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Problem 5.1: The Streda formula and the quantized Hall conductivity [**Oral** | 4 pt(s)]

ID: ex_hofstadter_model_Streda_formula_quantized_Hall_conductivity:tqp25

Learning objective

In Problem 4.1 you derived the Harper equation for the Hofstadter model which determines its spectrum and the eigenstates for a homogeneous magnetic field. The direct evaluation (first carried out by TKNN[a]) of the Chern numbers using the eigenstates is quite technical. Instead, in this exercise you derive the *Streda formula* and employ heuristic arguments to derive the Chern numbers and the quantized Hall conductivity for a general tight-binding model.

[a] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, "Quantized Hall Conductance in a Two-Dimensional Periodic Potential," Physical Review Letters, vol. 49, no. 6, pp. 405–408 (1982), doi:10.1103/physrevlett.49.405.

a) As a preliminary step, derive the *Streda formula*[1] for the Hall conductivity **1**pt(s)

$$\sigma_{xy} = \frac{\partial \rho}{\partial B}\,. \tag{1}$$

For a fixed position in space, the Streda formula relates the variation in *charge density* ρ to a change in the magnetic field B.

Hint: Use the continuity equation to relate the off-diagonal current response to the charge density. Then apply the Maxwell–Faraday law.

In the following, we consider a spinless *tight-binding model* [e.g. think of the Hofstadter model from Problem 4.1] on a two-dimensional square lattice $\mathcal{L}$ of size $L_x \times L_y$ with periodic boundary conditions. The number of unit cells in the i-th direction is denoted $N_i := L_i/a$ where a is the lattice constant. Additionally, we consider a perpendicular *homogeneous magnetic field* B.

The number of magnetic flux quanta through each plaquette is given by $\hat{\Phi} = \Phi/\Phi_0$, where $\Phi = Ba^2$ is the magnetic flux and $\Phi_0 = h/e$ is the quantum of flux. We assume that $\hat{\Phi} = \frac{p}{q} \in \mathbb{Q}_{\neq 0}$ is rational with p and $q > 0$ coprime integers. In Problem 4.1 you derived that this gives rise to *magnetic translation operators* that define an enlarged *magnetic unit cell* of size $aq \times a$. To preserve periodicity of the system, we assume that $N_x \in q\mathbb{N}$.

Bloch's theorem then yields the single-particle eigenstates in a contracted *magnetic Brillouin zone* $T^2 = [0, 2\pi/qa) \times [0, 2\pi/a)$. The q sites within a magnetic unit cell introduce additional degrees of freedom that yield q bands.

Our goal is to derive the Chern numbers of these bands using the Streda formula, and re-derive the quantization of the Hall conductivity via generic arguments[2]. To this end, we consider a generic

[1] P. Streda, "Theory of quantised Hall conductivity in two dimensions," J. Phys. C: Solid State Phys. 15, pp. 717–721 (1982), doi:10.1088/0022-3719/15/22/005

[2] I.e., without actually computing Chern numbers from Bloch functions as derived in the lecture. For this, we would first need to fix a model and solve for the eigenstates (e.g. the Harper equation in the Hofstadter model).

insulator where the Fermi level is in the r-th gap, i.e., there are $r \in \{0, \ldots, q\}$ filled bands below the Fermi level:

b) Use the Streda formula (1) to write the Hall conductivity in the form **1pt(s)**

$$\sigma_{xy} = \frac{e}{a^2}\partial_B(r/q)\,, \tag{2}$$

where r/q is the fraction of filled bands.

Hint: Express the charge within the magnetic unit cell via the number of filled bands.

Note: We assume that the density of states of the occupied bands r/q is a differentiable function of B.

A *linear Diophantine equation* is a linear equation with integer coefficients for which only integer solution are of interest. For three given integer parameters r, q and p, this is an equation of the form

$$r = qs_r + pt_r \tag{3}$$

in the two integer variables s_r and t_r. The subscript r indicates that the integers s_r and t_r depend on the value of r. The idea is to use the linear Diophantine equation to rewrite the integer quotient r/q in Eq. (2) in a more useful form:

c) Use the linear Diophantine equation (3) to derive the expression **2pt(s)**

$$\sigma_{xy} = \frac{e^2}{h}t_r \tag{4}$$

for the Hall conductivity. Then use the TKNN formula (derived in the lecture) to compute the Chern number $C^{[r]} = t_r - t_{r-1}$ of the r-th band with $t_0 = 0$ for $r = 0$.

Note: This result applies in particular to the Hofstadter model from Problem 4.1.

Concluding remarks

The solution space of the linear Diophantine equation (3) can be explicitly parametrized as

$$s_r = rq^{\varphi(p)-1} + pn \qquad \text{and} \qquad t_r = r\frac{1-q^{\varphi(p)}}{p} - qn \qquad \text{for} \qquad n \in \mathbb{Z}\,. \tag{5}$$

Here, $\varphi(p)$ denotes *Euler's totient function*[3] which counts the number of positive coprime integers that are smaller than p. $\varphi(p)$ varies wildly in the range $\{1, \ldots, p-1\}$ for different arguments $p \in \mathbb{N}_{\geq 2}$. Note that it is guaranteed that $s, t \in \mathbb{Z}$ thanks to Euler's totient theorem[4].

In Eq. (5), any two solutions of the linear Diophantine equation differ by an integer $\Delta t_r \in q\mathbb{Z}$. Therefore, to fix a unique solution t_r in expression (4), we can demand that $|t_r| \leq q/2$.

This choice can be motivated as follows:

(1) Mathematically, we can fix a specific model and just perform the rigorous calculation of the Chern numbers using the eigenstates. It can be shown that a quantized Hall conductance always implies the existence of a linear Diophantine equation which determines its value[5]. The direct calculation then yields the constraint $|t_r| \leq q/2$ for the solution of the linear Diophantine equation. This calculation is quite lengthy and not suited for an exercise sheet.

[3] In German: *Euler'sche Phi-Funktion*

[4] *Euler's totient theorem* states that if (and only if) $q, p \in \mathbb{N}$ are coprime, then $q^{\varphi(p)} = 1$ (mod p).

[5] B. A. Bernevig and T. L. Hughes, Topological Insulators and Topological Superconductors. Princeton University Press, 2013. [Section 5.3, pp. 50–51]

(2) Physically, there is Bragg scattering at the magnetic unit cell[6] which can generally yield negative Hall conductivities. Furthermore, for $r = 0$ it is $t_r = 0$. This makes $|t_r| \leq q/2$ the obvious choice.

The solutions t_r (and thereby the Chern numbers $C^{[r]}$) generally behave quite erratically for different bands r and magnetic fluxes p/q.

Note: To be precise, the constraint $|t_r| \leq q/2$ only fixes a unique solution for $r \neq q/2$. For q even with $r = q/2$, there is an ambiguity in the solution $t_r = \pm q/2$ for $s_r = (1 \mp p)/2$. In this case for $E = 0$ there are q zero nodes (Dirac nodes[7]) where the bands are degenerate [see Problem 4.2]. Thus in this case, the spectrum is actually not gapped and we cannot talk about the Hall conductivity of both bands separately. Depending on how this degeneracy is removed by perturbations, both $t_r = \pm q/2$ and even $t_r = 0$ is possible.

Problem 5.2: The Chern number as Skyrmion number

[**Written** | 6 pt(s)]

ID: ex_chern_number_skyrmion_number:tqp25

> **Learning objective**
>
> For the special case of two-band Bloch Hamiltonians, the expression for the Chern number can be interpreted as a winding number that counts how often the sphere S^2 is wrapped when traversing the Brillouin zone. This number counts the topological twists in the Bloch vector field on the Brillouin zone; these twists are known as *(Anti-)Skyrmions*. In this exercise, you derive the expression for the Chern number that leads to this interpretation.

Consider a translation invariant system in two dimensions. The most general *two-band Hamiltonian* is given by

$$H = \bigoplus_{\boldsymbol{k} \in T^2} \tilde{H}(\boldsymbol{k}) \qquad \text{where} \qquad \tilde{H}(\boldsymbol{k}) = \varepsilon(\boldsymbol{k})\mathbb{1} + \vec{d}(\boldsymbol{k}) \cdot \vec{\sigma} \tag{6}$$

is the *Bloch Hamiltonian*. Here $\varepsilon : T^2 \to \mathbb{R}$ and $\vec{d} : T^2 \to \mathbb{R}^3$ are some function on the Brillouin zone T^2 (= Torus) and σ_i for $i \in \{x, y, z\}$ are the Pauli matrices. We denote $d \equiv |\vec{d}|$ and $\hat{d} \equiv \vec{d}/d$.

The Bloch Hamiltonian possesses a ground state $|u_{\boldsymbol{k}}\rangle$ and an excited state $|v_{\boldsymbol{k}}\rangle$ with eigenenergies $E_\pm(\boldsymbol{k}) = \varepsilon(\boldsymbol{k}) \pm d(\boldsymbol{k})$, respectively. We assume the system to be gapped, in particular $\Delta E(\boldsymbol{k}) = 2d(\boldsymbol{k}) > 0$.

The expression for the *Chern number* of Bloch bands was derived in the lecture. For the lower band, it reads

$$C = \frac{i}{2\pi} \int_{T^2} \left\{ \left\langle \tilde{\partial}_y u_{\boldsymbol{k}} \middle| \tilde{\partial}_x u_{\boldsymbol{k}} \right\rangle - \left\langle \tilde{\partial}_x u_{\boldsymbol{k}} \middle| \tilde{\partial}_y u_{\boldsymbol{k}} \right\rangle \right\} \mathrm{d}^2 k \tag{7}$$

with $\tilde{\partial}_i \equiv \partial_{k_i}$.

The goal of this exercise is to convert this expression into a new form with a straightforward topological interpretation:

a) As a preliminary step, show that **1** pt(s)

[6] Fradkin, Eduardo. Field Theories of Condensed Matter Systems. Addison-Wesley Publishing Company, 1991. [Section 12.8, pp. 478]

[7] Wen, X. G., and A. Zee. "Winding number, family index theorem, and electron hopping in a magnetic field," Nuclear Physics B 316.3, p. 641–662 (1989), doi:10.1016/0550-3213(89)90062-X

$$\varepsilon_{ijk}\,\hat{d}_i(\tilde{\partial}_x\hat{d}_j)(\tilde{\partial}_y\hat{d}_k) = \varepsilon_{ijk}\,\frac{d_i(\tilde{\partial}_x d_j)(\tilde{\partial}_y d_k)}{d^3}\,. \tag{8}$$

b) Now show that **2**pt(s)

$$\left\langle v_{\boldsymbol{k}} \middle| \tilde{\partial}_x u_{\boldsymbol{k}} \right\rangle = \frac{\langle v_{\boldsymbol{k}}| \left[\tilde{\partial}_x H\right] |u_{\boldsymbol{k}}\rangle}{-2d(\boldsymbol{k})} \tag{9}$$

and use this to derive the expression for the Chern number

$$C = -\frac{1}{4\pi}\int_{T^2} \frac{\tilde{\partial}_y d_i \tilde{\partial}_x d_j}{d^2}\,\mathrm{Im}\left[\langle u_{\boldsymbol{k}}|\,\sigma^i\,|v_{\boldsymbol{k}}\rangle \langle v_{\boldsymbol{k}}|\,\sigma^j\,|u_{\boldsymbol{k}}\rangle\right]\,\mathrm{d}^2k\,. \tag{10}$$

Hint: Use that the Bloch functions $\{|u_{\boldsymbol{k}}\rangle\,, |v_{\boldsymbol{k}}\rangle\}$ for fixed $\boldsymbol{k}$ form a complete, orthonormal basis of $\mathcal{H}(\boldsymbol{k})$. You may use results from Problem 3.1.

c) Show that $\langle u_{\boldsymbol{k}}|\,\sigma^k\,|u_{\boldsymbol{k}}\rangle = -\hat{d}_k$ and use this to show that $\mathrm{Im}\left[\langle u_{\boldsymbol{k}}|\,\sigma^i\,|v_{\boldsymbol{k}}\rangle \langle v_{\boldsymbol{k}}|\,\sigma^j\,|u_{\boldsymbol{k}}\rangle\right] = -\varepsilon_{ijk}\hat{d}_k$. **3**pt(s)

Finally, using subtask a), derive the expression for the Chern number

$$C = -\frac{1}{4\pi}\int_{T^2} \hat{d}\cdot\left(\tilde{\partial}_x\hat{d}\times\tilde{\partial}_y\hat{d}\right)\,\mathrm{d}^2k\,. \tag{11}$$

Why is this an integer?

Identify the Berry curvature $\mathcal{F}_{xy}(\boldsymbol{k})$.

Hint: Use that $\vec{\sigma}$ is a vector-operator to show that the term $\langle u_{\boldsymbol{k}}|\,\vec{\sigma}\,|u_{\boldsymbol{k}}\rangle$ is a unit vector.

Geometrically, the *Berry curvature* in Eq. (11) is just the Jacobian for the (oriented) surface integral over the sphere S^2. The *Chern number* then counts how often $\hat{d}(\boldsymbol{k})$ covers S^2 when sweeping $\boldsymbol{k}$ over the Brillouin zone T^2.

In the lecture, you used this picture to motivate the interpretation of the Chern number and the Berry curvature in terms of a total *Skyrmion number* and a *Skyrmion density*, respectively. Skyrmions (after Tony Skyrme) are the localized "twists" or "knots" of $\hat{d}$ that live on the Brillouin zone. The total Skyrmion number C (counting Antiskyrmions negative) is then a topological invariant.

Problem 5.3: The Berry curvature of Dirac Hamiltonians

[**Oral** | 2 pt(s)]

ID: ex_berry_curvature_dirac_hamiltonians:tqp25

Learning objective

In the lecture, we identified Dirac Hamiltonians as useful tools to study *changes* in Chern numbers. Here you derive a simple expression for the integral of the Berry curvature of a general Dirac Hamiltonian over its (non-compact) momentum space $\mathbb{R}^2$.

Consider a general gapped *Dirac Hamiltonian*

$$H_D(\boldsymbol{k}) = \sum_{i,j=1}^{2} k_i h_{ij} \sigma^j + h_z \sigma^z \,, \tag{12}$$

linear in $\boldsymbol{k} \in \mathbb{R}^2$ with $h \in \mathbb{R}^{2\times 2}$ and "mass" $h_z \neq 0$.

Show that the integral of the Berry curvature for the lower band yields

$$C = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \mathcal{F}_{xy} \, \mathrm{d}^2 k = -\frac{\mathrm{sign}[h_z]\, \mathrm{sign}[\det(h)]}{2} \,. \tag{13}$$

Hint: Make the linear substitution $\boldsymbol{k}' = h^T \boldsymbol{k}$ and use the result derived in Problem 5.2. Why can you do this?