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Problem 1: The Hofstadter model and the magnetic Brillouin zone

Learning objective

The Hofstadter model is an exactly solvable model of non-interacting fermions hopping on a square lattice in a magnetic field, originally introduced and studied by Douglas Hofstadter[a]. It can be seen as a toy model for the integer quantum Hall effect as it features topological bands with non-zero Chern numbers and a quantized Hall response. Here you study this model analytically and numerically.

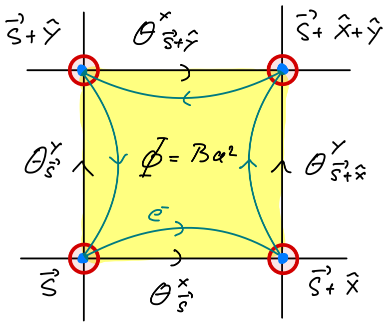
[a] D. R. Hofstadter, "Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields," Physical Review B, vol. 14, no. 6, Art. no. 6, Sep. 1976, doi: 10.1103/physrevb.14.2239. [Hofstadter is a quite unconventional scientist; to the public, he is best known for his Pulitzer 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 square lattice $\mathcal{L}$ of size $L_x \times L_y$ with periodic boundary conditions and lattice constant a; the number of unit cells in i-direction is $N_i = L_i/a$. We place a fermion mode $c_{\boldsymbol{s}}^{(\dagger)} = c_{m,n}^{(\dagger)}$ on each vertex $\boldsymbol{s} = (m,n)a$ with coordinates $m = 1,\dots,N_x$ and $n = 1,\dots,N_y$. Let $\hat{\boldsymbol{x}} = (a,0)$ and $\hat{\boldsymbol{y}} = (0,a)$ denote the lattice vectors in x- and y-direction.

In addition, we consider a two-component background gauge field $A_i(\boldsymbol{x}) \in \mathbb{R}$ on $\boldsymbol{x} \in \mathbb{R}^2$ with $i = x,y$. The phase accumulated by a particle that is coupled to this gauge field and hops to an adjacent site is then

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

Geometrically, one should think of $\theta_{\boldsymbol{s}}^x = \theta_{mn}^x$ ($\theta_{\boldsymbol{s}}^y = \theta_{mn}^y$) living on the horizontal (vertical) edges between $\boldsymbol{s} = (m,n)a$ and $\boldsymbol{s}+\hat{\boldsymbol{x}} = (m+1,n)a$ [$\boldsymbol{s}+\hat{\boldsymbol{y}} = (m,n+1)a$]:



Then the tight-binding Hamiltonian for charged, spinless fermions hopping on $\mathcal{L}$ is given by

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

a) To build trust in Eq. (2), show that the accumulated phase $e^{i\gamma}$ of an electron that hops anti-clockwise around a plaquette (see sketch above) is given by

$$\gamma = 2\pi\frac{Ba^2}{h/e} = 2\pi\frac{\Phi}{\Phi_0} = 2\pi\hat{\Phi} \quad \text{with magnetic field} \quad B := \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\,. \tag{3}$$

This describes exactly the Aharonov-Bohm phase that an electron picks up when moving around the magnetic flux $\Phi = Ba^2$ ($\Phi_0 = h/e = 2\pi\hbar/e$ denotes the quantum of flux, $\hat{\Phi}$ is the magnetic flux per plaquette in units of flux quanta).

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

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

b) Show that the Hamiltonian can now be written as

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

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

c) To this end, define the generic translation operators

$$\hat{T}_x = \sum_{m,n} e^{i\chi^x_{mn}}\,c^\dagger_{m+1,n}c_{m,n} \quad \text{and} \quad \hat{T}_y = \sum_{m,n} e^{i\chi^y_{mn}}\,c^\dagger_{m,n+1}c_{m,n} \tag{6}$$

where χ^x_{mn} and χ^y_{mn} are functions to be determined.

To construct a Brillouin zone, we would like these to be symmetries of the Hamiltonian:

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

Show that the choice $\chi^x_{mn} = 2\pi\hat{\Phi}n$ and $\chi^y_{mn} = 0$ solves this condition in the Landau gauge.

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

d) Show that the magnetic translation operators do in general *not* commute but rather

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

This is known as the *magnetic translation algebra.*

e) To construct a Brillouin zone we need *two* independent conserved momenta (“good quantum numbers”). The corresponding translation operators therefore *must* commute—and Eq. (8) is a problem! To solve this, define the new translation operators $\hat{T}_j^{n_j}$ for some integers $n_j \in \mathbb{N}$; these describe translations by n_j lattice vectors in direction j.

Show that whenvever $\hat{\Phi} = p/q$ is a rational number (where p and q are coprime), there are n_x and n_y such that

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

The smallest integers n_x, n_y that solve this equation define the *magnetic unit cell* which restores translational invariance of the Hamiltonian (but with more degrees of freedom per unit cell).

For $\hat{\Phi} = p/q$, we choose $n_x = q$ and $n_y = 1$. Then we can invoke Bloch's theorem to characterize the eigenstates $|\boldsymbol{k}\rangle = |k_x, k_y\rangle$ of H as simultaneous eigenstates of H, $\hat{T}_x^q$ and $\hat{T}_y$ with

$$H|\boldsymbol{k}\rangle = E(\boldsymbol{k})|\boldsymbol{k}\rangle \ , \quad \hat{T}_x^q|\boldsymbol{k}\rangle = e^{iqak_x}|\boldsymbol{k}\rangle \ , \quad \hat{T}_y|\boldsymbol{k}\rangle = e^{iak_y}|\boldsymbol{k}\rangle \tag{10}$$

where the momenta are periodic and define the *magnetic Brillouin zone* T^2 with

$$-\frac{\pi}{qa} < k_x \leq \frac{\pi}{qa} \quad \text{and} \quad -\frac{\pi}{a} < k_y \leq \frac{\pi}{a} \,. \tag{11}$$

Note that this Brillouin zone is contracted by a factor of $1/q$ in k_x-direction. In the following, we set $a = 1$ to simplify the notation.

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

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

g) Finally, let us compute these eigenenergies. To this end, let the system be periodic in both directions with extension $L_x \in q\mathbb{N}$ in x-direction and $L_y \in \mathbb{N}$ in y-direction. (Remember that the magnetic unit cell comprises q of the original unit cells in x-direction and 1 in y-direction.)

To diagonalize the system, insert the single particle wavefunction

$$|\Psi\rangle = \sum_{m=1}^{L_x}\sum_{n=1}^{L_y} \Psi_{m,n} c_{m,n}^\dagger |0\rangle \quad \text{with} \quad \Psi_{m,n} \in \mathbb{C} \tag{12}$$

into the time-independent Schrödinger equation for Eq. (5) and derive a coupled system of linear equations for the coefficients $\Psi_{m,n}$.

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

$$\tilde{\Psi}_r(k_x, k_y) := \sum_{m,n} e^{-i(k_x + 2\pi\hat{\Phi}r)m - ik_y n}\,\Psi_{m,n} \quad \text{with } k_x \in [0, 2\pi/q),\ k_y \in [0, 2\pi) \tag{13}$$

and where the index $r = 0, \dots, q-1$ takes into account the q sites within a single magnetic unit cell.

Then the inverse Fourier transform reads (use $\hat{\Phi} = p/q$ with p and q coprime to check this!)

$$\Psi_{m,n} = \frac{1}{L_x}\sum_{r=0}^{q-1}\sum_{k_x=0}^{2\pi/q}\frac{1}{L_y}\sum_{k_y=0}^{2\pi} e^{i(k_x+2\pi\hat{\Phi}r)m + ik_y n}\,\tilde{\Psi}_r(k_x, k_y)\,. \tag{14}$$

Show that with this transformation, the eigenvalue equation becomes a system of q coupled linear equations,

$$-2t\cos\left(k_x + 2\pi\hat{\Phi}r\right)\tilde{\Psi}_r(\boldsymbol{k}) - t\left[e^{ik_y}\tilde{\Psi}_{r+1}(\boldsymbol{k}) + e^{-ik_y}\tilde{\Psi}_{r-1}(\boldsymbol{k})\right] = E(\boldsymbol{k})\tilde{\Psi}_r(\boldsymbol{k}) \tag{15}$$

known as the *Harper equation*; it determines the spectrum of Eq. (2) for a homogeneous magnetic field with $\hat{\Phi} = p/q$ flux per unit cell.

With the Harper equation, you can compute the spectrum of the theory as a function of the magnetic flux $\hat{\Phi} = \Phi/\Phi_0$ per unit cell by solving the q-dimensional system of equations for discrete momenta on the magnetic Brillouin zone (i.e., for a finite system of size $L_x \times L_y$).

h) Use your favourite programming language (`C++`, `Python`, `Julia`, `Mathematica`, `Matlab`, ...) to implement and solve the Harper equation Eq. (15) numerically for given flux $\hat{\Phi} = p/q$ (set $t = 1$). Study the spectrum for $\hat{\Phi} = \frac{1}{2}, \frac{1}{3}, \frac{2}{3}, \frac{1}{4}, \frac{1}{5}, \frac{2}{5}$ in the limit of large systems ($\Delta k_i < 0.1$) by plotting the eigenenergies $E(\boldsymbol{k})$ as functions of $\boldsymbol{k} = (k_x, k_y)$ over the magnetic Brillouin zone in a 3D plot. The emerging bands, known as *Hofstadter bands*, are the lattice analogue of Landau levels.

i) Compute the spectrum as a function of magnetic flux for many (> 100) rational values in the range $0 \leq \hat{\Phi} \leq 1$ (what happens for $\hat{\Phi} > 1$?). Draw a black dot with coordinates $(\hat{\Phi}, E)$ for every eigenvalue E. The resulting picture is a fractal known as the *Hofstadter Butterfly*. Try to identify the bands that you plotted in h) in the Butterfly.

With the magnetic Brillouin zone at hand (for rational magnetic flux per unit cell), you are now prepared to compute the Chern numbers C_r for each of the q bands. However, since this exercise is already long enough (and the evaluation of C_r is far from trivial), we only state the result. If you are interested in the details, have a look at the original paper by TKNN[1] or (better *and*) the textbook by Eduardo Fradkin[2]; a very detailed account is also provided in the textbook by Andrei Bernevig[3].

To compute the Chern number of the rth band, one has to find integer solutions $(s_r, t_r) \in \mathbb{Z}^2$ to the *linear Diophantine equation*

$$r = qs_r + pt_r \,. \tag{16}$$

Since p and q are coprime (their greatest common divisor is 1), a unique solution with $|t_r| \leq q/2$ is guaranteed to exist (this is a well-known result in number theory). It can then be shown that

$$C_r = t_r - t_{r-1} \quad \text{with} \quad t_0 := 0 \,. \tag{17}$$

Using the TKNN formula derived in the lecture for a Fermi energy E_F that lies in the gap between bands r and $r+1$, the quantized Hall conductivity of the Hofstadter model is then simply (telescoping series!)

$$\sigma_{xy} = \frac{e^2}{2\pi\hbar} t_r \tag{18}$$

where r is the index of the last filled band. Note that the solutions $t_r \in \mathbb{Z}$ for $r = 1, 2, 3, \ldots$ are typically quite erratic, positive and negative integers (if you are in doubt, check this for a few fractions p/q).

[1] 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.

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

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