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Problem 4.1: The Hofstadter model and the magnetic Brillouin zone [**Written** | 10 pt(s)]

ID: ex_hofstadter_model_magnetic_brillouin_zone:tqp25

Learning objective

The Hofstadter model[a] (Douglas R. Hofstadter[b], 1976) is an exactly solvable model of non-interacting fermions hopping on a square lattice in a magnetic field. It is a toy model for the integer quantum Hall effect as it features topological bands with non-zero Chern numbers and a quantized Hall response. In this exercise you study this model analytically.

[a] D. R. Hofstadter, "Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields," Physical Review B, Vol. 14, No. 6 (1976), doi:10.1103/physrevb.14.2239.
[b] Hofstadter is quite an unconventional scientist. To the public he is best known for his Pulitzer Prize winning book *"Gödel, Escher, Bach: An Eternal Golden Braid"*; an inspiring read on a wide span of topics such as (in)completeness in mathematics, computability and the problem of (self-)consciousness.

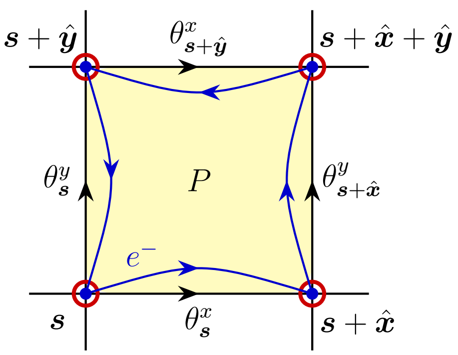
Consider a two-dimensional square lattice $\mathcal{L}$ of size $L_x \times L_y$ and lattice constant a with periodic boundary conditions. The number of unit cells in the i-th direction is denoted $N_i := L_i/a$. Let $\hat{\boldsymbol{x}} = (a,0)^T$ and $\hat{\boldsymbol{y}} = (0,a)^T$ denote the lattice vectors in x- and y-direction, respectively.

We now place a fermion mode $c_{\boldsymbol{s}}^{(\dagger)} \equiv c_{m,n}^{(\dagger)}$ on each site $\boldsymbol{s} = a(m,n)^T$ with coordinates $m \in \{1,\dots,N_x\}$ and $n \in \{1,\dots,N_y\}$. In addition, we consider a two-component background gauge field $\boldsymbol{A} : \mathbb{R}^2 \to \mathbb{R}^2$ that gives rise to the perpendicular magnetic field $B := \partial_x A_y - \partial_y A_x$.

The phase accumulated by a charged particle that hops from site $\boldsymbol{s}$ to an adjacent site $\boldsymbol{s}+\hat{\boldsymbol{i}}$ is then

$$\theta_{\boldsymbol{s}}^i := \frac{e}{\hbar}\int_{\boldsymbol{s}}^{\boldsymbol{s}+\hat{\boldsymbol{i}}} \boldsymbol{A}(\boldsymbol{x})\cdot \mathrm{d}\boldsymbol{x} \qquad \text{for} \qquad i \in \{x,y\}\,. \tag{1}$$

Geometrically, one should think of $\theta_{\boldsymbol{s}}^i \equiv \theta_{mn}^i$ for $i = x$ ($i = y$) as living on the horizontal (vertical) edges between $\boldsymbol{s}$ and $\boldsymbol{s}+\hat{\boldsymbol{i}}$:



In this setting, the tight-binding Hamiltonian of the *Hofstadter model* describes charged, spinless fermions hopping on $\mathcal{L}$:

$$H = -t\sum_{\boldsymbol{s}\in\mathcal{L}}\left[e^{i\theta_{\boldsymbol{s}}^x}c_{\boldsymbol{s}+\hat{\boldsymbol{x}}}^\dagger c_{\boldsymbol{s}} + e^{i\theta_{\boldsymbol{s}}^y}c_{\boldsymbol{s}+\hat{\boldsymbol{y}}}^\dagger c_{\boldsymbol{s}}\right] + \text{h.c.} \tag{2}$$

a) To build trust in the Hamiltonian (2), consider an electron e^- that hops anti-clockwise around a plaquette P (blue path in the sketch above). Show that the electron accumulates a phase **1pt(s)**

$$\gamma = 2\pi \frac{\Phi_P}{\Phi_0}\,, \tag{3}$$

where Φ_P is the magnetic flux through P and $\Phi_0 = h/e$ denotes the quantum of flux.

Note: This describes exactly the *Aharonov-Bohm phase* that an electron picks up when moving around a magnetic flux, and makes Eq. (2) a reasonable discretization for charged particles in a magnetic field.

In the following, we consider a *homogeneous magnetic field* B and choose the Landau gauge:

$$A_x = 0 \qquad \text{and} \qquad A_y = Bx\,. \tag{4}$$

The (constant[1]) number of magnetic flux quanta through each plaquette is denoted by $\hat{\Phi} = \Phi/\Phi_0$.

b) Show that the Hamiltonian (2) can be written in this gauge in the form **1pt(s)**

$$H = -t \sum_{m,n} \left[c^\dagger_{m+1,n} c_{m,n} + e^{i2\pi\hat{\Phi}m} c^\dagger_{m,n+1} c_{m,n} \right] + \text{h.c.} \tag{5}$$

Since the Hamiltonian (5) is quadratic in fermion operators, the fermions are not interacting. Consequently, the many-body spectrum of the Hamiltonian is completely determined by the spectrum in the single-particle sector of Fock space. In the following, we will therefore restrict our analysis to *single-particle states.*

Note that the Hamiltonian (5) is generally *not translation invariant* in x-direction! This begs the questions how this Hamiltonian can be diagonalized and whether a Brillouin zone can still be defined (which would be needed to compute Chern numbers and the Hall response).

To make progress, we define generic *translation operators* on the single-particle sector of Fock space:

$$\hat{T}_j := \sum_{\boldsymbol{s}\in\mathcal{L}} e^{i\chi^j_{\boldsymbol{s}}}\, c^\dagger_{\boldsymbol{s}+\hat{\boldsymbol{j}}} c_{\boldsymbol{s}} \qquad \text{for} \qquad j \in \{x, y\}\,. \tag{6}$$

Here $\chi^j_{\boldsymbol{s}} \equiv \chi^j_{m,n}$ are yet undetermined functions.

c) To construct a Brillouin zone, the translation operators should be symmetries of the Hamiltonian: **2pt(s)**

$$\left[H, \hat{T}_j\right] \stackrel{!}{=} 0 \qquad \text{for} \qquad j \in \{x, y\}\,. \tag{7}$$

Show that the choice $\chi^j_{mn} := 2\pi\delta_{j,x}\hat{\Phi}\, n$ solves this condition in Landau gauge.

Hint: For single-particle operators, it is sufficient to show that they commute in the single-particle sector of Fock space.

The operators $\hat{T}_j$ with the property Eq. (7) are known as *magnetic translation operators.*

d) Show that the magnetic translation operators fulfill the *magnetic translation algebra* **1pt(s)**

$$\hat{T}_x \hat{T}_y = e^{2\pi i\hat{\Phi}} \hat{T}_y \hat{T}_x \tag{8}$$

within the single-particle sector (i.e., they do *not* commute in general).

[1] As $\hat{\Phi}_P$ is the same for each plaquette, we drop the index P in the following.

We need *two* independent conserved momenta as good quantum numbers to label the eigenstates in the Brillouin zone. The translation operators that realize the corresponding symmetry therefore must *commute* (to diagonalize them simultaneously). However, due to the magnetic translation algebra (8), the magnetic translation operators obtain a phase factor $e^{2\pi i\hat{\Phi}}$ when commuted!

To fix this problem, we define the new translation operators $\hat{T}_j^{n_j}$ for some integers $n_j \in \mathbb{N}$, which describe a translation by $n_j \cdot \hat{\boldsymbol{j}}$ on the lattice.

e) Show that whenever $\hat{\Phi} \in \mathbb{Q}$ is a *rational number*, there exist $n_x, n_y \in \mathbb{N}$ such that **1**pt(s)

$$\left[\hat{T}_x^{n_x}, \hat{T}_y^{n_y}\right] = 0\,. \tag{9}$$

Solutions $n_x, n_y \in \mathbb{N}$ with the smallest product $n_x \cdot n_y$ define a *magnetic unit cell*.

What is the size of the magnetic unit cell?

Hint: Every non-zero rational number $\hat{\Phi} \in \mathbb{Q}$ can be uniquely expressed as $\hat{\Phi} = p/q$ with p and $q > 0$ *coprime* integers.

For $\hat{\Phi} = p/q$ with p and $q > 0$ coprime integers, we can choose $n_x = q$ and $n_y = 1$ without loss of generality. Then the magnetic unit cell comprises q of the original unit cells in x-direction and one unit cell in y-direction, i.e., the magnetic unit cell is of size $qa \times a$. This enlarged unit cell restores translation invariance of the Hamiltonian at the price of more degrees of freedom per unit cell. To keep the periodicity of the system, we assume a size $L_x \in q\mathbb{N}$ in x-direction in the following.

We can now invoke *Bloch's theorem* to characterize the single-particle eigenstates $|\boldsymbol{k}\rangle \equiv |k_x, k_y\rangle$ of H as simultaneous eigenstates of $\hat{T}_x^q$ and $\hat{T}_y$:

$$H\,|\boldsymbol{k}\rangle = E(\boldsymbol{k})\,|\boldsymbol{k}\rangle\;, \qquad \hat{T}_x^q\,|\boldsymbol{k}\rangle = e^{ik_x qa}\,|\boldsymbol{k}\rangle\;, \qquad \hat{T}_y\,|\boldsymbol{k}\rangle = e^{ik_y a}\,|\boldsymbol{k}\rangle\;. \tag{10}$$

The momenta are periodic and define the *magnetic Brillouin zone* T^2 with $k_x \in [0, 2\pi/qa)$ and $k_y \in [0, 2\pi/a)$. Note that this Brillouin zone is contracted by a factor of $1/q$ in k_x-direction!

f) Show that every eigenenergy $E = E(\boldsymbol{k})$ is (at least) q-fold degenerate. **1**pt(s)

Hint: Use $\hat{T}_x$ to construct q linearly independent states with the same energy.

g) To (partially) diagonalize the system, insert the *single-particle wave function* $|\Psi\rangle = \sum_{\boldsymbol{s}\in\mathcal{L}} \Psi_{\boldsymbol{s}} c_{\boldsymbol{s}}^\dagger\,|0\rangle$ with coefficients $\Psi_{\boldsymbol{s}} \equiv \Psi_{m,n} \in \mathbb{C}$ into the time-independent Schrödinger equation for the Hamiltonian (5). Derive a coupled system of linear equations for the coefficients $\Psi_{m,n}$. **3**pt(s)

To solve this equation, use a *discrete Fourier transform* on the magnetic Brillouin zone,

$$\tilde{\Psi}_r(k_x, k_y) := \sum_{m,n} e^{-i(k_x a + 2\pi\hat{\Phi}r)m - ik_y na}\,\Psi_{m,n}\;, \tag{11}$$

with $\boldsymbol{k} \in T^2$ and $r \in \{0, \ldots, q-1\}$ (show that this is bijective!).

Show that the eigenvalue problem becomes the *Harper equation*

$$-2t\cos\left(k_x a + 2\pi\hat{\Phi}r\right)\tilde{\Psi}_r(\boldsymbol{k}) - t\left[e^{ik_y a}\tilde{\Psi}_{r+1}(\boldsymbol{k}) + e^{-ik_y a}\tilde{\Psi}_{r-1}(\boldsymbol{k})\right] = E(\boldsymbol{k})\tilde{\Psi}_r(\boldsymbol{k})\,, \tag{12}$$

which is a system of q coupled linear equations.

Hint: Show that the *inverse Fourier transform* reads

$$\Psi_{m,n} = \frac{1}{L_x L_y} \sum_{r=0}^{q-1} \sum_{\boldsymbol{k} \in T^2} e^{i(k_x a + 2\pi \hat{\Phi} r)m + i k_y n a} \, \tilde{\Psi}_r(k_x, k_y) \,, \tag{13}$$

given that $\hat{\Phi} = p/q$ with p and $q > 0$ coprime integers.

The Harper equation determines the spectrum and eigenstates of the Hamiltonian (2) for a homogeneous magnetic field with $\hat{\Phi} = p/q$ flux quanta per unit cell. The index $r \in \{0, \ldots, q-1\}$ takes into account the q sites within a single magnetic unit cell, i.e., there are q bands. Solving Eq. (12) is best done numerically (which you will do in Problem 4.2).

With the eigenstates of the r-th band at hand, you could now apply the TKNN formula introduced in the lecture to compute the Chern number $C^{[r]}$ and the corresponding Hall conductivity σ_{xy} directly. This calculation was first carried out by Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) in their famous 1982 paper[2]. However, the full derivation is quite technical, so we will not pursue it here. If you are interested in the details, have a look at the textbook by Eduardo Fradkin [3] or the textbook by Andrei Bernevig [4].

Instead, on the next problem set, we choose a different approach: using on the Streda formula we are going to (heuristically) derive the Chern numbers and the quantized Hall conductivity by employing high-level arguments for a general tight-binding model.

[2]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.

[3] Fradkin, Eduardo. Field Theories of Condensed Matter Systems. Addison-Wesley Publishing Company, 1991. [Section 9.8, pp. 287–292]

[4]B. A. Bernevig and T. L. Hughes, Topological Insulators and Topological Superconductors. Princeton University Press, 2013. [Section 5.4, pp. 51–59]

Problem 4.2: Hofstadter bands and Hofstadter butterfly (Numerics) [**Oral** | 6 pt(s)]

ID: ex_hofstadter_model_numerics:tqp25

Learning objective

In Problem 4.1 you studied the physics of charged fermions hopping on a square lattice in a perpendicular magnetic field (the *Hofstadter model*). As final result, you obtained the *Harper equation* which determines the spectrum of the Hofstadter Hamiltonian on a lattice with periodic boundaries. In this exercise, you solve the Harper equation numerically to compute the topological bands. You will find a remarkable spectrum with fractal structure known as the *Hofstadter butterfly*.

We assume a homogeneous magnetic field with $\hat{\Phi} = p/q$ flux quanta per unit cell, where p and $q > 0$ are coprime integers. As derived in Problem 4.1, the eigenvalue problem of the Hofstadter model is given by the *Harper equation*

$$-2\cos\left(k_x a + 2\pi\hat{\Phi}r\right)\tilde{\Psi}_r(\boldsymbol{k}) - \left[e^{ik_y a}\tilde{\Psi}_{r+1}(\boldsymbol{k}) + e^{-ik_y a}\tilde{\Psi}_{r-1}(\boldsymbol{k})\right] = \tilde{E}(\boldsymbol{k})\tilde{\Psi}_r(\boldsymbol{k})\,. \tag{14}$$

For every $\boldsymbol{k} = (k_x, k_y)^T \in T^2$ in the magnetic Brillouin zone, this is a system of q coupled linear equations in $\tilde{\Psi}_r(\boldsymbol{k})$, where the index $r \in \{1, \ldots, q\}$ (counted modulo q) corresponds to the q bands. Here $\tilde{E}(\boldsymbol{k}) \equiv E(\boldsymbol{k})/t$ is the eigenenergy in units of the hopping strength t.

To compute the spectrum of the theory (i.e., the q values of $\tilde{E}(\boldsymbol{k})$ for each $\boldsymbol{k}$ such that non-trivial solutions $\tilde{\Psi}_r(\boldsymbol{k})$ exist), we consider finite but large system sizes $N_i \approx 100$ such that the discrete steps between momenta $\Delta k_i a = 2\pi/N_i < 0.1$ are small (to produce smooth plots):

a) Use your favorite programming language to implement and solve the Harper Eq. (14) numerically. 4pt(s)

   Study the spectrum for fluxes $\hat{\Phi} \in \left\{\frac{1}{2}, \frac{1}{3}, \frac{2}{3}, \frac{1}{4}, \frac{1}{5}, \frac{2}{5}\right\}$ by plotting the eigenenergies $\tilde{E}(\boldsymbol{k})$ over the magnetic Brillouin zone $\boldsymbol{k} \in T^2$ (in a 3D plot).

   Are the bands always fully gapped?

   For which flux do you find bands that resemble Landau levels most closely?

The bands you plotted are known as *Hofstadter bands*, they are the lattice analogue of Landau levels.

b) Compute the spectrum as a function of the magnetic flux for many (> 100) rational values $\hat{\Phi} \in \mathbb{Q}_{[0,1]}$. Draw a black dot with coordinates $(\hat{\Phi}, E)$ for every eigenvalue E. 2pt(s)

   Try to identify the bands that you plotted in a).

   What happens for $\hat{\Phi} > 1$?

The spectrum you plotted as a function of magnetic flux quanta per unit cell is a fractal known as *Hofstadter's Butterfly*. Its fractal structure is rooted in the fact that in the neighbourhood of every rational flux $\hat{\Phi} = p/q$ there are other rational values with arbitrarily large denominator q (= numbers of bands).

Fun fact: Hofstadter discussed this spectrum in his famous book *Gödel, Escher, Bach*.