Hofstadter spectrum of TBG

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May 30, 2023

1 BM Hamiltonian

Twisted bilayer graphene (TBG) has the continuum BM Hamiltonian. In this note we only focus on valley $\eta = +$, which under magnetic field $\boldsymbol{B} = B\boldsymbol{e}_z$ is written as

$$
\begin{aligned}
H &= \begin{pmatrix} v_F(\boldsymbol{\pi} - \hbar\boldsymbol{K}_1)\cdot\boldsymbol{\sigma} & U(\boldsymbol{r}) \\ U^\dagger(\boldsymbol{r}) & v_F(\boldsymbol{\pi} - \hbar\boldsymbol{K}_2)\cdot\boldsymbol{\sigma} \end{pmatrix}, \\
U(\boldsymbol{r}) &= W_1 + W_2 e^{-i(\boldsymbol{g}_1+\boldsymbol{g}_2)\cdot\boldsymbol{r}} + W_3 e^{-i\boldsymbol{g}_2\cdot\boldsymbol{r}} = e^{i(\boldsymbol{K}_1-\boldsymbol{K}_2)\cdot\boldsymbol{r}}(W_1 e^{i\boldsymbol{q}_1\cdot\boldsymbol{r}} + W_2 e^{i\boldsymbol{q}_2\cdot\boldsymbol{r}} + W_3 e^{i\boldsymbol{q}_3\cdot\boldsymbol{r}}), \\
W_1 &= \begin{pmatrix} u_0 & u_1 \\ u_1 & u_0 \end{pmatrix}, \quad W_2 = \begin{pmatrix} u_0 & u_1\omega^{-1} \\ u_1\omega & u_0 \end{pmatrix}, \quad W_3 = \begin{pmatrix} u_0 & u_1\omega \\ u_1\omega^{-1} & u_0 \end{pmatrix},
\end{aligned} \tag{1}
$$

where $\boldsymbol{\pi} = \boldsymbol{p} + e\boldsymbol{A}$, and in this note we take the Landau gauge $\boldsymbol{A} = Bx\boldsymbol{e}_y$. The lattice vectors in real and reciprocal spaces are respectively

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

and $\boldsymbol{q}_1 = \frac{4\pi}{3L_\theta}(0,1)$, $\boldsymbol{q}_2 = \frac{4\pi}{3L_\theta}\left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$, $\boldsymbol{q}_3 = \frac{4\pi}{3L_\theta}\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$. Notice that we have change the basis choice to make $\boldsymbol{a}_2^m$ along $\boldsymbol{e}_y$. The momentum shift of the two layers are ($\boldsymbol{\Gamma}_G$ is the offset, i.e., center of the reciprocal cutoff)

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

2 LL basis for graphene, momentum shift

Although the theory is the same, one cannot simply use the conventional Landau level (LL) basis which put the momentum center $\boldsymbol{k} = 0$. They are not eigenstates of TBG in the absence of moire potential. We'd better use the LL basis of monolayer graphene as the starting point. The monolayer graphene has the Hamiltonian (omit the layer tensor ϱ_l)

$$
h_l(\boldsymbol{\pi}) = v_F(\boldsymbol{\pi} - \hbar\boldsymbol{K}_l)\cdot\boldsymbol{\sigma} = i\frac{\sqrt{2}\hbar v_F}{l_B}\begin{pmatrix} & -a \\ a^\dagger & \end{pmatrix} - \hbar v_F \boldsymbol{K}_l\cdot\boldsymbol{\sigma}, \tag{4}
$$

where $l_B = \sqrt{\hbar/(eB)}$, and the ladder operator is the normal one: $a \sim i(\pi_x - i\pi_y)$, $a^\dagger \sim -i(\pi_x + i\pi_y)$. The operators $a^\dagger a$ and p_y has common eigenstates $\phi_{n,k_y} = \langle\boldsymbol{r}|n, k_y\rangle$ (see my note "Landau level formulation"). But be careful here we have the momentum shift $\boldsymbol{K}_l$ in Eq. (4). Correspondingly, we define the LLs with modified momentum (the p_y eigenvalue is $\hbar k_y$)

$$
\phi^{(l)}_{n,k_y}(\boldsymbol{r}) = \langle\boldsymbol{r}|l, n, k_y\rangle = \frac{1}{\sqrt{L_y}} e^{iK_{lx}x} e^{ik_y y}\langle x + (k_y - K_{ly})l_B^2|n\rangle = e^{i\boldsymbol{K}_l\cdot\boldsymbol{r}}\phi_{n,k_y-K_{ly}}(\boldsymbol{r}). \tag{5}
$$

The only difference with ϕ_{n,k_y} (see Section 4) is the prefactor $\exp(i\boldsymbol{K}_l \cdot \boldsymbol{r})$ to eliminate the shift in $\boldsymbol{\pi} - \hbar \boldsymbol{K}_l$. Under t_1^s it translates like

$$t_1^s \phi^{(l)}_{n,k_y} = e^{i\frac{s(s-1)}{2}\boldsymbol{q}_\phi \cdot \boldsymbol{a}_1} e^{-isK_{lx}a_{1x}} e^{-isk_y a_{1y}} \phi^{(l)}_{n,k_y - s\frac{2\pi}{L_\theta}\frac{p}{q}}(\boldsymbol{r}). \tag{6}$$

The plane wave matrix under $\phi^{(l)}_{n,k_y}$ is thus

$$\begin{aligned}
\langle l', n', k_y' | e^{i\boldsymbol{q}\cdot\boldsymbol{r}} | l, n, k_y \rangle &= \langle n', k_y' - K_{l'y} | e^{i(\boldsymbol{q} - \boldsymbol{K}_{l'} + \boldsymbol{K}_l)\cdot \boldsymbol{r}} | n, k_y - K_{ly} \rangle \\
&= \delta_{k_y', k_y + q_y} e^{-i\left[(q_{l'l})_x (k_y - K_{ly}) + \frac{(q_{l'l})_x (q_{l'l})_y}{2}\right] l_B^2} F_{n'n}(\boldsymbol{q}_{l'l}) \\
&= \delta_{k_y', k_y + q_y} e^{-i\left[(q_{l'l})_x (k_y' - K_{l'y}) - \frac{(q_{l'l})_x (q_{l'l})_y}{2}\right] l_B^2} F_{n'n}(\boldsymbol{q}_{l'l}),
\end{aligned} \tag{7}$$

where $\boldsymbol{q}_{l'l} = \boldsymbol{q} - \boldsymbol{K}_{l'} + \boldsymbol{K}_l$, and $F_{n'n}(\boldsymbol{q})$ can be found in another note.

The actual eigenstates with eigenenergy $\mathrm{sgn}(n)\sqrt{2|n|}\hbar v_F / l_B$, i.e., LLs of Eq. (4) is

$$\Phi^{(l)}_{n,k_y}(\boldsymbol{r}) = \alpha_n \begin{pmatrix} -i\,\mathrm{sgn}(n)\phi^{(l)}_{|n|-1,k_y}(\boldsymbol{r}) \\ \phi^{(l)}_{|n|,k_y}(\boldsymbol{r}) \end{pmatrix} = \alpha_n e^{i\boldsymbol{K}_l \cdot \boldsymbol{r}} \begin{pmatrix} -i\,\mathrm{sgn}(n)\phi_{|n|-1,k_y - K_{ly}}(\boldsymbol{r}) \\ \phi_{|n|,k_y - K_{ly}}(\boldsymbol{r}) \end{pmatrix}, \tag{8}$$

where n takes all integer values: $n = 0, \pm 1, \pm 2, \ldots$, and $\alpha_0 = 1$, $\alpha_n = 2^{-1/2}$ for $n \neq 0$. We can use $\Phi^{(l)}_{n,k_y}$ to construct eigenstates of the magnetic translation group (MTG), as we did for the cases without momentum shift.

3 MTG basis, and matrix element

However, a more convenient choice of basis to avoid $\mathrm{sgn}(n)$ and α_n before that should be to use state $|l, \alpha, n, k_y\rangle$ where the only component $|l, n, k_y\rangle$ is on layer $l = 1, 2$ and sublattice α, and n takes non-negative integers. It is clear that $|l, \alpha, n, k_y\rangle, n = 0, 1, 2, \ldots$ and $|\Phi^{(l)}_{n,k_y}\rangle, n = 0, \pm 1, \pm 2, \ldots$ can be transformed to each other easily. But we have to be careful that, if the LL cutoff for B sublattice is N_c, then the cutoff for A sublattice should better be $N_c - 1$, to make the cutoff subspace closed. For commensurate field with $\phi/\phi_0 = p/q$, the MTG basis can then be defined as ($\mathcal{X}_{l\alpha}$ is the vector whose only nonzero element is indexed by $l\alpha$ and has value 1)

$$|l, \alpha, n, r, k_1, k_2\rangle = \frac{\mathcal{X}_{l\alpha}}{\sqrt{N_1}} \sum_s e^{i2\pi k_1 s} t_1^s \left| l, n, \frac{2\pi}{L_\theta}\left(k_2 + \frac{r}{q}\right)\right\rangle, \tag{9}$$

for $k_1 \times k_2 \in [0, 1) \times [0, 1/q)$, $r = 0, 1, \ldots, p-1$, $n = 0, 1, \ldots, N_c$ for $\alpha = B$ and $n = 0, 1, \ldots, N_c - 1$ for $\alpha = A$. One may prove (notice that the eigenvalue of t_2^q is shifted)

$$\begin{aligned}
t_1 |l, \alpha, n, r, k_1, k_2\rangle &= e^{-i2\pi k_1} |l, \alpha, n, r, k_1, k_2\rangle, \\
t_2^q |l, \alpha, n, r, k_1, k_2\rangle &= e^{-i2\pi k_2 q} |l, \alpha, n, r, k_1, k_2\rangle, \\
\langle l', \alpha', n', r', k_1', k_2' | l, \alpha, n, r, k_1, k_2\rangle &= \delta_{l'l}\delta_{\alpha'\alpha}\delta_{n'n}\delta_{r'r}\delta_{k_1'k_1}\delta_{k_2'k_2}.
\end{aligned} \tag{10}$$

The plane wave matrix under the MTG basis then becomes ($\mathcal{X}_{l'\alpha',l\alpha}$ is the matrix whose only nonzero element is at $(l'\alpha', l\alpha)$ and has value 1)

$$
\begin{aligned}
&\langle l', \alpha, n', r', k_1', k_2'| e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\mathcal{X}_{l'\alpha',l\alpha}|l,\alpha,n,r,k_1,k_2\rangle \\
=&\frac{1}{N_1}\sum_{s's} e^{i2\pi k_1 s - i2\pi k_1' s'}\left\langle l', n', \frac{2\pi}{L_\theta}\left(k_2' + \frac{r'}{q}\right)\right| t_1^{-s'} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} t_1^{s}\left| l, n, \frac{2\pi}{L_\theta}\left(k_2 + \frac{r}{q}\right)\right\rangle \\
=&\frac{1}{N_1}\sum_{s's} e^{i2\pi (k_1 s - k_1' s')} e^{is'\boldsymbol{q}\cdot\boldsymbol{a}_1}\left\langle l', n', \frac{2\pi}{L_\theta}\left(k_2' + \frac{r'}{q}\right)\right| e^{i\boldsymbol{q}\cdot\boldsymbol{r}} t_1^{s-s'}\left| l, n, \frac{2\pi}{L_\theta}\left(k_2 + \frac{r}{q}\right)\right\rangle \\
=&\frac{1}{N_1}\sum_{s's} e^{i2\pi k_1 s} e^{i[2\pi(k_1-k_1')+\boldsymbol{q}\cdot\boldsymbol{a}_1]s'}\left\langle l', n', \frac{2\pi}{L_\theta}\left(k_2' + \frac{r'}{q}\right)\right| e^{i\boldsymbol{q}\cdot\boldsymbol{r}} t_1^{s}\left| l, n, \frac{2\pi}{L_\theta}\left(k_2 + \frac{r}{q}\right)\right\rangle \\
=&\delta_{k_1',[k_1+q_1]_1}\sum_s e^{i2\pi k_1 s} e^{i\frac{s(s-1)}{2}\boldsymbol{q}_\phi\cdot\boldsymbol{a}_1} e^{-isK_{lx}a_{1x}} e^{-is\pi\left(k_2+\frac{r}{q}\right)} \\
&\times\left\langle l', n', \frac{2\pi}{L_\theta}\left(k_2' + \frac{r'}{q}\right)\right| e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\left| l, n, \frac{2\pi}{L_\theta}\left(k_2 + \frac{r-sp}{q}\right)\right\rangle \\
=&\delta_{k_1',[k_1+q_1]_1}\sum_s \delta_{k_2'+\frac{r'}{q},k_2+\frac{r-sp}{q}+q_2} e^{i2\pi k_1 s} e^{i\frac{\pi}{2}\frac{p}{q}s(s-1)-is\pi\left(k_2+\frac{r}{q}+1\right)} \\
&\times e^{-i\left[(q_{l'l})_x\left(\frac{2\pi}{L_\theta}\left(k_2'+\frac{r'}{q}\right)-K_{l'y}\right)-\frac{(q_{l'l})_x(q_{l'l})_y}{2}\right]l_B^2} F_{n'n}(\boldsymbol{q}_{l'l}).
\end{aligned}
\tag{11}
$$

Now we write down the matrix element under MTG basis (8). First the BM Hamiltonian can be decomposed as

$$
H(\boldsymbol{\pi},\boldsymbol{r}) = \varrho_1 h_1(\boldsymbol{\pi}) + \varrho_2 h_2(\boldsymbol{\pi}) + [\varrho_+ W_1 + \varrho_+ W_2 e^{-i(\boldsymbol{g}_1+\boldsymbol{g}_2)\cdot\boldsymbol{r}} + \varrho_+ W_3 e^{-i\boldsymbol{g}_2\cdot\boldsymbol{r}} + h.c.], \tag{12}
$$

where ϱ_i represents 2×2 matrices in layer space. It is diagonal in $\boldsymbol{k} = (k_1, k_2)$.

The monolayer kinetic term $h_l(\boldsymbol{\pi})$ has the following elements

$$
\langle l'\alpha' n' r' \boldsymbol{k}|\varrho_t h_t|l\alpha n r\boldsymbol{k}\rangle = i\frac{\sqrt{2}\hbar v_F}{l_B}\delta_{l't}\delta_{lt}\begin{pmatrix} & -\sqrt{n}\delta_{n'+1,n} \\ \sqrt{n'}\delta_{n',n+1} & \end{pmatrix}_{\alpha'\alpha}\delta_{r'r}, \tag{13}
$$

$$
\langle l'\alpha' n' r' \boldsymbol{k}|\varrho_+ W_1|l\alpha n r\boldsymbol{k}\rangle = \delta_{l'1}\delta_{l2}(W_1)_{\alpha'\alpha}F_{n'n}(\boldsymbol{q}_1), \tag{14}
$$

$$
\begin{aligned}
\langle l'\alpha' n' r \boldsymbol{k}|\varrho_+ W_2 e^{-i(\boldsymbol{g}_1+\boldsymbol{g}_2)\cdot\boldsymbol{r}}|l\alpha n r\boldsymbol{k}\rangle =& \delta_{l'1}\delta_{l2}(W_2)_{\alpha'\alpha}F_{n'n}(\boldsymbol{q}_2) \\
&\times\sum_s \delta_{r',r-sp-q} e^{i2\pi k_1 s} e^{i\frac{\pi}{2}\frac{p}{q}s(s-1)-is\pi\left(k_2+\frac{r}{q}+1\right)} e^{i\pi\frac{q}{p}\left(k_2+\frac{r'}{q}+\frac{1}{2}\right)},
\end{aligned}
\tag{15}
$$

$$
\begin{aligned}
\langle l'\alpha' n' r' \boldsymbol{k}|\varrho_+ W_3 e^{-i\boldsymbol{g}_2\cdot\boldsymbol{r}}|l\alpha n r\boldsymbol{k}\rangle =& \delta_{l'1}\delta_{l2}(W_3)_{\alpha'\alpha}F_{n'n}(\boldsymbol{q}_3) \\
&\times\sum_s \delta_{r',r-sp-q} e^{i2\pi k_1 s} e^{i\frac{\pi}{2}\frac{p}{q}s(s-1)-is\pi\left(k_2+\frac{r}{q}+1\right)} e^{-i\pi\frac{q}{p}\left(k_2+\frac{r'}{q}+\frac{1}{2}\right)}.
\end{aligned}
\tag{16}
$$

The parameters are: $k_1 \in [0, 1)$ (effectively $k_1 \in [0, 1/q)$ is enough to produce the Hofstadter spectrum since other stripes are degenerate with this part), $k_2 \in [0, 1/q)$, $l = 1, 2$, $\alpha = A, B$, $r = 0, 1, \ldots, p-1$, and $n = 0, 1, \ldots, N_c - 2$ for $\alpha = A$, $n = 0, 1, \ldots, N_c - 1$ for $\alpha = B$.

4 Another set of MTG basis

Now we switch to the most original MTG basis to diagonalize the BM Hamiltonian. We use exactly the same MTG LLs like in the square and triangular cases, i.e., we neglect the momentum shift in monolayer terms and treat them as some kind of constant potentials. Becareful, it is important to keep the cutoff of LLs on sublattice A smaller than that on sublattice B by 1. We list the formula briefly in this section under such basis.

The LL basis is defined as

$$
|l,\alpha,n,r,\boldsymbol{k}\rangle = \frac{\mathcal{X}_{l\alpha}}{\sqrt{N_1}}\sum_s e^{i2\pi k_1 s} t_1^s\left| n, \frac{2\pi}{L_\theta}\left(k_2 + \frac{r}{q}\right)\right\rangle, \tag{17}
$$

where $|n,k_y\rangle$ is the bare LL wavefunction, $\langle r|n,k_y\rangle = \frac{1}{\sqrt{L_y}}e^{ik_y y}\langle x+k_y l_B^2|n\rangle = \phi_{n,k_y}(\boldsymbol{r})$. Written in this basis, the matrix elements can be directly read from "Note_Hofstadter_physics"

$$
\begin{aligned}
\langle l'\alpha'n'r'\boldsymbol{k}|\varrho_t h_t|l\alpha n r\boldsymbol{k}\rangle =& i\frac{\sqrt{2}\hbar v_F}{l_B}\delta_{l't}\delta_{lt}\begin{pmatrix} & -\sqrt{n}\delta_{n'+1,n} \\ \sqrt{n'}\delta_{n',n+1} & \end{pmatrix}_{\alpha'\alpha}\delta_{r'r} \\
&-\hbar v_F\delta_{l't}\delta_{lt}(\boldsymbol{K}_t\cdot\boldsymbol{\sigma})_{\alpha'\alpha}\delta_{n'n}\delta_{r'r}, &(18)\\
\langle l'\alpha'n'r'\boldsymbol{k}|\varrho_+ W_1|l\alpha n r\boldsymbol{k}\rangle =& \delta_{l'1}\delta_{l2}(W_1)_{\alpha'\alpha}\delta_{n'n}\delta_{r'r}, &(19)\\
\langle l'\alpha'n'r\boldsymbol{k}|\varrho_+ W_2 e^{-i(\boldsymbol{g}_1+\boldsymbol{g}_2)\cdot\boldsymbol{r}}|l\alpha n r\boldsymbol{k}\rangle =& \delta_{l'1}\delta_{l2}(W_2)_{\alpha'\alpha}F_{n'n}(-\boldsymbol{g}_1-\boldsymbol{g}_2) \\
&\times\sum_s \delta_{r',r-sp-q}e^{i2\pi k_1 s}e^{i\frac{\pi}{2}\frac{p}{q}s(s-1)-is\pi\left(k_2+\frac{r}{q}\right)}e^{i\pi\frac{q}{p}\left(k_2+\frac{r'}{q}+\frac{1}{2}\right)}, &(20)\\
\langle l'\alpha'n'r'\boldsymbol{k}|\varrho_+ W_3 e^{-i\boldsymbol{g}_2\cdot\boldsymbol{r}}|l\alpha n r\boldsymbol{k}\rangle =& \delta_{l'1}\delta_{l2}(W_3)_{\alpha'\alpha}F_{n'n}(-\boldsymbol{g}_2) \\
&\times\sum_s \delta_{r',r-sp-q}e^{i2\pi k_1 s}e^{i\frac{\pi}{2}\frac{p}{q}s(s-1)-is\pi\left(k_2+\frac{r}{q}\right)}e^{-i\pi\frac{q}{p}\left(k_2+\frac{r'}{q}+\frac{1}{2}\right)}. &(21)
\end{aligned}
$$

I have checked that this set of basis could also correctly reproduce the Hofstadter spectrum (at low-field regime it behaves worse than the previous basis considering the momentum shift with the same LL cutoff).