Tight-binding Hamiltonian

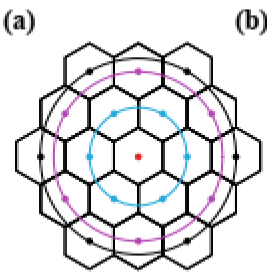
First, we introduce the tight-binding Hamiltonian we use to describe Gamma valley twisted TMD here following 'Γ valley transition metal dichalcogenide moire bands'.

$$H_t = -\frac{\hbar^2 \boldsymbol{k}^2}{2m^*} - \sum_s V_s \sum_{j=1}^{6} e^{i\boldsymbol{g}_j^s \cdot \boldsymbol{r}}$$

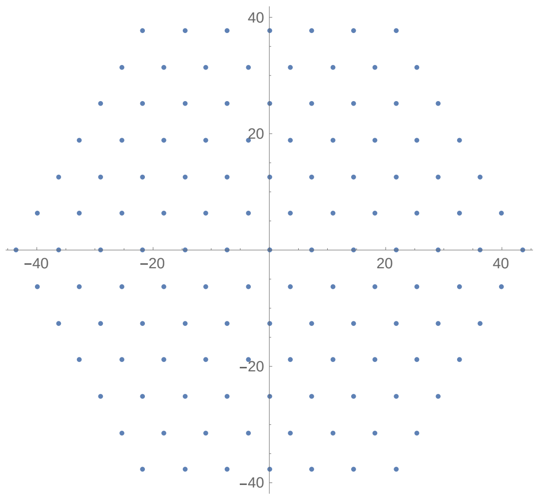
After Fourier transformation for moire potential,

$$H_t(k) = -\sum_{\boldsymbol{G}} \frac{\hbar^2(\boldsymbol{k}+\boldsymbol{G})^2}{2m^*} c_{\boldsymbol{k}+\boldsymbol{G}}^{\dagger} c_{\boldsymbol{k}+\boldsymbol{G}} - \sum_{\boldsymbol{G}} \sum_s V_s \sum_{j=1}^{6} c_{\boldsymbol{k}+\boldsymbol{G}}^{\dagger} c_{\boldsymbol{k}+\boldsymbol{G}+\boldsymbol{g}_j^s}$$

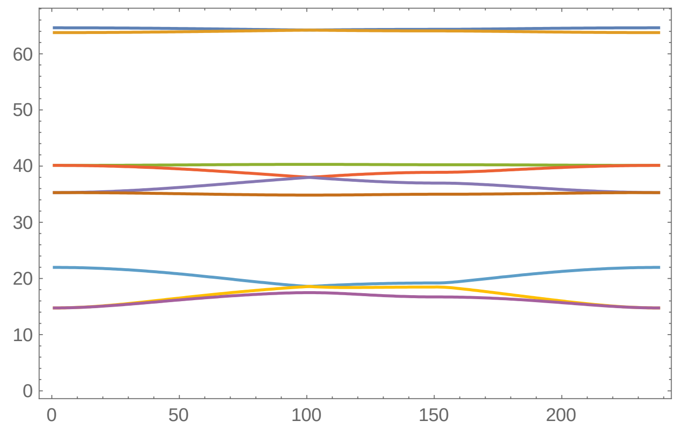
Here, parameter $\theta = 1.2°, V_1 = 33.5, V_2 = 4, V_3 = 5.5, m^* = 0.87m_e, a_0 = 0.318nm$, $\boldsymbol{g_j^s}$ are reciprocal lattice vector linking the 's' nearest shell like below



We choose cut-off of G points from Gamma point as below



After diagonalization, we plot up-most 9 bands as the picture shown in MacDonald's paper



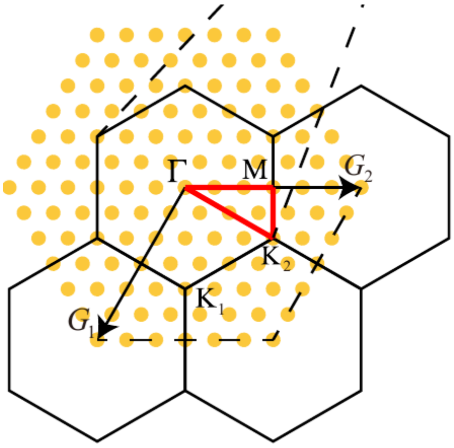
Flat band Hamiltonian with Coulomb interaction at half filling

Next, we project Coulomb interaction on top-most two bands and assume flat band limit at half filling. The Hamiltonian now is

$$H_I = \frac{1}{2\Omega} \sum_{q+G\neq 0} V(q+G)\rho_{q+G}\rho_{-q-G}$$

$$\rho_{q+G} = \sum_{k,m,n} \lambda_{m,n}(k, k+q+G)\left(c^{\dagger}_{k,m,s}c_{k+q,n,s} + c^{\dagger}_{k,m,-s}c_{k+q,n,-s} - \delta_{q,0}\delta_{m,n}\right) = \rho^{\dagger}_{-q-G}$$

Here $\lambda_{m,n}(k, k+q+G) \equiv \sum_{G'} u^{*}_{m,G'}(k)u_{n,G'}(k+q+G)$, $u_{n,G'}(k+q+G)$ is the eigenvector of band n at momentum point $k+q+G$. $\frac{V(q+G)}{\Omega} \approx \frac{\theta}{\epsilon_r N_k}\frac{4\pi}{\sqrt{3}}\frac{\tanh(q\cdot d)}{q\cdot a_M}$, here we take $\theta = 1.2, \epsilon_r = 1, d = 2a_M$ for computation for now. Again, we make a cut-off for momentum transfer $q+G$ as the yellow points below (take 6×6 momentum points as an example)



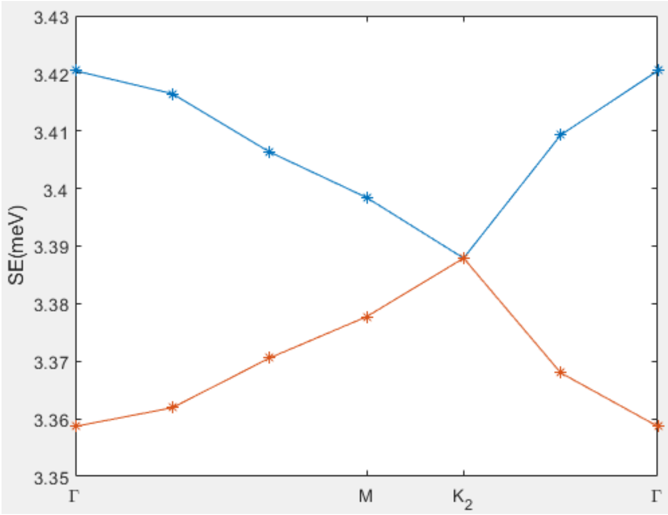
Ground states, Single-particle excitations and correlations

Here we introduce how we get ground states, single-particle excitations and correlations by noticing SU(2) symmetry for spin. First, one notice spin-polarize (SP) is one of degenerated ground states for this positive semidefinite Hamiltonian since $\lambda_{m,m}(k,k) = 1$ and $\rho_{q+G}|\psi^{Full}_{-s}\rangle = 0$. Then we can define a raising operator $\Delta^{\dagger} = \sum_{k,m} c^{\dagger}_{k,m,s}c_{k,m,-s}$, one can easily check $[\rho_{q+G}, \Delta^{\dagger}] = 0$ so that $[H_I, \Delta^{\dagger}] = 0$ and $(\Delta^{\dagger})^n|\psi^{Full}_{-s}\rangle$ is also a ground state. Since here $n = 0,1,2,\ldots,2N$, there are $2N+1$ degenerate ground states because of spin SU(2).

One can see the energy for exciting a particle with spin s on state $|\psi^{Full}_{-s}\rangle$ is equal to the energy for exciting a particle from empty, which can be achieved by diagonalizing H_I in single-particle basis

$$H_I = \frac{1}{2\Omega} \sum_{q+G\neq 0} V(q+G) \sum_{k,m,n,n'} \lambda_{m,n'}(k, k+q+G)\lambda_{n',n}(k+q+G, k)c^{\dagger}_{k,m,s}c_{k,n,s}$$

Then one finds one single-particle excitation state from $|\psi^{Full}_{-s}\rangle$ with excitation energy $\varepsilon_{k,1}$ is $c^{\dagger}_{k,1,s}|\psi^{Full}_{-s}\rangle$, $H_I c^{\dagger}_{k,1,s}|\psi^{Full}_{-s}\rangle = \varepsilon_{k,1}c^{\dagger}_{k,1,s}|\psi^{Full}_{-s}\rangle$. And single-particle excitation from $(\Delta^{\dagger})^n|\psi^{Full}_{-s}\rangle$ will have the same excitation energy $\varepsilon_{k,1}$ since $H_I c^{\dagger}_{k,1,s}(\Delta^{\dagger})^n|\psi^{Full}_{-s}\rangle = (\Delta^{\dagger})^n H_I c^{\dagger}_{k,1,s}|\psi^{Full}_{-s}\rangle = \varepsilon_{k,1}c^{\dagger}_{k,1,s}(\Delta^{\dagger})^n|\psi^{Full}_{-s}\rangle$. Plot single-particle excitation (SE) for 6×6 momentum points as an example



Single-particle correlations (or single-particle Green's functions) can also be achieved by normalizing all ground states and single-particle states. First, $\langle\psi_{-s}^{Full}|\psi_{-s}^{Full}\rangle = 1$ so that $|\psi_{-s}^{Full}\rangle$ is already normalized. Since $[\Delta,\Delta^{\dagger}] = \sum_{k,m}(c_{k,m,-s}^{\dagger}c_{k,m,-s} - c_{k,m,s}^{\dagger}c_{k,m,s}) = \widehat{N}_{-s} - \widehat{N}_s$, $\langle\psi_{-s}^{Full}|\Delta^n(\Delta^{\dagger})^n|\psi_{-s}^{Full}\rangle = n(2N-n+1)\langle\psi_{-s}^{Full}\left|\Delta^{n-1}(\Delta^{\dagger})^{n-1}\right|\psi_{-s}^{Full}\rangle = \frac{n!(2N)!}{(2N-n)!}$. Then we define normalized ground states $|\psi_n\rangle = \sqrt{\frac{(2N-n)!}{n!(2N)!}}(\Delta^{\dagger})^n|\psi_{-s}^{Full}\rangle$. For normalizing $c_{k,1,s}^{\dagger}(\Delta^{\dagger})^n|\psi_{-s}^{Full}\rangle$, one notice $\Delta c_{k,1,s}^{\dagger}|\psi_{-s}^{Full}\rangle = 0$ so that $\langle\psi_{-s}^{Full}|c_{k,1,s}\Delta^n(\Delta^{\dagger})^n c_{k,1,s}^{\dagger}|\psi_{-s}^{Full}\rangle = n(2N-n)\langle\psi_{-s}^{Full}\left|c_{k,1,s}\Delta^{n-1}(\Delta^{\dagger})^{n-1}c_{k,1,s}^{\dagger}\right|\psi_{-s}^{Full}\rangle = \frac{n!(2N-1)!}{(2N-1-n)!}$. We define normalized single-particle excitation states $|\psi_{n,k,1}\rangle = \sqrt{\frac{(2N-1-n)!}{n!(2N-1)!}}c_{k,1,s}^{\dagger}(\Delta^{\dagger})^n|\psi_{-s}^{Full}\rangle = \sqrt{\frac{2N}{2N-n}}c_{k,1,s}^{\dagger}|\psi_n\rangle$. At the same time, one can compute $\langle\psi_{-s}^{Full}|\Delta^n c_{k,1,s}^{\dagger}c_{k,1,s}(\Delta^{\dagger})^n|\psi_{-s}^{Full}\rangle = \langle\psi_{-s}^{Full}|\Delta^n(\Delta^{\dagger})^n|\psi_{-s}^{Full}\rangle - \langle\psi_{-s}^{Full}|c_{k,1,s}\Delta^n(\Delta^{\dagger})^n c_{k,1,s}^{\dagger}|\psi_{-s}^{Full}\rangle = \frac{n!(2N)!}{(2N-n)!} - \frac{n!(2N-1)!}{(2N-1-n)!} = \frac{n!(2N-1)!}{(2N-1-n)!}\left(\frac{n}{2N-n}\right)$, so that we can define $|\psi_{n,k,-1}\rangle = \sqrt{\frac{(2N-1-n)!(2N-n)}{n!(2N-1)!n}}c_{k,1,s}(\Delta^{\dagger})^n|\psi_{-s}^{Full}\rangle = \sqrt{\frac{2N}{n}}c_{k,1,s}|\psi_n\rangle$. Now we are ready to write down single-particle correlations at low temperature limit

$$G_{k,1,s}(\tau) = \langle c_{k,1,s}(\tau)c_{k,1,s}^{\dagger}(0)\rangle = \frac{Tr\left(e^{-(\beta-\tau)H}c_{k,1,s}e^{-\tau H}c_{k,1,s}^{\dagger}\right)}{Tr(e^{-\beta H})}$$

$$\underset{\beta\to\infty}{\overset{\lim}{=}}\frac{1}{2N+1}\left[\sum_n e^{-\tau\varepsilon_{k,1}}\left|\langle c_{k,1,s}^{\dagger}\psi_n|\psi_{n,k,1}\rangle\right|^2 + \sum_n e^{-(\beta-\tau)\varepsilon_{k,1}}\left|\langle\psi_{n,k,-1}|c_{k,1,s}\psi_n\rangle\right|^2\right]$$

$$= \frac{1}{2N+1}\left[e^{-\tau\varepsilon_{k,1}}\sum_n\frac{2N-n}{2N} + e^{-(\beta-\tau)\varepsilon_{k,1}}\sum_n\frac{n}{2N}\right]$$

$$= \frac{1}{2}e^{-\tau\varepsilon_{k,1}} + \frac{1}{2}e^{-(\beta-\tau)\varepsilon_{k,1}}$$

With the same spirit, $G_{k,2,s}(\tau) = \frac{1}{2}e^{-\tau\varepsilon_{k,2}} + \frac{1}{2}e^{-(\beta-\tau)\varepsilon_{k,2}}$.

Order parameter, continuous exciton excitations

For 2D system, we know SU(2) symmetry cannot spontaneously break so that there should be no magnetism. But magnet susceptibility is allowed. According to SU(2) symmetry, we define 'order parameters' $O_{x,q}, O_{z,q}$ as below

$$O_{x,q} = \sum_{k,m}(c_{k,m,s}^{\dagger}c_{k+q,m,-s} + c_{k,m,-s}^{\dagger}c_{k+q,m,s})$$

$$O_{z,q} = \sum_{k,m} \left(c^{\dagger}_{k,m,s} c_{k+q,m,s} - c^{\dagger}_{k,m,-s} c_{k+q,m,-s} \right)$$

We discuss this part according to $q = 0$ and $q \neq 0$ two cases.

When $q = 0$, one can check $[O_{x,0}, \rho_{q+G}] = [O_{z,0}, \rho_{q+G}] = 0$ so that $[O_{x,0}, H_I] = [O_{z,0}, H_I] = 0$. By noticing commutation relation $[O_{x,0}, \Delta^{\dagger}] = -O_{z,0} = \hat{N}_{-s} - \hat{N}_s$, we can normalize state $O_{x,0}(\Delta^{\dagger})^n \left|\psi^{Full}_{-s}\right\rangle = n(2N - n + 1)(\Delta^{\dagger})^{n-1}\left|\psi^{Full}_{-s}\right\rangle + (\Delta^{\dagger})^{n+1}|\psi^{Full}_{-s}\rangle$. That will be $O_{x,0}|\psi_n\rangle = \sqrt{n(2N-n+1)}|\psi_{n-1}\rangle + \sqrt{(n+1)(2N-n)}|\psi_{n+1}\rangle$. Combine all results above, we can see the excitation defined by $O_{x,0}$ at low temperature limit should be

$$\begin{aligned}
\langle O_{x,0}(\tau) O_{x,0}(0)\rangle &= \langle O_{x,0}(0) O_{x,0}(0)\rangle \\
&= \frac{Tr\left(e^{-\beta H} O_{x,0} O_{x,0}\right)}{Tr(e^{-\beta H})} \\
&\underset{\beta\to\infty}{\overset{\lim}{=}} \frac{1}{2N+1} \sum_n \langle \psi_n | O_{x,0} O_{x,0} | \psi_n \rangle \\
&= \frac{2}{2N+1} \sum_n n(2N - n + 1) \\
&= \frac{2N(2N+2)}{3}
\end{aligned}$$

At the same time, $\langle O_{z,0}(\tau) O_{z,0}(0)\rangle$ at low temperature limit can also be easily calculated

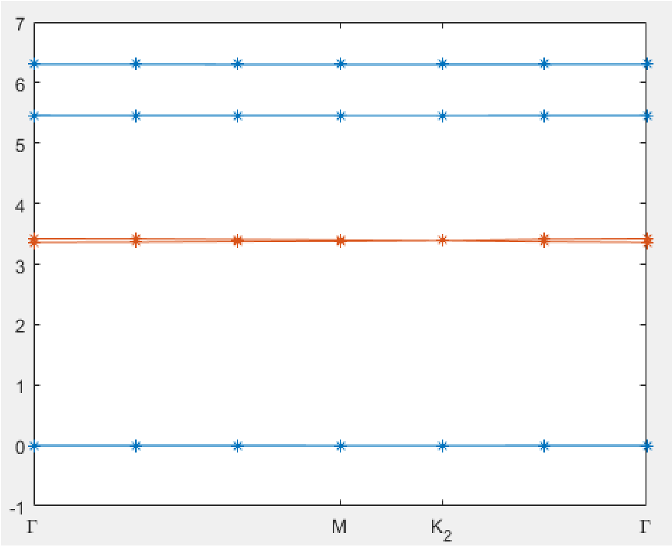
$$\begin{aligned}
\langle O_{z,0}(\tau) O_{z,0}(0)\rangle &= \langle O_{z,0}(0) O_{z,0}(0)\rangle \\
&= \frac{Tr\left(e^{-\beta H} O_{z,0} O_{z,0}\right)}{Tr(e^{-\beta H})} \\
&\underset{\beta\to\infty}{\overset{\lim}{=}} \frac{1}{2N+1} \sum_n (2N - 2n)^2 \\
&= \frac{2N(2N+2)}{3}
\end{aligned}$$

One can see $\langle O_{x,0}(\tau) O_{x,0}(0)\rangle = \langle O_{z,0}(\tau) O_{z,0}(0)\rangle$ and both do not decay with τ, which should be a natural result from SU(2) symmetry.

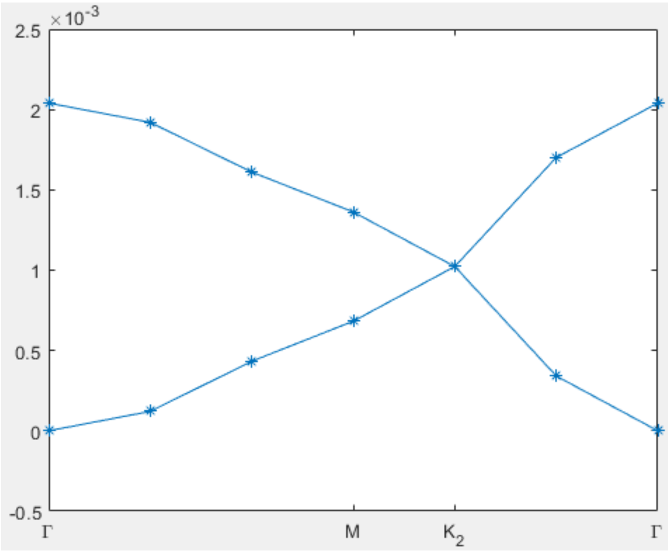
When $q \neq 0$, one can check $[O_{x,q}, H_I] \neq 0, [O_{z,q}, H_I] \neq 0$ generally, so that $\langle O_{x,q}(\tau) O_{x,q}(0)\rangle$ and $\langle O_{z,q}(\tau) O_{z,q}(0)\rangle$ will decay with τ (But it seems it is not the case in this single band model, maybe one need a better tight-binding model). Anyway, the steps below are general and can be applied when there is a better model. First, one can see for $p \neq 0$, $\langle \psi^{Full}_{-s} \left| \Delta^n c^{\dagger}_{k_2+p,n_2,s_2} c_{k_2,m_2,s_1} c^{\dagger}_{k_1,m_1,s_1} c_{k_1+p,n_1,s_2} (\Delta^{\dagger})^n \right| \psi^{Full}_{-s} \rangle = \delta_{k_1,k_2} \delta_{m_1,m_2} \delta_{n_1,n_2} A$, which means $c^{\dagger}_{k,m_1,s_1} c_{k+p,n_1,s_2} (\Delta^{\dagger})^n |\psi^{Full}_{-s}\rangle$ can form a group of orthogonal basis. Of course, one can derive Green's function by computing A here like what we have done in single-particle case, we will not discuss this part since there should be lots of exponential components at a single momentum p for $O_{x,q}$ or $O_{z,q}$ generally (Again, not the case here where $[O_{x,q}, H_I] \approx 0, [O_{z,q}, H_I] \approx 0$ because of $\lambda_{m,n}(k+p, k+p+q+G) \approx \lambda_{m,n}(k, k+q+G)$). By computing

$$\begin{aligned}
&[H_I, c^{\dagger}_{k,m_1,s} c_{k+p,n_1,-s}] (\Delta^{\dagger})^n |\psi^{Full}_{-s}\rangle \\
&= \sum_{q+G\neq 0} V(q+G) \sum_{m,n} \Big[\lambda_{n,m}(k, k+q+G) \lambda_{m,m_1}(k+q+G, k) c^{\dagger}_{k,n,s} c_{k+p,n_1,-s} \\
&\quad - 2\lambda_{n_1,n}(k+p, k+p+q+G) \lambda_{m,m_1}(k+q+G, k) c^{\dagger}_{k+q,m,s} c_{k+q+p,n,-s} \\
&\quad + \lambda_{n,m}(k+p+q+G, k+p) \lambda_{n_1,n}(k+p, k+p+q+G) c^{\dagger}_{k,m_1,s} c_{k+p,m,-s} \Big] (\Delta^{\dagger})^n |\psi^{Full}_{-s}\rangle
\end{aligned}$$

one can diagonalize and derive exciton excitations with different momentum p



Here the blue line represents the lowest 10 $c^{\dagger}_{k,m_1,s_1} c_{k+p,n_1,s_2}$ excitations with momentum p and red line represents single-particle excitations with momentum p. Zoom in for observing the lowest two excitations, one will see figure below



Contrast with TBG at chiral limit with neutral filling below, one can see different p all have almost zero-energy excitations. This result comes from $\lambda_{m,n}(k+p, k+p+q+G) \approx \lambda_{m,n}(k, k+q+G)$, which is the result we only fold one band to form moire flat band and wavefunctions of this band are very similar at little moire dispersion region.