Hofstadter physics (v2)

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May 30, 2025

Contents

1 Lattice in magnetic field

For a general 2D lattice with unit vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ (we set $\boldsymbol{a}_2 = a_2\boldsymbol{e}_y$ and $a_{1x} > 0$) and reciprocal basis vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$ ($\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$), the Hamiltonian can be written as

$$H(\boldsymbol{p}, \boldsymbol{r}) = T(\boldsymbol{p}) + V(\boldsymbol{r}), \tag{1}$$

where $T(\boldsymbol{p})$ is the kinetic energy, and $V(\boldsymbol{r})$ is the periodic potential satisfying $V(\boldsymbol{r}) = V(\boldsymbol{r} + n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2)$ for any integers n_1, n_2. The Hamiltonian has the lattice translation symmetry $[H(\boldsymbol{p}, \boldsymbol{r}), e^{-i\boldsymbol{p}\cdot\boldsymbol{a}_i/\hbar}] = 0$.

Now under magnetic field $\boldsymbol{B} = -B\boldsymbol{e}_z$, the Hamiltonian becomes

$$H(\boldsymbol{p} + e\boldsymbol{A}) = T(\boldsymbol{\pi}) + V(\boldsymbol{r}), \tag{2}$$

where $\boldsymbol{A}$ is the vector potential, $\boldsymbol{\pi} = \boldsymbol{p} + e\boldsymbol{A}$. In calculations we choose the Landau gauge: $\boldsymbol{A} = -Bx\boldsymbol{e}_y$. The vector potential breaks the usual translation symmetry, but we still can find two magnetic translation operators $t(\boldsymbol{a}_i)$ so that $[H(\boldsymbol{\pi}, \boldsymbol{r}), t(\boldsymbol{a}_i)] = 0$. The two operators are

$$t(\boldsymbol{a}_1) = e^{-i\boldsymbol{\pi}'\cdot\boldsymbol{a}_1/\hbar}, \quad t(\boldsymbol{a}_2) = e^{-i\boldsymbol{\pi}'\cdot\boldsymbol{a}_2/\hbar} = e^{-i\boldsymbol{p}\cdot\boldsymbol{a}_2/\hbar}. \tag{3}$$

where $\boldsymbol{\pi}' = \boldsymbol{\pi} - e\boldsymbol{B}\times\boldsymbol{r}$. Although $t(\boldsymbol{a}_i)$ commute with H, they do not commute with each other: $t(\boldsymbol{a}_1)t(\boldsymbol{a}_2) = \exp(i2\pi\phi/\phi_0)t(\boldsymbol{a}_2)t(\boldsymbol{a}_1)$, where $\phi = a_{1x}a_2B$ is the magnetic flux in a unit cell and $\phi_0 = h/e$ is the flux quantum. We consider the case $\phi/\phi_0 = p/q$, where p and q are co-prime integers, we then have

$$[t(\boldsymbol{a}_1), t^q(\boldsymbol{a}_2)] = 0. \tag{4}$$

So the Hilbert space of H can be classified according to eigenvalues of $t(\boldsymbol{a}_1)$ and $t^q(\boldsymbol{a}_2)$.

2 Landau levels as basis

If $V(\boldsymbol{r})$ is absent, the problem is the traditional Landau level (LL) problem. In this case we only need to diagonalize $T(\boldsymbol{\pi})$. The torus system can be viewed as a magnetic lattice with $N_\phi = N_1 \times N_2$ sites ($N_\phi = A/(2\pi l_B^2)$ is the LL degeneracy) and lattice vectors $\boldsymbol{m}_1, \boldsymbol{m}_2$ ($\boldsymbol{m}_2 = m_2 \boldsymbol{e}_y$, $m_{1x} > 0$). The Bloch LLs are (see the note "Landau level formulation")

$$\begin{aligned} |\psi_{n,\boldsymbol{k}}\rangle =& \frac{e^{-i\pi k_2^2 m_{1y}/m_2}}{\sqrt{N_1 N_t}} \sum_{s=0}^{N_1-1} \sum_{l\in\mathbb{Z}} e^{i2\pi(s+lN_1)k_1} t^{s+lN_1}(\boldsymbol{m}_1)|\varphi_{n,\frac{2\pi}{m_2}k_2}\rangle \\ =& \frac{1}{\sqrt{N_1 N_t}} \sum_{s\in\mathbb{Z}} e^{is2\pi k_1} e^{-i\pi\frac{m_{1y}}{m_2}(k_2+s)^2} |\varphi_{n,\frac{2\pi}{m_2}(k_2+s)}\rangle, \end{aligned} \tag{5}$$

where $\boldsymbol{k} = k_1\boldsymbol{g}_1 + k_2\boldsymbol{g}_2 \in$MBZ (magnetic Brillouin zone, $k_1, k_2 \in [0,1)$), $|\varphi\rangle$ are LLs on the cylinder, and $\boldsymbol{g}_i$ are magnetic reciprocal vectors ($\boldsymbol{g}_i \cdot \boldsymbol{m}_j = 2\pi\delta_{ij}$). Each magnetic unit cell has area $2\pi l_B^2$. The Bloch LLs are eigenstates of magnetic translations

$$t(\boldsymbol{m}_1)|\psi_{n,\boldsymbol{k}}\rangle = e^{-i2\pi k_1}|\psi_{n,\boldsymbol{k}}\rangle, \quad t(\boldsymbol{m}_2)|\psi_{n,\boldsymbol{k}}\rangle = e^{-i2\pi k_2}|\psi_{n,\boldsymbol{k}}\rangle. \tag{6}$$

The plane wave matrix element under such basis is ($\boldsymbol{q} = q_1\boldsymbol{g}_1 + q_2\boldsymbol{g}_2$)

$$\langle n', \boldsymbol{k}'|e^{i\boldsymbol{q}\cdot\boldsymbol{r}}|n, \boldsymbol{k}\rangle = \delta_{k_1',[k_1+q_1]}\delta_{k_2',[k_2+q_2]} e^{i2\pi k_1'(k_2'-k_2-q_2)} e^{i2\pi q_1\left(k_2+\frac{q_2}{2}\right)} F_{n'n}\left(\frac{q_x+iq_y}{\sqrt{2}}l_B\right), \tag{7}$$

where $[k_i]$ represents the fractional part of k_i, and (L_n^α is the associated Laguerre polynomial)

$$F_{n'n}(Q) = \begin{cases} e^{-\frac{|Q|^2}{2}}\sqrt{\frac{n'!}{n!}}(i\bar{Q})^{n-n'}L_{n'}^{n-n'}(|Q|^2) & (n' \le n) \\ e^{-\frac{|Q|^2}{2}}\sqrt{\frac{n!}{n'!}}(iQ)^{n'-n}L_n^{n'-n}(|Q|^2) & (n' \ge n) \end{cases}. \tag{8}$$

In the case of $\phi/\phi_0 = p/q$, i.e., $a_{1x}a_2 = 2\pi l_B^2 p/q$, the magnetic and lattice cells are commensurate: $p\boldsymbol{m}_1 \times \boldsymbol{m}_2 = q\boldsymbol{a}_1 \times \boldsymbol{a}_2$, so we set the magnetic lattice $\boldsymbol{m}_1 = \boldsymbol{a}_1$, $\boldsymbol{m}_2 = \frac{q}{p}\boldsymbol{a}_2$ and $\boldsymbol{g}_1 = \boldsymbol{b}_1$, $\boldsymbol{g}_2 = \frac{p}{q}\boldsymbol{b}_2$. The momentum $\tilde{\boldsymbol{k}} \in$MBZ can be parameterized as $\tilde{k}_1\boldsymbol{g}_1 + \tilde{k}_2\boldsymbol{g}_2 = k_1\boldsymbol{b}_1 + \frac{k_2+r}{q}\boldsymbol{b}_2$, with $k_1 \in [0,1)$, $k_2 \in [0,1)$, and $r = 0, 1, ..., p-1$. We thus relabel Eq. (5) as

$$|n, r, \boldsymbol{k}\rangle = |\psi_{n,\tilde{k}_1=k_1,\tilde{k}_2=\frac{k_2+r}{p}}\rangle = \frac{1}{\sqrt{N_1 N_t}} \sum_{s\in\mathbb{Z}} e^{is2\pi k_1} e^{-i\pi\frac{a_{1y}}{a_2}\frac{p}{q}\left(\frac{k_2+r}{p}+s\right)^2} |\varphi_{n,\frac{2\pi}{a_2}\frac{p}{q}\left(\frac{k_2+r}{p}+s\right)}\rangle. \tag{9}$$

We can check $|n, r+p, \boldsymbol{k}\rangle = e^{-i2\pi k_1}|n, r, \boldsymbol{k}\rangle$. Using Eq. (6), we have

$$t(\boldsymbol{a}_1)|n, r, \boldsymbol{k}\rangle = e^{-i2\pi k_1}|n, r, \boldsymbol{k}\rangle, \quad t^q(\boldsymbol{a}_2)|n, r, \boldsymbol{k}\rangle = t^p(\boldsymbol{m}_2)|n, r, \boldsymbol{k}\rangle = e^{-i2\pi k_2}|n, r, \boldsymbol{k}\rangle, \tag{10}$$

so Eq. (9) are suitable to diagonalize H (the orthonormality follows easily from Eq. (5): $\langle n'r'\boldsymbol{k}'|nr\boldsymbol{k}\rangle = \delta_{n'n}\delta_{r'r}\delta_{\boldsymbol{k}'\boldsymbol{k}}$). The following target is to determine the matrix elements.

Before calculation, we prove that the spectrum of H is q-fold degenerate when $q > 1$. First we have

$$t(\boldsymbol{a}_2)|n, r, \boldsymbol{k}\rangle = \frac{e^{-\frac{i}{\hbar}p_y a_2}}{\sqrt{N_1 N_t}} \sum_{s\in\mathbb{Z}} e^{is2\pi k_1} e^{-i\pi\frac{a_{1y}}{a_2}\frac{p}{q}\left(\frac{k_2+r}{p}+s\right)^2} |\varphi_{n,\frac{2\pi}{a_2}\frac{p}{q}\left(\frac{k_2+r}{p}+s\right)}\rangle = e^{-i2\pi\frac{k_2+r}{q}}|n, r, [k_1-\frac{p}{q}], k_2\rangle, \tag{11}$$

and $k_1 \neq [k_1 - \frac{p}{q}]$ since p, q are co-prime. This means that $t(\boldsymbol{a}_2)$ alters k_1. For each eigenstate $|\Phi_{m\boldsymbol{k}}\rangle$ of H, $t^s(\boldsymbol{a}_2)|\Phi_{m\boldsymbol{k}}\rangle$ ($s = 1, 2, ..., q-1$) are also eigenstates of H since $[H, t(\boldsymbol{a}_2)] = 0$. They share the same energy and k_2 index, but have different k_1 indices: $[k_1 - s\frac{p}{q}]$, $s = 0, 1, ..., q-1$. This proves the q-fold degeneracy.

3 Matrix element

We calculate the Hamiltonian matrix elements in basis (9). The kinetic energy is simple since the involved operator $\boldsymbol{\pi}$ is related to the ladder operators

$$\pi_x = i\frac{\hbar}{\sqrt{2}l_B}(a^\dagger - a), \quad \pi_y = -\frac{\hbar}{\sqrt{2}l_B}(a^\dagger + a), \tag{12}$$

which act only on the LL energy index n, and is diagonal in $\boldsymbol{k}$ and r. The results are

$$\langle n'r'\boldsymbol{k}|a|nr\boldsymbol{k}\rangle = \sqrt{n}\delta_{n'+1,n}\delta_{r'r}, \quad \langle n'r'\boldsymbol{k}|a^\dagger|nr\boldsymbol{k}\rangle = \sqrt{n'}\delta_{n',n+1}\delta_{r'r}, \quad \langle n'r'\boldsymbol{k}|a^\dagger a|nr\boldsymbol{k}\rangle = n\delta_{n'n}\delta_{r'r}. \tag{13}$$

For $V(\boldsymbol{r})$, in general it is expanded as plane waves $V(\boldsymbol{r}) = \sum_{\boldsymbol{q}} V_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{r}}$, where $\boldsymbol{q} = q_1\boldsymbol{b}_1 + q_2\boldsymbol{b}_2 = q_1\boldsymbol{g}_1 + q_2\frac{q}{p}\boldsymbol{g}_2$ (q_i are integers). So we only need the plane wave matrix elements. Rewriting Eqs. (7), we have

$$\begin{aligned}
\langle n'r'\boldsymbol{k}'|e^{i\boldsymbol{q}\cdot\boldsymbol{r}}|nr\boldsymbol{k}\rangle =& F_{n'n}\left(\frac{q_x+iq_y}{\sqrt{2}}l_B\right)\delta_{k_1',[k_1+q_1]}\delta_{\frac{k_2'+r'}{p},[\frac{k_2+r+q_2q}{p}]}e^{i\frac{2\pi}{p}k_1'(k_2'+r'-k_2-r-q_2q)}e^{i\frac{2\pi}{p}q_1\left(k_2+r+\frac{q_2q}{2}\right)} \\
=& F_{n'n}\left(\frac{q_x+iq_y}{\sqrt{2}}l_B\right)\delta_{k_1'k_1}\delta_{k_2'k_2}\delta_{\frac{r'}{p},[\frac{r+q_2q}{p}]}e^{i\frac{2\pi}{p}k_1(r'-r-q_2q)}e^{i\frac{2\pi}{p}q_1\left(k_2+r+\frac{q_2q}{2}\right)} \\
=& F_{n'n}\left(\frac{q_x+iq_y}{\sqrt{2}}l_B\right)\delta_{k_1'k_1}\delta_{k_2'k_2}\sum_{s\in\mathbb{Z}}\delta_{r',r+q_2q+sp}e^{i2\pi sk_1}e^{i\frac{2\pi}{p}q_1\left(k_2+r+\frac{q_2q}{2}\right)}.
\end{aligned} \tag{14}$$

For each (r', r), at most one s survives in the summation. Eq. (14) is dense in n. In calculations we make a cutoff, i.e., we truncate N_c LLs, corresponding to an energy window $\sim \hbar^2 N_c/(ml_B^2)$. The computation cost increases when $B \to 0$.

To conveniently calculate $F_{n'n}(Q)$, we rewrite Eq. (8) as

$$F_{n'n}(Q) = \begin{cases} e^{i(\frac{\pi}{2}-\theta_Q)(n-n')}\exp\left[\frac{\ln\gamma(n'+1)-\ln\gamma(n+1)}{2} - \frac{|Q|^2}{2} + (n-n')\ln|Q|\right] L_{n'}^{n-n'}(|Q|^2) & (n' \le n) \\ e^{i(\frac{\pi}{2}+\theta_Q)(n'-n)}\exp\left[\frac{\ln\gamma(n+1)-\ln\gamma(n'+1)}{2} - \frac{|Q|^2}{2} + (n'-n)\ln|Q|\right] L_{n}^{n'-n}(|Q|^2) & (n' \ge n) \end{cases}, \tag{15}$$

where $\theta_Q = \arg(Q)$, $\gamma(n)$ is the gamma function, and for the Laguerre polynomials we recursively use

$$L_{n+1}^{\alpha}(x) = \frac{(2n+1+\alpha-x)L_n^{\alpha}(x) - (n+\alpha)L_{n-1}^{\alpha}(x)}{n+1}, \tag{16}$$

starting from $L_0^\alpha(x) = 1$, $L_1^\alpha(x) = 1+\alpha-x$.

4 Examples

4.1 Square lattice

For square lattice, $\boldsymbol{a}_1 = (a, 0)$, $\boldsymbol{a}_2 = (0, a)$, the Hamiltonian reads ($V_0 > 0$)

$$H(\boldsymbol{\pi}, \boldsymbol{r}) = \frac{\boldsymbol{\pi}^2}{2m} + V(\boldsymbol{r}) = \frac{\hbar^2}{l_B^2 m}\left(a^\dagger a + \frac{1}{2}\right) - V_0(e^{i\boldsymbol{g}_1\cdot\boldsymbol{r}} + e^{i\boldsymbol{g}_2\cdot\boldsymbol{r}} + e^{-i\boldsymbol{g}_1\cdot\boldsymbol{r}} + e^{-i\boldsymbol{g}_2\cdot\boldsymbol{r}}), \tag{17}$$

the matrix elements are

$$\begin{aligned}
\langle n'r'\boldsymbol{k}|\frac{\hbar^2}{ml_B^2}\left(a^\dagger a + \frac{1}{2}\right)|nr\boldsymbol{k}\rangle &= \frac{\hbar^2}{ml_B^2}\left(n+\frac{1}{2}\right)\delta_{n'n}\delta_{r'r}, \\
\langle n'r'\boldsymbol{k}|e^{i\boldsymbol{g}_1\cdot\boldsymbol{r}}|nr\boldsymbol{k}\rangle &= F_{n'n}\left(\frac{g_{1x}+ig_{1y}}{\sqrt{2}}l_B\right)\delta_{r'r}e^{i\frac{2\pi}{p}(k_2+r)}, \\
\langle n'r'\boldsymbol{k}|e^{i\boldsymbol{g}_2\cdot\boldsymbol{r}}|nr\boldsymbol{k}\rangle &= F_{n'n}\left(\frac{g_{2x}+ig_{2y}}{\sqrt{2}}l_B\right)\sum_s\delta_{r',r+q+sp}e^{i2\pi sk_1}.
\end{aligned} \tag{18}$$

4.2 Triangle lattice

The lattice vectors $\boldsymbol{a}_1 = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \boldsymbol{a}_2 = a(0,1)$, $\boldsymbol{g}_1 = \frac{4\pi}{\sqrt{3}a}(1,0), \boldsymbol{g}_2 = \frac{4\pi}{\sqrt{3}a}\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$. The kinetic energy is same to the square one, while the potential term becomes ($\boldsymbol{g}_3 = \boldsymbol{g}_1 + \boldsymbol{g}_2$)

$$V(\boldsymbol{r}) = -V_0[e^{i\boldsymbol{g}_1\cdot\boldsymbol{r}} + e^{i\boldsymbol{g}_2\cdot\boldsymbol{r}} + e^{i\boldsymbol{g}_3\cdot\boldsymbol{r}} + e^{-i\boldsymbol{g}_1\cdot\boldsymbol{r}} + e^{-i\boldsymbol{g}_2\cdot\boldsymbol{r}} + e^{-i\boldsymbol{g}_3\cdot\boldsymbol{r}}]. \tag{19}$$

The matrix elements are

$$\begin{aligned}
\langle n'r'\boldsymbol{k}|e^{i\boldsymbol{g}_1\cdot\boldsymbol{r}}|nr\boldsymbol{k}\rangle &= F_{n'n}\left(\frac{g_{1x}+ig_{1y}}{\sqrt{2}}l_B\right)\delta_{r'r}e^{i\frac{2\pi}{p}(k_2+r)},\\
\langle n'r'\boldsymbol{k}|e^{i\boldsymbol{g}_2\cdot\boldsymbol{r}}|nr\boldsymbol{k}\rangle &= F_{n'n}\left(\frac{g_{2x}+ig_{2y}}{\sqrt{2}}l_B\right)\sum_s\delta_{r',r+q+sp}e^{i2\pi sk_1},\\
\langle n'r'\boldsymbol{k}|e^{i\boldsymbol{g}_3\cdot\boldsymbol{r}}|nr\boldsymbol{k}\rangle &= F_{n'n}\left(\frac{g_{3x}+ig_{3y}}{\sqrt{2}}l_B\right)\sum_s\delta_{r',r+q+sp}e^{i2\pi sk_1}e^{i\frac{2\pi}{p}(k_2+r+\frac{q}{2})}.
\end{aligned}\tag{20}$$

4.3 Twisted bilayer graphene

Twisted bilayer graphene (TBG) has the continuum model, so under magnetic field it can also be diagonalized using the above method. We leave this part in another note called "Note_TBG_Hofstadter".

5 The Diophantine equation

For simple lattice with flux $\phi/\phi_0 = p/q$, where p and q are co-prime, the energy spectrum splits into a set of Hofstadter bands. The ν-th gap (from low- to high-energy) is characterized by a pair of integers (t_ν, s_ν), which satisfies the Diophantine equation (for $\boldsymbol{B} = -B\boldsymbol{e}_z$, $B > 0$)

$$-\nu = t_\nu p + s_\nu q. \tag{21}$$

Specifically, t_ν is the Chern number of the ν-th gap, i.e., the Chern number of the ν-th band is $\sigma_\nu = t_\nu - t_{\nu-1}$. In the following we give a proof to the Diophantine equation, which is modified from I. Dana's paper (J. Phys. C: Solid State Phys 18 L679).

5.1 A heuristic proof

We only consider the non-degenerate (at each $\boldsymbol{k}$) case. Suppose the ν-th band with Chern number σ_ν has the wave function $|\Phi_{\nu,k_1,k_2}\rangle$, i.e., $H|\Phi_{\nu,k_1,k_2}\rangle = E_{\nu,k_1,k_2}|\Phi_{\nu,k_1,k_2}\rangle$, where $k_1 \in [0,1)$, $k_2 \in [0,1)$, satisfying $t(\boldsymbol{a}_1)|\Phi_{\nu,k_1,k_2}\rangle = e^{-i2\pi k_1}|\Phi_{\nu,k_1,k_2}\rangle$, $\quad t^q(\boldsymbol{a}_2)|\Phi_{\nu,k_1,k_2}\rangle = e^{-i2\pi k_2}|\Phi_{\nu,k_1,k_2}\rangle$.

In consistency with the Chern number σ_ν, we may choose the boundary condition (BC) (one may easily check that the following BC could give the correct Chern number by calculating the phase accumulation along the closed path $(k_1,k_2) = (0,0) \to (1,0) \to (1,1) \to (0,1) \to (0,0)$)

$$|\Phi_{\nu,k_1+1,k_2}\rangle = e^{-i2\pi\sigma_\nu k_2}|\Phi_{\nu,k_1,k_2}\rangle, \quad |\Phi_{\nu,k_1,k_2+1}\rangle = |\Phi_{\nu,k_1,k_2}\rangle. \tag{22}$$

We know $t(\boldsymbol{a}_2)|\Phi_{\nu,k_1,k_2}\rangle \sim |\Phi_{\nu,[k_1-\frac{p}{q}],k_2}\rangle$ is still an eigenstate with the same energy, so in general we assume

$$t(\boldsymbol{a}_2)|\Phi_{\nu,k_1,k_2}\rangle = e^{i2\pi m_\nu k_2}|\Phi_{\nu,k_1-\frac{p}{q},k_2}\rangle, \tag{23}$$

which then gives

$$t^q(\boldsymbol{a}_2)|\Phi_{\nu,k_1,k_2}\rangle = e^{i2\pi m_\nu k_2 q}|\Phi_{\nu,k_1-p,k_2}\rangle = e^{i2\pi k_2(m_\nu q+\sigma_\nu p)}|\Phi_{\nu,k_1,k_2}\rangle = e^{-i2\pi k_2}|\Phi_{\nu,k_1,k_2}\rangle, \tag{24}$$

meaning $m_\nu q + \sigma_\nu p = -1$. This equation is equivalent to the Diophantine equation above by noting $\sigma_\nu = t_\nu - t_{\nu-1}$, $m_\nu = s_\nu - s_{\nu-1}$, and m_ν actually is an integer because

$$\begin{aligned}
e^{i2\pi m_\nu k_2}|\Phi_{\nu,k_1-\frac{p}{q},k_2}\rangle =& t(\boldsymbol{a}_2)|\Phi_{\nu,k_1,k_2}\rangle = t(\boldsymbol{a}_2)|\Phi_{\nu,k_1,k_2+1}\rangle = e^{i2\pi m_\nu(k_2+1)}|\Phi_{\nu,k_1-\frac{p}{q},k_2+1}\rangle\\
=& e^{i2\pi m_\nu}e^{i2\pi m_\nu k_2}|\Phi_{\nu,k_1-\frac{p}{q},k_2}\rangle.
\end{aligned}\tag{25}$$

The Diophantine equation is a general rule to tell us the Chern number or Hall conductance of the system. It is irrelative about the specific lattice, and is purely a result of the magnetic translation symmetry.

5.2 Relation with the Streda formula

For the case with flux $\phi/\phi_0 = p/q$, the electron density, i.e., the number of electrons per original unit cell, is $\rho = \nu/q$. From Diophantine equation we know

$$\rho = \frac{\nu}{q} = -t_\nu \frac{p}{q} - s_\nu = -t_\nu \frac{e}{h} BS - s_\nu. \tag{26}$$

Taking the gradients with respect to the flux, we reach the Streda formula

$$\sigma_{xy}^\nu = \frac{e^2}{h} t_\nu = -\frac{e}{S} \frac{\partial \rho}{\partial B}. \tag{27}$$

6 Numerical method for Chern numbers

Suppose at flux $\phi/\phi_0 = p/q$ the ν-th eigenstate satisfying $H|\Phi_{\nu\boldsymbol{k}}\rangle = E_{\nu\boldsymbol{k}}|\Phi_{\nu\boldsymbol{k}}\rangle$ is

$$|\Phi_{\nu\boldsymbol{k}}\rangle = \sum_{n,r} |nr\boldsymbol{k}\rangle P_{nr,\nu}(\boldsymbol{k}). \tag{28}$$

We define the Bloch functions $|u_{\nu\boldsymbol{k}}\rangle = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}|\Phi_{\nu\boldsymbol{k}}\rangle$, which satisfy (using $t(\boldsymbol{a})e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}t(\boldsymbol{a})e^{i\boldsymbol{k}\cdot\boldsymbol{a}}$)

$$t(\boldsymbol{a}_1)|u_{\nu\boldsymbol{k}}\rangle = |u_{\nu\boldsymbol{k}}\rangle, \quad t^q(\boldsymbol{a}_2)|u_{\nu\boldsymbol{k}}\rangle = |u_{\nu\boldsymbol{k}}\rangle. \tag{29}$$

One should be careful here $\boldsymbol{k} = k_1\boldsymbol{b}_1 + k_2\frac{\boldsymbol{b}_2}{q} = k_1\boldsymbol{g}_1 + \frac{k_2}{p}\boldsymbol{g}_2$.

The ν-th band Chern number can then be numerically calculated. For multiple bands, we simply replace U below by the determinant. First we discretize $\boldsymbol{k}_{ij} = (\frac{i}{N_1}, \frac{j}{N_2})$, for $i = 0, 1, \ldots, N_1 - 1$, $j = 0, 1, \ldots, N_2 - 1$. The U and $\mathcal{F}$ matrices are

$$U_1^\nu(\boldsymbol{k}_{ij}) = \frac{\langle u_{\nu,\boldsymbol{k}_{ij}}|u_{\nu,\boldsymbol{k}_{i+1,j}}\rangle}{|\langle u_{\nu,\boldsymbol{k}_{ij}}|u_{\nu,\boldsymbol{k}_{i+1,j}}\rangle|}, \quad U_2^\nu(\boldsymbol{k}_{ij}) = \frac{\langle u_{\nu,\boldsymbol{k}_{ij}}|u_{\nu,\boldsymbol{k}_{i,j+1}}\rangle}{|\langle u_{\nu,\boldsymbol{k}_{ij}}|u_{\nu,\boldsymbol{k}_{i,j+1}}\rangle|}, \quad \mathcal{F}^\nu(\boldsymbol{k}_{ij}) = \ln\left[\frac{U_1^\nu(\boldsymbol{k}_{ij})U_2^\nu(\boldsymbol{k}_{i+1,j})}{U_1^\nu(\boldsymbol{k}_{i,j+1})U_2^\nu(\boldsymbol{k}_{ij})}\right], \tag{30}$$

where the phase of $\mathcal{F}$ is confined as $[-\pi, \pi)$. The band Chern number reads

$$t_\nu = \frac{i}{2\pi}\sum_{ij} \mathcal{F}^\nu(\boldsymbol{k}_{ij}). \tag{31}$$

One should be careful about the inner product of $|u_{\nu\boldsymbol{k}}\rangle$, which reads ($\boldsymbol{k} = k_1\boldsymbol{b}_1 + \frac{k_2}{q}\boldsymbol{b}_2 = k_1\boldsymbol{g}_1 + \frac{k_2}{p}\boldsymbol{g}_2$)

$$\langle u_{\nu'\boldsymbol{k}'}|u_{\nu\boldsymbol{k}}\rangle = \sum_{n'r'}\sum_{nr} P^*_{n'r',\nu'}(\boldsymbol{k}')\langle n'r'\boldsymbol{k}'|e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}|nr\boldsymbol{k}\rangle P_{nr,\nu}(\boldsymbol{k}) = [P^\dagger(\boldsymbol{k}')X(\boldsymbol{k}',\boldsymbol{k})P(\boldsymbol{k})]_{\nu'\nu}, \tag{32}$$

$$\begin{aligned}
[X(\boldsymbol{k}',\boldsymbol{k})]_{n'r',nr} =& \langle \psi_{n,k_1',\frac{k_2'+r'}{p}}|e^{i[(k_1'-k_1)\boldsymbol{g}_1+\frac{k_2'-k_2}{p}\boldsymbol{g}_2]\cdot\boldsymbol{r}}|\psi_{n,k_1,\frac{k_2+r}{p}}\rangle \\
=& \delta_{k_1',[k_1+k_1'-k_1]}\delta_{\frac{k_2'+r'}{p},[\frac{k_2+r}{p}+\frac{k_2'-k_2}{p}]}\exp[i2\pi k_1'(\frac{k_2'+r'}{p} - \frac{k_2+r}{p} - \frac{k_2'-k_2}{p})] \\
& \times e^{i2\pi(k_1'-k_1)\left(\frac{k_2+r}{p}+\frac{k_2'-k_2}{2p}\right)} F_{n'n}\left(\frac{(k_1'-k_1)\boldsymbol{g}_1 + (k_2'-k_2)\boldsymbol{g}_2/p}{\sqrt{2}}l_B\right) \\
=& \delta_{r'r}e^{i\frac{\pi}{p}(k_1'-k_1)(k_2'+k_2+2r)}F_{n'n}\left(\frac{(k_1'-k_1)\boldsymbol{g}_1 + (k_2'-k_2)\boldsymbol{g}_2/p}{\sqrt{2}}l_B\right),
\end{aligned} \tag{33}$$

where Eq. (7) has been used.

7 Connection with Peierls substitution in TB model

7.1 Peierls substitution

Suppose we have a spinless TB model (atomic gauge)

$$H = \sum_{\alpha\beta}\sum_{\boldsymbol{R}_\alpha\boldsymbol{R}_\beta} t_{\alpha\beta}(\boldsymbol{R}_\beta - \boldsymbol{R}_\alpha)c^\dagger_{\boldsymbol{R}_\alpha,\alpha}c_{\boldsymbol{R}_\beta,\beta}, \tag{34}$$

where $\boldsymbol{R}_\alpha$, $\boldsymbol{R}_\beta$ denote the atomic positions of sublattice α, β. The Peierls substitution suggests that, under magnetic field $\boldsymbol{B} = \nabla \times \boldsymbol{A}$, the model is modified into

$$H_{\boldsymbol{A}} = \sum_{\alpha\beta} \sum_{\boldsymbol{R}_\alpha \boldsymbol{R}_\beta} t^{\boldsymbol{A}}_{\alpha\beta}(\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta) \tilde{c}^\dagger_{\boldsymbol{R}_\alpha,\alpha} \tilde{c}_{\boldsymbol{R}_\beta,\beta}, \quad t^{\boldsymbol{A}}_{\alpha\beta}(\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta) = t_{\alpha\beta}(\boldsymbol{R}_\beta - \boldsymbol{R}_\alpha) e^{i\theta(\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta)}, \tag{35}$$

where the phase is a line-integral of $\boldsymbol{A}$ between the two sites

$$\theta(\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta) = -\frac{e}{\hbar} \int_{\boldsymbol{R}_\beta}^{\boldsymbol{R}_\alpha} \boldsymbol{A}(\boldsymbol{r}') \cdot d\boldsymbol{r}'. \tag{36}$$

The relation between the new basis $\tilde{c}_{\boldsymbol{R}_\alpha,\alpha}$ and original basis $c_{\boldsymbol{R}_\alpha,\alpha}$ will become clear below.

7.2 A derivation from continuum model

The Peierls substitution can be derived using Wannier functions. Assume a small enough B field, so that $\boldsymbol{A}$ changes gradually in the lattice ($l_B \gg a$). When $B = 0$, the Hamiltonian $H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})$ has Wannier orbital $\phi_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}n} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_\alpha} U_{n,\alpha}(\boldsymbol{k}) \psi_{n\boldsymbol{k}}(\boldsymbol{r})$, and the hopping reads

$$t_{\alpha\beta}(\boldsymbol{R}_\beta - \boldsymbol{R}_\alpha) = \int d\boldsymbol{r} \phi^*_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha) \left[\boldsymbol{p}^2/(2m) + V(\boldsymbol{r})\right] \phi_\beta(\boldsymbol{r} - \boldsymbol{R}_\beta). \tag{37}$$

All $\phi_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha)$ span the complete Hilbert space, but they are inconvenient to use when $B \neq 0$. We instead adopt the gauged orbitals

$$\tilde{\phi}_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha) = \exp\left(-i\frac{e}{\hbar} \int_{\boldsymbol{R}_\alpha}^{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r}') \cdot d\boldsymbol{r}'\right) \phi_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha). \tag{38}$$

In such basis we have

$$\begin{aligned} \boldsymbol{\pi}\tilde{\phi}_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha) =& \exp\left(-i\frac{e}{\hbar} \int_{\boldsymbol{R}_\alpha}^{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r}') \cdot d\boldsymbol{r}'\right) \left(\boldsymbol{\pi} - e\nabla \int_{\boldsymbol{R}_\alpha}^{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r}') \cdot d\boldsymbol{r}'\right) \phi_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha) \\ \approx& \exp\left(-i\frac{e}{\hbar} \int_{\boldsymbol{R}_\alpha}^{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r}') \cdot d\boldsymbol{r}'\right) \boldsymbol{p}\phi_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha), \end{aligned} \tag{39}$$

where the third step is valid when $\boldsymbol{A}$ changes gradually over the lattice constant and ϕ_α is well-localized. The error of this step is $\sim |\nabla \times \boldsymbol{A}| a^2 = Ba^2$, which is much smaller when the flux quanta $Ba^2 \ll h/e \Rightarrow a \ll l_B$. Written in these "magnetic Wannier orbitals", the hoppings are

$$\begin{aligned} t^{\boldsymbol{A}}_{\alpha\beta}(\boldsymbol{R}_\alpha, \boldsymbol{R}_\beta) =& \langle \tilde{\phi}_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha) | H^{\boldsymbol{A}} | \tilde{\phi}_\beta(\boldsymbol{r} - \boldsymbol{R}_\beta) \rangle \\ \approx& \int d\boldsymbol{r} \phi^*_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha) e^{i\frac{e}{\hbar}\int_{\boldsymbol{R}_\alpha}^{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r}')\cdot d\boldsymbol{r}' - i\frac{e}{\hbar}\int_{\boldsymbol{R}_\beta}^{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r}')\cdot d\boldsymbol{r}'} \left[\frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})\right] \phi_\beta(\boldsymbol{r} - \boldsymbol{R}_\beta) \\ =& e^{-i\frac{e}{\hbar}\int_{\boldsymbol{R}_\beta}^{\boldsymbol{R}_\alpha} \boldsymbol{A}(\boldsymbol{r}')d\cdot\boldsymbol{r}'} \int d\boldsymbol{r} e^{-i\frac{e}{\hbar}\Theta_{\boldsymbol{R}_\alpha\boldsymbol{R}_\beta}(\boldsymbol{r})} \phi^*_\alpha(\boldsymbol{r} - \boldsymbol{R}_\alpha) \left[\frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})\right] \phi_\beta(\boldsymbol{r} - \boldsymbol{R}_\beta), \end{aligned}$$

where the phase is a triangular-shaped closed loop integral (flux)

$$\Theta_{\boldsymbol{R}_\alpha\boldsymbol{R}_\beta}(\boldsymbol{r}) = \int_{\boldsymbol{R}_\beta \to \boldsymbol{r} \to \boldsymbol{R}_\alpha \to \boldsymbol{R}_\beta} \boldsymbol{A}(\boldsymbol{r}') \cdot d\boldsymbol{r}'. \tag{40}$$

Since the spread of $\tilde{\phi}_\alpha$ is much smaller than l_B, the main part in (40) should come from the integral of $\boldsymbol{r}$ around $\boldsymbol{R}_\alpha$ and $\boldsymbol{R}_\beta$, i.e., from the region $|\boldsymbol{r} - \boldsymbol{R}_\alpha|, |\boldsymbol{r} - \boldsymbol{R}_\beta| \sim a \ll l_B$. This makes the triangle very thin and the flux integral tiny. Neglecting $\Theta_{\boldsymbol{R}_\alpha\boldsymbol{R}_\beta}(\boldsymbol{r}) \approx 0$ gives the Peierls substitution.