

Hofstadter spectrum of TBG (v2)

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May 30, 2025

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1 BM Hamiltonian

The lattice vectors of TBG in real and reciprocal spaces are respectively (in basis $\mathbf{e}_x, \mathbf{e}_y$)

$$\mathbf{a}_1 = L_\theta \left(\frac{\sqrt{3}}{2}, \frac{1}{2} \right), \quad \mathbf{a}_2 = L_\theta(0, 1); \quad \mathbf{b}_1 = \frac{4\pi}{\sqrt{3}L_\theta}(1, 0), \quad \mathbf{b}_2 = \frac{4\pi}{\sqrt{3}L_\theta} \left(-\frac{1}{2}, \frac{\sqrt{3}}{2} \right), \quad (1)$$

Under external field $\mathbf{B} = -B\mathbf{e}_z$ ($B > 0$), the BM Hamiltonian reads ($\boldsymbol{\sigma}_\eta = (\eta\sigma_x, \sigma_y)$)

$$H^\eta = \begin{pmatrix} v_F(\boldsymbol{\pi} - \hbar\mathbf{K}_1^\eta) \cdot \boldsymbol{\sigma}_\eta & U_\eta(\mathbf{r}) \\ U_\eta^\dagger(\mathbf{r}) & v_F(\boldsymbol{\pi} - \hbar\mathbf{K}_2^\eta) \cdot \boldsymbol{\sigma}_\eta \end{pmatrix}, \quad (2)$$

where $\boldsymbol{\pi} = \mathbf{p} + e\mathbf{A}$ in the Landau gauge $\mathbf{A} = -Bx\mathbf{e}_y$. The moiré potential is

$$U_\eta(\mathbf{r}) = T_1^\eta + T_2^\eta e^{-i\eta\mathbf{b}_2 \cdot \mathbf{r}} + T_3^\eta e^{-i\eta(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}}, \quad (3)$$

with

$$T_1^\eta = \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix}, \quad T_2^\eta = \begin{pmatrix} u_0 & u_1\omega^\eta \\ u_1\omega^{-\eta} & u_0 \end{pmatrix}, \quad T_3^\eta = \begin{pmatrix} u_0 & u_1\omega^{-\eta} \\ u_1\omega^\eta & u_0 \end{pmatrix}, \quad (4)$$

The Dirac points in the layer l is

$$\mathbf{K}_l^\eta = \eta(\boldsymbol{\Gamma} + \bar{\mathbf{K}}_l), \quad \bar{\mathbf{K}}_1 = \frac{4\pi}{3L_\theta} \left(\frac{\sqrt{3}}{2}, -\frac{1}{2} \right), \quad \bar{\mathbf{K}}_2 = \frac{4\pi}{3L_\theta} \left(\frac{\sqrt{3}}{2}, \frac{1}{2} \right), \quad (5)$$

where the momentum shift $\boldsymbol{\Gamma}$ can be gauged out.

We focus on the case with flux $\frac{\phi}{\phi_0} = \frac{p}{q}$, where $\phi = \frac{\sqrt{3}L_\theta^2 B}{2}$ and $\phi_0 = h/e$, i.e.,

$$\frac{\sqrt{3}L_\theta^2/2}{2\pi l_B^2} = \frac{p}{q} \quad \Rightarrow \quad l_B = L_\theta \sqrt{\frac{\sqrt{3}}{4\pi} \frac{q}{p}}, \quad (6)$$

where $l_B = \sqrt{\hbar/(eB)}$.

2 LL basis for graphene

We use the LL basis of moiré-less monolayer graphene as the starting point. The monolayer graphene has the Hamiltonian (omit the momentum offset)

$$h_l^+(\boldsymbol{\pi}) = v_F \boldsymbol{\pi} \cdot \boldsymbol{\sigma}_+ = i \frac{\sqrt{2} \hbar v_F}{l_B} \begin{pmatrix} & -a \\ a^\dagger & \end{pmatrix}, \quad h_l^-(\boldsymbol{\pi}) = v_F \boldsymbol{\pi} \cdot \boldsymbol{\sigma}_- = i \frac{\sqrt{2} \hbar v_F}{l_B} \begin{pmatrix} & -a^\dagger \\ a & \end{pmatrix}. \quad (7)$$

Both valleys have LL energies $\epsilon_n = \text{sgn}(n) \sqrt{2|n|} \hbar v_F / l_B$, with LL wave functions

$$\tilde{\phi}_{n=0, \mathbf{k}}^+ = \begin{pmatrix} 0 \\ \psi_{0\mathbf{k}} \end{pmatrix}, \quad \tilde{\phi}_{n \neq 0, \mathbf{k}}^+ = \frac{1}{\sqrt{2}} \begin{pmatrix} -i \text{sgn}(n) \psi_{|n|-1, \mathbf{k}} \\ \psi_{|n| \mathbf{k}} \end{pmatrix}, \quad (8)$$

in the $\eta = +$ valley, and

$$\tilde{\phi}_{n=0, \mathbf{k}}^- = \begin{pmatrix} \psi_{0\mathbf{k}} \\ 0 \end{pmatrix}, \quad \tilde{\phi}_{n \neq 0, \mathbf{k}}^- = \frac{1}{\sqrt{2}} \begin{pmatrix} \psi_{|n| \mathbf{k}} \\ i \text{sgn}(n) \psi_{|n|-1, \mathbf{k}} \end{pmatrix}, \quad (9)$$

in the $\eta = -$ valley. Here $\psi_{n\mathbf{k}}$ are LL wave functions of quadratic electrons on torus

$$\psi_{n\mathbf{k}} = \frac{e^{-i\pi k_2^2 \frac{m_1 y}{m_2}}}{\sqrt{N_1 N_t}} \sum_{s \in \mathbb{Z}} e^{i2\pi s k_1} t^s(\mathbf{m}_1) \varphi_{n, \frac{2\pi}{m_2} k_2} = \frac{1}{\sqrt{N_1 N_t}} \sum_{s \in \mathbb{Z}} e^{is2\pi k_1} e^{-i\pi \frac{m_1 y}{m_2} (k_2 + s)^2} \varphi_{n, \frac{2\pi}{m_2} (k_2 + s)}, \quad (10)$$

and φ_{n, k_y} are LLs on cylinder. From Eqs. (8), (9), it is important to keep the LL cutoff on sublattice A smaller than that on B by 1 in valley $\eta = +$, and reversely in valley $\eta = -$.

3 TBG matrix elements

3.1 Basis set

For rational flux p/q , we set the magnetic lattice in real and reciprocal space as

$$\mathbf{m}_1 = \mathbf{a}_1, \quad \mathbf{m}_2 = \frac{q}{p} \mathbf{a}_2, \quad \mathbf{g}_1 = \mathbf{b}_1, \quad \mathbf{g}_2 = \frac{p}{q} \mathbf{b}_2. \quad (11)$$

The momentum $\tilde{\mathbf{k}} \in \text{MBZ}$ can be parameterized as $\tilde{\mathbf{k}}_1 \mathbf{g}_1 + \tilde{\mathbf{k}}_2 \mathbf{g}_2 = k_1 \mathbf{b}_1 + \frac{k_2 + r}{q} \mathbf{b}_2$, with $k_1 \in [0, 1)$, $k_2 \in [0, 1)$, and $r = 0, 1, \dots, p-1$. Following note ‘Hofstadter’ and gauging out the offset $\boldsymbol{\Gamma}$, we define the following basis

$$|\eta l \alpha n \mathbf{r} \mathbf{k}\rangle = e^{i\eta \boldsymbol{\Gamma} \cdot \mathbf{r}} \chi_{l\alpha} |\psi_{n, k_1 \mathbf{g}_1 + \frac{k_2 + r}{p} \mathbf{g}_2}\rangle = e^{i\eta \boldsymbol{\Gamma} \cdot \mathbf{r}} \chi_{l\alpha} |\psi_{n, k_1 \mathbf{b}_1 + \frac{k_2 + r}{q} \mathbf{b}_2}\rangle, \quad (12)$$

where $\chi_{l\alpha}$ is a 4-vector whose $(l\alpha)$ element is 1 and 0 for others. The plane wave matrix elements are derived in note ‘Hofstadter’, so we directly list the Hamiltonian matrix elements below, which is diagonal in \mathbf{k} .

3.2 Matrix elements in + valley

First focus on the valley $\eta = +$. The kinetic term is diagonal in l, r , with elements

$$\begin{aligned} & \langle +l \alpha' n' r \mathbf{k} | v_F (\boldsymbol{\pi} - \hbar \mathbf{K}_l^+) \cdot \boldsymbol{\sigma}_+ | +l \alpha n r \mathbf{k} \rangle \\ &= i \frac{\sqrt{2} \hbar v_F}{l_B} \begin{pmatrix} & -\sqrt{n} \delta_{n'+1, n} \\ \sqrt{n'} \delta_{n', n+1} & \end{pmatrix}_{\alpha' \alpha} - v_F \hbar [\bar{\mathbf{K}}_l \cdot \boldsymbol{\sigma}_+]_{\alpha' \alpha} \delta_{n' n}. \end{aligned} \quad (13)$$

For the moiré potential,

$$\langle +1 \alpha' n' r \mathbf{k} | U_+ | +2 \alpha n r \mathbf{k} \rangle = [T_1^+]_{\alpha' \alpha} \delta_{n' n} \delta_{r' r} + [T_2^+]_{\alpha' \alpha} [e^{-i \mathbf{b}_2 \cdot \mathbf{r}}]_{n' r' \mathbf{k}, n r \mathbf{k}} + [T_3^+]_{\alpha' \alpha} [e^{-i (\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}}]_{n' r' \mathbf{k}, n r \mathbf{k}}, \quad (14)$$

where

$$[e^{-i \mathbf{b}_2 \cdot \mathbf{r}}]_{n' r' \mathbf{k}, n r \mathbf{k}} = F_{n' n} \left(-\frac{\mathbf{b}_2}{\sqrt{2}} l_B \right) \sum_{s \in \mathbb{Z}} \delta_{r', r - q + sp} e^{i2\pi s k_1}, \quad (15)$$

$$[e^{-i (\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}}]_{n' r' \mathbf{k}, n r \mathbf{k}} = F_{n' n} \left(-\frac{\mathbf{b}_1 + \mathbf{b}_2}{\sqrt{2}} l_B \right) \sum_{s \in \mathbb{Z}} \delta_{r', r - q + sp} e^{i2\pi s k_1} e^{-i \frac{2\pi}{p} (k_2 + r - \frac{q}{2})}. \quad (16)$$

The form factor reads (for $\mathbf{Q} = (Q_x, Q_y)$, we define $Q = Q_x + iQ_y$, $\bar{Q} = Q_x - iQ_y$)

$$F_{n'n}(\mathbf{Q}) = \begin{cases} e^{-\frac{|Q|^2}{2}} \sqrt{\frac{n!}{n'}} (i\bar{Q})^{n-n'} L_{n'}^{n-n'}(|Q|^2) & (n' \leq n) \\ e^{-\frac{|Q|^2}{2}} \sqrt{\frac{n!}{n'}} (iQ)^{n'-n} L_n^{n'-n}(|Q|^2) & (n' \geq n) \end{cases}. \quad (17)$$

3.3 Matrix elements in - valley

In the valley $\eta = -$, the kinetic term is

$$\begin{aligned} & \langle -l\alpha'n'r\mathbf{k} | v_F(\boldsymbol{\pi} - \hbar\mathbf{K}_l^+) \cdot \boldsymbol{\sigma}_+ | -l\alpha n r \mathbf{k} \rangle \\ &= i \frac{\sqrt{2}\hbar v_F}{l_B} \begin{pmatrix} -\sqrt{n'}\delta_{n',n+1} \\ \sqrt{n}\delta_{n'+1,n} \end{pmatrix}_{\alpha'\alpha} + v_F \hbar [\bar{\mathbf{K}}_l \cdot \boldsymbol{\sigma}_-]_{\alpha'\alpha} \delta_{n'n}. \end{aligned} \quad (18)$$

The moiré potential is

$$\langle -l\alpha'n'r'\mathbf{k} | U_- | -l\alpha n r \mathbf{k} \rangle = [T_1^-]_{\alpha'\alpha} \delta_{n'n} \delta_{r'r} + [T_2^-]_{\alpha'\alpha} [e^{i\mathbf{b}_2 \cdot \mathbf{r}}]_{n'r'\mathbf{k}, nr\mathbf{k}} + [T_3^-]_{\alpha'\alpha} [e^{i(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}}]_{n'r'\mathbf{k}, nr\mathbf{k}}, \quad (19)$$

where

$$[e^{i\mathbf{b}_2 \cdot \mathbf{r}}]_{n'r'\mathbf{k}, nr\mathbf{k}} = F_{n'n} \left(\frac{\mathbf{b}_2}{\sqrt{2}} l_B \right) \sum_{s \in \mathbb{Z}} \delta_{r', r+q+sp} e^{i2\pi s k_1}, \quad (20)$$

$$[e^{i(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}}]_{n'r'\mathbf{k}, nr\mathbf{k}} = F_{n'n} \left(\frac{\mathbf{b}_1 + \mathbf{b}_2}{\sqrt{2}} l_B \right) \sum_{s \in \mathbb{Z}} \delta_{r', r+q+sp} e^{i2\pi s k_1} e^{i\frac{2\pi}{p}(k_2 + r + \frac{q}{2})}. \quad (21)$$

4 Chern number

For the Hofstadter state $|\Phi_{\nu\mathbf{k}}^\eta\rangle = \sum_{l\alpha n r} |\eta l \alpha n r \mathbf{k}\rangle P_{l\alpha n r, \nu}^\eta(\mathbf{k})$ satisfying $H^\eta |\Phi_{\nu\mathbf{k}}^\eta\rangle = E_{\nu\mathbf{k}}^\eta |\Phi_{\nu\mathbf{k}}^\eta\rangle$, we define the Bloch wave function $|u_{\nu\mathbf{k}}^\eta\rangle = e^{-i\mathbf{k} \cdot \mathbf{r}} |\Phi_{\nu\mathbf{k}}^\eta\rangle$. The (valley) Chern number of band ν can be calculated as follows. We discretize $\mathbf{k}_{ij} = (\frac{i}{N_1}, \frac{j}{N_2})$, $i = 0, 1, \dots, N_1 - 1$, $j = 0, 1, \dots, N_2 - 1$, and define

$$U_1^{\eta\nu}(\mathbf{k}_{ij}) = \frac{\langle u_{\nu, \mathbf{k}_{ij}}^\eta | u_{\nu, \mathbf{k}_{i+1, j}}^\eta \rangle}{|\langle u_{\nu, \mathbf{k}_{ij}}^\eta | u_{\nu, \mathbf{k}_{i+1, j}}^\eta \rangle|}, \quad U_2^{\eta\nu}(\mathbf{k}_{ij}) = \frac{\langle u_{\nu, \mathbf{k}_{ij}}^\eta | u_{\nu, \mathbf{k}_{i, j+1}}^\eta \rangle}{|\langle u_{\nu, \mathbf{k}_{ij}}^\eta | u_{\nu, \mathbf{k}_{i, j+1}}^\eta \rangle|}, \quad \mathcal{F}^{\eta\nu}(\mathbf{k}_{ij}) = \ln \left[\frac{U_1^{\eta\nu}(\mathbf{k}_{ij}) U_2^{\eta\nu}(\mathbf{k}_{i+1, j})}{U_1^{\eta\nu}(\mathbf{k}_{i, j+1}) U_2^{\eta\nu}(\mathbf{k}_{ij})} \right], \quad (22)$$

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

$$t_\nu = \frac{i}{2\pi} \sum_{ij} \mathcal{F}^{\eta\nu}(\mathbf{k}_{ij}). \quad (23)$$

The inner product of $|u_{\nu\mathbf{k}}^\eta\rangle$ reads $(\mathbf{k} = k_1 \mathbf{b}_1 + \frac{k_2}{q} \mathbf{b}_2 = k_1 \mathbf{g}_1 + \frac{k_2}{p} \mathbf{g}_2)$

$$\langle u_{\nu'\mathbf{k}'}^\eta | u_{\nu\mathbf{k}}^\eta \rangle = \sum_{l\alpha n' r' \nu'} P_{l\alpha n' r', \nu'}^{\eta*}(\mathbf{k}') [e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}}]_{n'r'\mathbf{k}', nr\mathbf{k}} P_{l\alpha n r, \nu}^\eta(\mathbf{k}) = [P^{\eta\dagger}(\mathbf{k}') X(\mathbf{k}', \mathbf{k}) P^\eta(\mathbf{k})]_{\nu'\nu}, \quad (24)$$

where

$$[X(\mathbf{k}', \mathbf{k})]_{\nu'\alpha' n' r', l\alpha n r} = \delta_{l'l} \delta_{\alpha'\alpha} \delta_{r'r} e^{i\frac{\pi}{p}(k'_1 - k_1)(k'_2 + k_2 + 2r)} F_{n'n} \left(\frac{(k'_1 - k_1)\mathbf{g}_1 + (k'_2 - k_2)\mathbf{g}_2/p}{\sqrt{2}} l_B \right). \quad (25)$$

For a collective bands, we only need replace U by the multi-band determinant.