecture
Hall conductance as a topological invariant

Niclas Heinsdorf

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Contents

1 Quantum Hall effect continued

These notes continue where section 2.6 left off and aims to deepen the understanding of the quantum Hall effect. For an introduction to this effect please refer to the aforementioned part in Prof. Valentis script.

Let us consider the Hamiltonian of a charged particle coupled to an external magnetic field again as we did in section 2.4 Landau diamagnetism. Now, we will consider an electric field **E** in the x-direction additionally

$$H = \frac{1}{2m}\left(p_x^2 + (p_y + eBx)^2\right) - eEx \tag{1}$$

Notice that we reduced our problem to two dimensions and that we set $c = 1$. We can use the ansatz we used before to obtain the same states, but with a shifted argument

$$\psi(x, y) = \psi_{nk}(x - mE/eB^2, y) \tag{2}$$

and our energies are now given by

$$E_{nk} = \hbar\omega_0\left(n + \frac{1}{2}\right) + eE\left(k_y\lambda^2 - \frac{eE}{m\omega_0^2}\right) + \frac{m}{2}\frac{E^2}{B^2} \tag{3}$$

with

$$\omega_0 = \frac{eB}{m} \tag{4}$$

$$\lambda = \frac{\hbar}{eB} \tag{5}$$

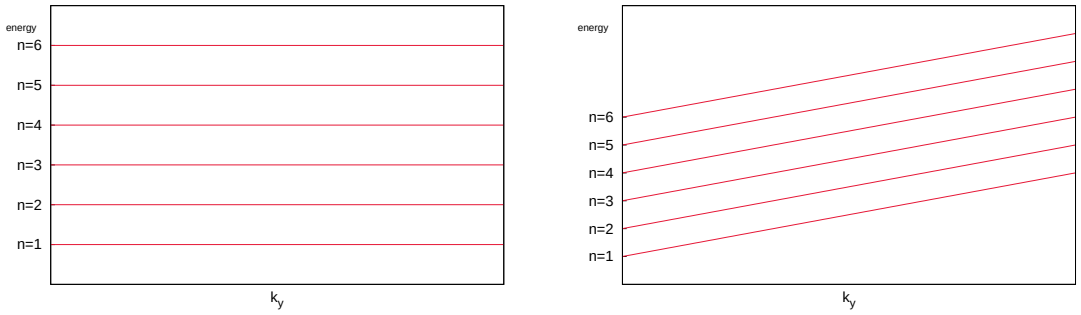

Figure 1: Landau levels with and without an electric field applied

As the energies E_{nk} depend linearly on k now the degeneracy of the Landau has been lifted (Fig.1). It is worth noting that the states drift neither in the **E** nor in the **B**-direction, but in the $\mathbf{E} \times \mathbf{B}$-direction. With the group velocity being

$$v_y = \frac{1}{\hbar}\frac{\partial E_{nk}}{\partial k_y} = e\hbar E\lambda^2 = \frac{E}{B} \tag{6}$$

we can think of the third term of Eq. 3 as the kinetic energy while the middle part corresponds to the potential energy of a wave packet; now localized around $-k_y\lambda^2 + eE/m\omega_0^2$. Let us now put the Fermi energy between the first two Landau levels (Fig.2) and vary the strength of the magnetic field **B** adiabatically. Remember that the spacing between the Landau levels or rather the cyclotron frequency ω_0 is proportional to **B** (Eq.4), so via changing **B** we can shift the Fermi Energy up and down. Since the Landau Energy levels are linearly dependent on k_y each intersection of the Fermi energy with a landau energy level contributes a fixed amount of conductivity to the overall Hall conductivity σ_{xy}, independently on where this intersection is. In Figure 2 we can see two differently placed Fermi energies and their intersections with the Landau levels. Since the upper Fermi energy has overstepped one more level it has one more intersection and thereby the Hall conductivity is higher by $\frac{e^2}{2\pi\hbar}$.

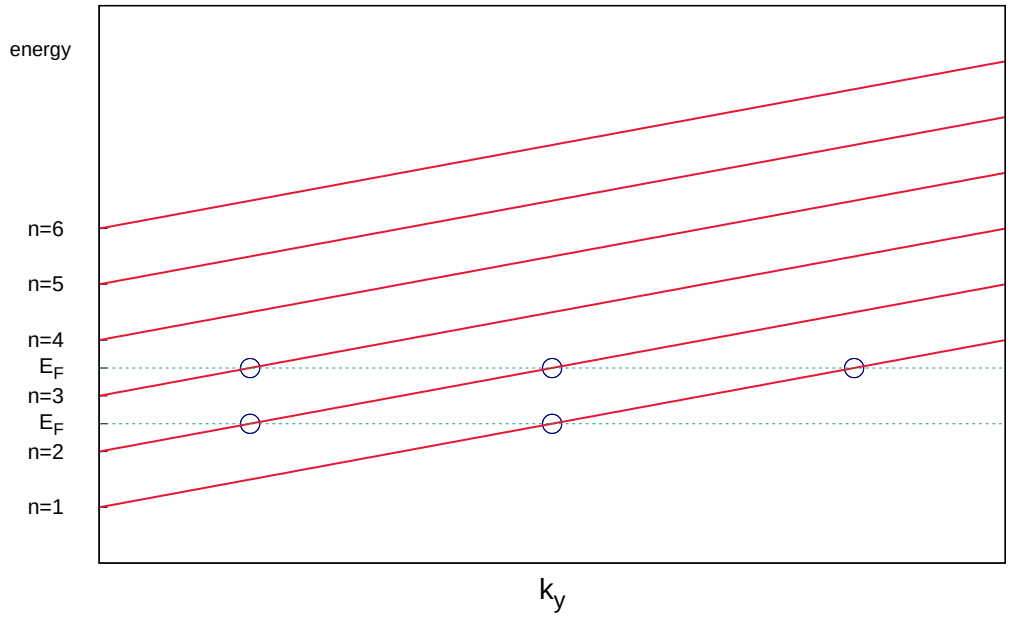

Figure 2: Landau levels intersected by two Fermi levels

2 Edge states

Section 1 aimed to clarify why the Hall conductivity σ_{xy} is quantized. Now we will elaborate on why the states that are localized in the bulk of our material do not contribute to the total conductivity whereas the edge states carry all the current.
The bending of the Landau levels due to an electric field has already been object to our discussion. Up to now, we have only considered periodic boundary conditions. Let us now factor in that our material has in fact open boundaries, so that we consider a potential well with very steep walls Fig 3.

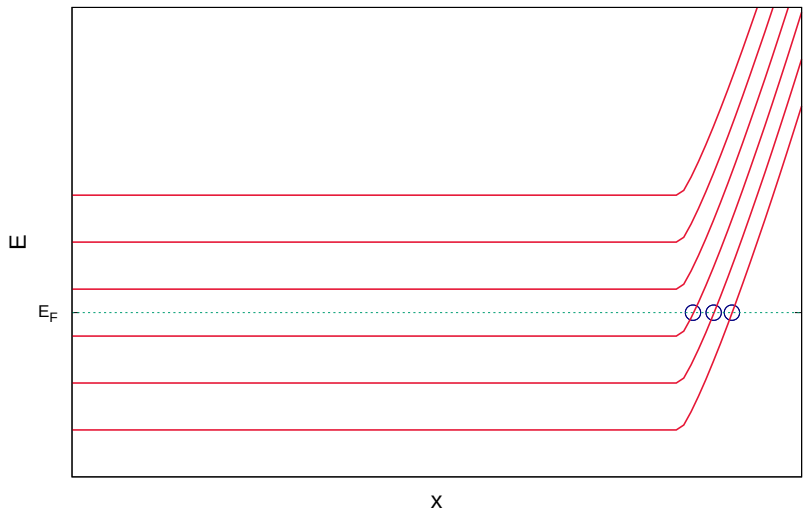

Figure 3: Landau levels in potential well

Please be aware that we are in real and not in k-space, although in the particular case of $\mathbf{E} = (E, 0, 0)^\top$ k_y and x are proportional to each other, anyway (Eq. 3), with the proportionality constant being λ^2.
Regarding the quantization of the Hall conductivity σ_{xy} the same argument holds as in the previous section. However, looking at Fig. 3 we would argue that the bulk of our material is an insulator whereas the edges are metallic, because that is where our intersections with the (arbitrarily chosen) Fermi energy sit.
Another way of understanding the appearance of conducting edge states in a classical fashion is to think about the cyclotron orbits of the particles. In the bulk of the material the particles will just describe a circular movement due to the applied magnetic field and the resulting Lorentz force. On the edges however the open boundaries of our system put a constraint on their movement. Imagine the particles bouncing of the boundary and thereby moving on skipping orbits (Fig.4). This results in an overall, chiral charge transport along the edges of our system.
This behaviour can also account for the robustness of the effect. If the edges are the only

places where charge is transported, the electrons have to travel a macroscopical distance (namely the width of the sample) in order to scatter other electrons.

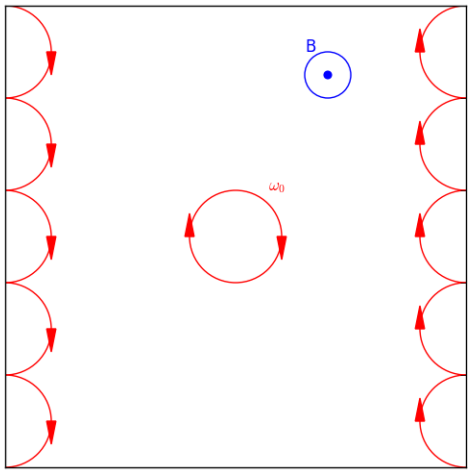

Figure 4: Particles performing skipping orbits along the boundary of the Hall system

3 Berry phase

Moving away for now from our Hall system, let us consider a parameter dependent Hamiltonian $H(\mathbf{R}(t))$ where $\mathbf{R}$ is a n-dimensional, time dependent vector, which is moving on a closed loop $\mathcal{C}$ in parameter space and $|n(\mathbf{R}(t))\rangle$ as the normalized instantaneous eigenstate of $H(\mathbf{R}(t))$ with

$$H(\mathbf{R}(t))\,|n(\mathbf{R}(t))\rangle = E_n(\mathbf{R}(t))\,|n(\mathbf{R}(t))\rangle \tag{7}$$

Equation (1.1) determines the eigenstate $|n(\mathbf{R}(t))\rangle$ only up to a phase and we know per adiabatic theorem, that for slow variation of $\mathbf{R}$ the system remains in its eigenstate. We will now consider the phase $\theta(t)$ of the state $|\psi(t)\rangle = e^{-i\theta(t)}\,|n(\mathbf{R}(t))\rangle$ during an adiabatic evolution along the loop $\mathcal{C}$. The time evolution of the system is given by

$$H(\mathbf{R}(t))\,|\psi(t)\rangle = i\hbar\frac{d}{dt}\,|\psi(t)\rangle \tag{8}$$

Which yields

$$E_n(\mathbf{R}(t))\,|n(\mathbf{R}(t))\rangle = \hbar\left(\frac{d}{dt}\theta(t)\right)|n(\mathbf{R}(t))\rangle + i\hbar\frac{d}{dt}\,|n(\mathbf{R}(t))\rangle \tag{9}$$

Taking the scalarproduct with $\langle n(\mathbf{R}(t))|$ and integrating we obtain

$$\theta(t) = \frac{1}{\hbar}\int_0^t E_n(\mathbf{R}(t')) - i\int_0^t \langle n(\mathbf{R}(t'))| \frac{d}{dt'} |n(\mathbf{R}(t'))\rangle \, dt' \tag{10}$$

The first part is the dynamical phase factor, which we already know, whereas the negative of the second term is the so called Berry or geometrical Phase γ_n

$$\gamma_n = i\int_0^t \langle n(\mathbf{R}(t'))| \frac{d}{dt'} |n(\mathbf{R}(t'))\rangle \, dt' \tag{11}$$

Via a transformation we obtain

$$\gamma_n = i\int_0^t \langle n(\mathbf{R}(t'))| \nabla_{\mathbf{R}} |n(\mathbf{R}(t'))\rangle \frac{d\mathbf{R}}{dt'} dt' = i\int_{\mathcal{C}} \langle n(\mathbf{R})| \nabla_{\mathbf{R}} |n(\mathbf{R})\rangle \, d\mathbf{R} \tag{12}$$

Where we have dropped the time dependence of $\mathbf{R}$.
We can now define a vector potential called Berry connection

$$\mathcal{A}_n(\mathbf{R}) = i \langle n(\mathbf{R})| \nabla_{\mathbf{R}} |n(\mathbf{R})\rangle \tag{13}$$

Or in components (we now omit the subscript n, as well as the $\mathbf{R}$-dependence of n and assume we stay in the eigenstate n)

$$\mathcal{A}_n = i \langle n| \nabla_{\mathbf{R}} |n\rangle \tag{14}$$

Lastly, we define the curvature of our vector potential.

$$\mathcal{F} = \nabla_{\mathbf{R}} \times \mathcal{A} \tag{15}$$

Or in components:

$$\mathcal{F}_{ij} = \frac{\partial \mathcal{A}_j}{\partial R_i} - \frac{\partial \mathcal{A}_i}{\partial R_j} \tag{16}$$

Notice, how the expressions above resemble those that are defined in electrodynamics. A lot of authors refer to the Berry curvature as magnetic field in parameter space.

4 Gauß-Bonnet theorem

Via the Gauß-Bonnet theorem it is possible to establish a relation between the curvature $\mathcal{K}$ of a surface and its genus g, which is a topological invariant under homeomorphisms (a continuous function that has a continious inverse function). Let M be a compact two-dimensional Riemannian manifold without boundary and with a compact orientable surface. Let $\mathcal{K}$ be

the Gaussian curvature of M and dA the element of area. Then

$$\int_M \mathcal{K} dA = 2\pi(2 - 2g) \tag{17}$$

The genus g is basically the number of holes in the object. A sphere (whose Gaussian curvature $\mathcal{K}$ equals 1 in each point) has therefore a genus of $g = 0$, whereas a torus has a genus of $g = 1$. Notice, that the genus g can only take integer values.

5 Chern number

In the previous section, we have been reminded that the integration over the curvature on a surface yields integers, which are topologically invariant (for another analogy just think of the winding number which yields an integer value depending on how often a point is encircled counterclockwise by a closed curve). Two sections before (Sec.3), we have obtained the Berry curvature $\mathcal{F}$, which describes the geometry of parameter space. Integrating the Berry Curvature $\mathcal{F}$ over the surface $\mathcal{S}$ gives the Chern number C (where $\mathcal{S}$ is the surface whose boundary is the closed loop $\mathcal{C}$)

$$C = \frac{1}{2\pi} \int_{\mathcal{S}} \mathcal{F} \tag{18}$$

The Chern number C can be used to classify electronic bandstructures. In that case the parameter $\mathbf{R}$ corresponds to $\mathbf{k}$ and the path $\mathcal{C}$ can be considered closed due to the periodicity of the lattice. In the following section we will see how to Chern number and the Hall conductivity relate to each other.

6 Kubo Formula

Putting aside the previous discussions for a while, we should now think of how to calculate the Hall conductivity. To this end, yet another technique has to be introduced.

The Kubo formula expresses the *linear response* of an observable quantity due to a time-dependent perturbation. Let H_0 be our unperturbed Hamiltonian and $|m\rangle$ its energy eigenstates with

$$H_0 |m\rangle = E_m |m\rangle \tag{19}$$

We now add a pertubation in the form of

$$\Delta H = -\mathbf{JA} \tag{20}$$

With $\mathbf{J}$ as the current density operator and $\mathbf{A}$ as the electro-magnetic potential. We choose as gauge

$$\mathbf{A}_t = 0 \qquad \Rightarrow \qquad -\partial_t \mathbf{A} = \mathbf{E} \tag{21}$$

Ultimately, we would like to consider a DC, but it is easier to work with an AC first and then take the limit $\omega \to 0$, where ω is the frequency of the current. We get

$$\mathbf{E}(t) = \mathbf{E}e^{-i\omega t} \qquad and \qquad \mathbf{A} = \frac{\mathbf{E}}{i\omega}e^{-i\omega t} \tag{22}$$

In the following we will work in the Dirac Picture, so that operators evolve with $\mathbf{J}(t) = V^{-1}\mathbf{J}V$ with $V = e^{-iH_0 t/\hbar}$, but the states with

$$|\psi(t)\rangle_D = U(t, t_0)\,|\psi(t_0)\rangle_D \tag{23}$$

$$U(t, t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} \Delta H(t')dt'} \tag{24}$$

Let us prepare the system in its ground state $|\psi_0\rangle$ at time $t \to -\infty$.

$$\langle \mathbf{J}(t)\rangle = \langle\psi_0(t)|\,\mathbf{J}(\mathbf{t})\,|\psi_0(t)\rangle = \langle\psi_0|\,U^{-1}(t)\mathbf{J}(t)U(t)\,|\psi_0\rangle \tag{25}$$

$$\approx \langle\psi_0|\,\frac{i}{\hbar}\int_{-\infty}^{t} dt'[\Delta H(t'), \mathbf{J}(t)]\,|\psi_0\rangle \tag{26}$$

Where we have used the time evolution of the states $\langle\psi_0|$ and $|\psi_0\rangle$, as well as the linear expansion of $U(t)$ while assuming that the zeroth order vanishes. Using Eq.(20) and Eq.(22) we get

$$\langle J_i(t)\rangle = \frac{1}{\hbar\omega}\int_{-\infty}^{t} dt'\,\langle\psi_0|\,[J_j(t'), J_i(t)]\,|\psi_0\rangle\,E_j e^{-i\omega t'} \tag{27}$$

But due to the system's time translational invariane we can write this expression as

$$\langle J_i(t)\rangle = \frac{1}{\hbar\omega}\left(\int_0^{\infty} dt'' e^{i\omega t''}\,\langle\psi_0|\,[J_j(0), J_i(t'')]\,|\psi_0\rangle\right)E_j e^{-i\omega t} \tag{28}$$

As we can see, the current responds by oscillating at the same frequency ω when an electric field with that frequency is applied. The proportionality constant corresponds to our Hall conductivity. We are interested in the off-diagonal part, which is the *Kubo formula* for the Hall conductivity:

$$\sigma_{xy}(\omega) = \frac{1}{\hbar\omega}\int_0^{\infty} dt e^{i\omega t}\,\langle\psi_0|\,[J_y(0), J_x(t)]\,|\psi_0\rangle \tag{29}$$

Now we take into account that the current operator evolves as $\mathbf{J}(\mathbf{t}) = V^{-1}\mathbf{J}V$ with $V = e^{-iH_0 t/\hbar}$ and insert some complete basis sets of the eigenstates of H_0.

$$\sigma_{xy}(\omega) = \frac{1}{\hbar\omega}\int_0^{\infty} dt e^{i\omega t}\sum_n \langle\psi_0|\,J_y\,|n\rangle\,\langle n|\,J_x\,|\psi_0\rangle\,e^{i(E_n - E_0)t/\hbar} - \sum_n \langle\psi_0|\,J_x\,|n\rangle\,\langle n|\,J_y\,|\psi_0\rangle\,e^{i(E_0 - E_n)t/\hbar} \tag{30}$$

Before we perform the integral we should substitute ω with $\omega + i\epsilon$ in order to circumvent poles on the real axis. After the integration we take the limit $\epsilon \to 0$. Doing this yields the following expression:

$$\sigma_{xy}(\omega) = -i\frac{1}{\omega}\sum_{n\neq 0}\left(\frac{\langle\psi_0|\, J_y\,|n\rangle\,\langle n|\, J_x\,|\psi_0\rangle}{\hbar\omega + E_n - E_0} - \frac{\langle\psi_0|\, J_x\,|n\rangle\,\langle n|\, J_y\,|\psi_0\rangle}{\hbar\omega + E_0 - E_n}\right) \tag{31}$$

In the DC Limit $\omega \to 0$ the denominators become

$$\frac{1}{\hbar\omega + E_n - E_0} \approx \frac{1}{E_n + E_0} - \frac{\hbar\omega}{(E_n - E_0)^2} + \mathcal{O}(\omega^2) \tag{32}$$

Assuming rotational variance (or conservation of current) it can be shown, that the zeroth order terms must vanish. We are left with

$$\sigma_{xy} = i\hbar\sum_{n\neq 0}\frac{\langle\psi_0|\, J_y\,|n\rangle\,\langle n|\, J_x\,|\psi_0\rangle - \langle\psi_0|\, J_x\,|n\rangle\,\langle n|\, J_y\,|\psi_0\rangle}{(E_n - E_0)^2} \tag{33}$$

7 Hall conductivity as a Chern number

Finally, we are in a position to combine what we have learnt so far and show the relationship between the Hall conductivity σ_{xy} and topology.
Let us consider a cubic lattice with lattice constant a and periodic boundary conditions. We will neglect electron-electron interaction, so the wavefunctions in a given band n can be given by Bloch waves.

$$\psi^n_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{kx}}u^n_{\mathbf{k}}(\mathbf{x}) \tag{34}$$

With $u^n_{\mathbf{k}}(\mathbf{x})$ being periodic on the unit cell.
Furthermore, we will assume that we are dealing with an insulator at $T = 0$ so that all bands below E_F are completely filled and those above are completely empty. Let me remind you of the Berry connection defined in section 3.

$$\mathcal{A}_i = i\,\langle u_{\mathbf{k}}|\,\frac{\partial}{\partial k_i}\,|u_{\mathbf{k}}\rangle \tag{35}$$

We can see that a $U(1)$ gauge transformation of $\mathcal{A}$ corresponds to a change of phase of $|u^n_{\mathbf{k}}\rangle$. Let us calculate the corresponding Berry curvature

$$\mathcal{F}_{xy} = \frac{\partial\mathcal{A}_y}{\partial k_x} - \frac{\partial\mathcal{A}_x}{\partial k_y} = i\langle\frac{\partial u^n_{\mathbf{k}}}{\partial k_x}|\frac{\partial u^n_{\mathbf{k}}}{\partial k_y}\rangle - i\langle\frac{\partial u^n_{\mathbf{k}}}{\partial k_y}|\frac{\partial u^n_{\mathbf{k}}}{\partial k_x}\rangle \tag{36}$$

Our Chern number in 2d is given by

$$C = \frac{1}{2\pi}\int_{BZ} d^2k \mathcal{F}_{xy} \tag{37}$$

For particles on the lattice our Kubo formula (Eq.33) becomes

$$\sigma_{xy} = i\hbar \sum_n \sum_m \int_{BZ} \frac{d^2k}{(2\pi)^2} \int_{BZ} \frac{d^2k'}{(2\pi)^2} \frac{\langle u^n_{\mathbf{k}}| J_y |u^m_{\mathbf{k}'}\rangle \langle u^m_{\mathbf{k}'}| J_x |u^n_{\mathbf{k}}\rangle - \langle u^n_{\mathbf{k}}| J_x |u^m_{\mathbf{k}'}\rangle \langle u^m_{\mathbf{k}'}| J_y |u^n_{\mathbf{k}}\rangle}{(E_m(\mathbf{k}) - E_n(\mathbf{k}))^2} \tag{38}$$

Where n runs over the filled bands and m runs over *all* bands so that the following completeness relation is fulfilled:

$$\sum_m \int_{BZ} \frac{d^2k'}{(2\pi)^2} |u^m_{\mathbf{k}'}\rangle \langle u^m_{\mathbf{k}'}| = \mathbb{1} \tag{39}$$

Let us define $\mathbf{J}$ in terms of the group velocity of the wave packets,

$$\mathbf{J} = \frac{e}{\hbar}\frac{\partial H}{\partial \mathbf{k}} \tag{40}$$

We would like to work with $|u^n_{\mathbf{k}}\rangle$ rather than with $|\psi^n_{\mathbf{k}}\rangle$, so we take a look at the eigenproblem of our Bloch functions again and define,

$$\begin{aligned} H_0 |\psi^n_{\mathbf{k}}\rangle = E_n(\mathbf{k}) |\psi^n_{\mathbf{k}}\rangle &\Rightarrow e^{-i\mathbf{kx}} H_0 e^{i\mathbf{kx}} |u^n_{\mathbf{k}}\rangle \\ &\Rightarrow H |u^n_{\mathbf{k}}\rangle = E_n(\mathbf{k}) |u^n_{\mathbf{k}}\rangle \end{aligned}$$

Where we defined $H = e^{-i\mathbf{kx}} H_0 e^{i\mathbf{kx}}$.
The Kubo formula becomes

$$\sigma_{xy} = \frac{ie^2}{\hbar} \sum_n \sum_m \int_{BZ} \frac{d^2k}{(2\pi)^2} \int_{BZ} \frac{d^2k'}{(2\pi)^2} \frac{\langle u^n_{\mathbf{k}}| \partial_y H |u^m_{\mathbf{k}'}\rangle \langle u^m_{\mathbf{k}'}| \partial_x H |u^n_{\mathbf{k}}\rangle - \langle u^n_{\mathbf{k}}| \partial_x H |u^m_{\mathbf{k}'}\rangle \langle u^m_{\mathbf{k}'}| \partial_y |u^n_{\mathbf{k}}\rangle}{(E_m(\mathbf{k}) - E_n(\mathbf{k}))^2} \tag{41}$$

with $\partial_x \equiv \frac{\partial}{\partial k_x}$ and $\partial_y \equiv \frac{\partial}{\partial k_y}$.
For i being either x or y respectively, consider the product rule

$$\begin{aligned} \langle u^n_{\mathbf{k}}| \partial_i \big(H |u^m_{\mathbf{k}'}\rangle\big) &= \langle u^n_{\mathbf{k}}| \partial_i H |u^m_{\mathbf{k}'}\rangle + \langle u^n_{\mathbf{k}}| H |\partial_i u^m_{\mathbf{k}'}\rangle \\ \Leftrightarrow \langle u^n_{\mathbf{k}}| \partial_i H |u^m_{\mathbf{k}'}\rangle &= \langle u^n_{\mathbf{k}}| \partial_i \big(H |u^m_{\mathbf{k}'}\rangle\big) - \langle u^n_{\mathbf{k}}| H |\partial_i u^m_{\mathbf{k}'}\rangle \\ &= \big(E_m(\mathbf{k}') - E_n(\mathbf{k})\big) \langle u^n_{\mathbf{k}}| |\partial_i u^m_{\mathbf{k}'}\rangle \\ &= -\big(E_m(\mathbf{k}') - E_n(\mathbf{k})\big) \langle \partial_i u^n_{\mathbf{k}}| |u^m_{\mathbf{k}'}\rangle \end{aligned}$$

Substituting this into the Kubo formula (Eq. 33) yields

$$\sigma_{xy} = \frac{ie^2}{\hbar} \sum_n \int_{BZ} \frac{d^2k}{(2\pi)^2} \langle \partial_x u^n_{\mathbf{k}} | \partial_y u^n_{\mathbf{k}} \rangle - \langle \partial_y u^n_{\mathbf{k}} | \partial_x u^n_{\mathbf{k}} \rangle \tag{42}$$

With equation 36 and 37 we finally get

$$\sigma_{xy} = \frac{e^2}{\hbar} \sum_n \int_{BZ} \frac{d^2k}{(2\pi)^2} \mathcal{F}_{xy} \tag{43}$$

$$= \frac{e^2}{2\pi\hbar} \sum_n C_n \tag{44}$$

This equation states that the Hall conductivity σ_{xy} is the sum over the Chern numbers of the filled bands of our material (with the exception of some prefactor). We see that the behaviour of such a system is a manifestly topological property, which can account for the robustness of the effect.

8 Topological edge states

In the last section, we saw that the Hall conductivity is a topological invariant and it has also been discussed that the states which contribute to the overall Hall conductivity σ_{xy} live on the edges of our system. We have also learnt that we can explain this behaviour by considering the bending of the Landau levels due to the 2d box-potential of the system. The previous calculation enables us to discuss the appearance of the edge conductivity under a new aspect.
To this end, remember section 5 concerning the Chern number and that it is somewhat analogous to the genus of a geometric object. Let us remind ourselves that no homeomorphism between two objects with different genera can be found.
In the same way the band structure of materials belonging to different Chern classes can not be adiabatically transformed into one another. At the transition between two insulating materials, having two different Chern numbers, metallic edge states appear in order to have a smooth transition between a topological non-trivial and a trivial material (e.g. vacuum).
Imagine two bands that have to unwind in order to unravel a knot representing the topological non-triviality in that case (Fig. 5). This is not possible without closing the band gap somewhere, which is why at the edges the topological non-trivial material becomes metallic.

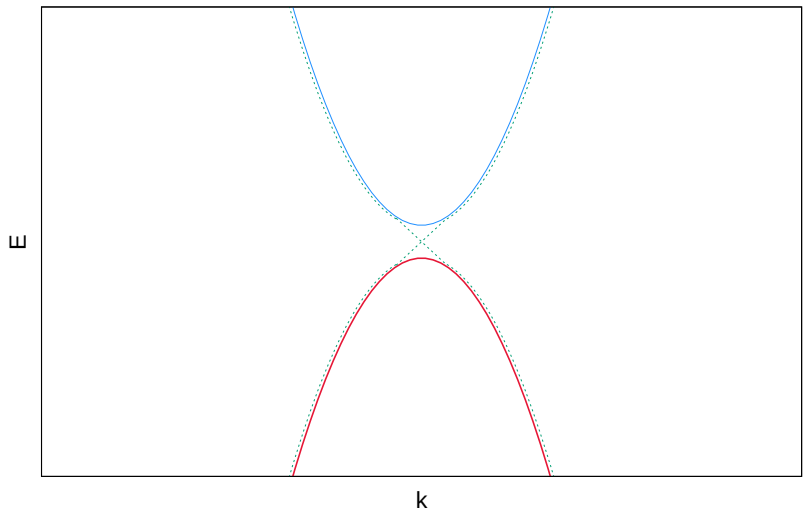

Figure 5: A "twist" between two bands renders the material topological non-trivial

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