Hofstadter spectrum of TBG (v2)

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Contents

1 BM Hamiltonian

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

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

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

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

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

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

with

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

The Dirac points in the layer l is

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

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.,

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

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

2 LL basis for graphene, momentum shift

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

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

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

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

in the $\eta = +$ valley, and

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

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

$$\psi_{n\boldsymbol{k}} = \frac{e^{-i\pi k_2^2\frac{m_{1y}}{m_2}}}{\sqrt{N_1N_t}}\sum_{s\in\mathbb{Z}} e^{i2\pi sk_1}t^s(\boldsymbol{m}_1)\varphi_{n,\frac{2\pi}{m_2}k_2} = \frac{1}{\sqrt{N_1N_t}}\sum_{s\in\mathbb{Z}} e^{is2\pi k_1}e^{-i\pi\frac{m_{1y}}{m_2}(k_2+s)^2}\varphi_{n,\frac{2\pi}{m_2}(k_2+s)}, \tag{10}$$

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

$$\boldsymbol{m}_1 = \boldsymbol{a}_1, \quad \boldsymbol{m}_2 = \frac{q}{p}\boldsymbol{a}_2, \quad \boldsymbol{g}_1 = \boldsymbol{b}_1, \quad \boldsymbol{g}_2 = \frac{p}{q}\boldsymbol{b}_2. \tag{11}$$

The momentum $\tilde{\boldsymbol{k}}$ ∈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 $r = 0, 1, ..., p-1$. Following note 'Hofstadter' and gauging out the offset $\boldsymbol{\Gamma}$, we define the following basis

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

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 $\boldsymbol{k}$.

3.2 Matrix elements in + valley

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

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

For the moiré potential,

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

where

$$[e^{-i\boldsymbol{b}_2\cdot\boldsymbol{r}}]_{n'r'\boldsymbol{k},nr\boldsymbol{k}} = F_{n'n}\left(-\frac{\boldsymbol{b}_2}{\sqrt{2}}l_B\right)\sum_{s\in\mathbb{Z}}\delta_{r',r-q+sp}e^{i2\pi sk_1}, \tag{15}$$

$$[e^{-i(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{r}}]_{n'r'\boldsymbol{k},nr\boldsymbol{k}} = F_{n'n}\left(-\frac{\boldsymbol{b}_1+\boldsymbol{b}_2}{\sqrt{2}}l_B\right)\sum_{s\in\mathbb{Z}}\delta_{r',r-q+sp}e^{i2\pi sk_1}e^{-i\frac{2\pi}{p}\left(k_2+r-\frac{q}{2}\right)}. \tag{16}$$

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

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

3.3 Matrix elements in - valley

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

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

The moiré potential is

$$\langle -1\alpha' n' r'\boldsymbol{k}|U_{-}|-2\alpha n r\boldsymbol{k}\rangle=[T_1^{-}]_{\alpha'\alpha}\delta_{n'n}\delta_{r'r}+[T_2^{-}]_{\alpha'\alpha}[e^{i\boldsymbol{b}_2\cdot\boldsymbol{r}}]_{n'r'\boldsymbol{k},nr\boldsymbol{k}}+[T_3^{-}]_{\alpha'\alpha}[e^{i(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{r}}]_{n'r'\boldsymbol{k},nr\boldsymbol{k}}, \tag{19}$$

where

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

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

4 Chern number

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

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

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

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

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

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

where

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

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