Tight-binding Hamiltonian

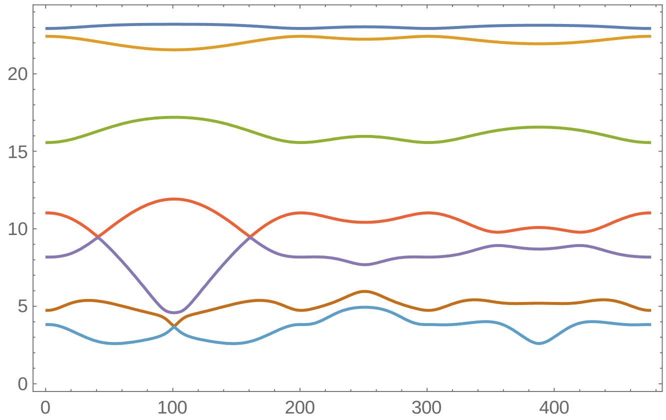
First, we introduce the tight-binding Hamiltonian we use to describe K valley twisted TMD here following 'Topological Insulators in Twisted Transition Metal Dichalcogenide Homobilayers' and 'Spontaneous fractional Chern insulators in transition metal dichalcogenides Moiré superlattices'.

$$H_+(k,r) = \begin{pmatrix} -\frac{\hbar^2(k-K_b)^2}{2m^*} + \Delta_b(r) & \Delta_T(r) \\ \Delta_T^\dagger(r) & -\frac{\hbar^2(k-K_t)^2}{2m^*} + \Delta_t(r) \end{pmatrix}$$

$$\Delta_l(r) = 2w_z \sum_{j=1,3,5} \cos\left(G_j \cdot r + l\psi\right), l \in \{b,t\} = \{+1,-1\}$$

$$\Delta_T(r) = w\left(1 + e^{-iG_2\cdot r} + e^{-iG_3\cdot r}\right)$$

Here, parameters $\left(\frac{\hbar^2}{2m^* a_0^2}, w_z, w, \psi, \theta\right) = (495meV, 8meV, -8.5meV, -89.6°, 1.2°)$. After Fourier transformation, taking topmost 7 bands, we plot energy dispersion below as the picture shown in MacDonald's paper



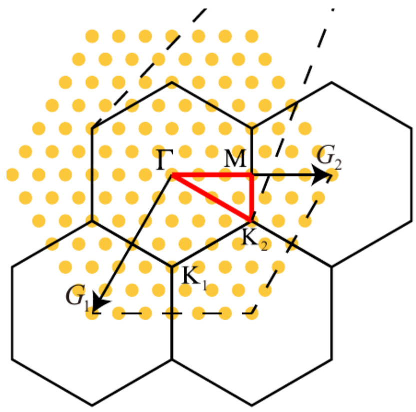
Flat band Hamiltonian with Coulomb interaction at half filling

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

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

$$\rho_{q+G} = \sum_{k,m,n,\tau} \lambda_{m,n,\tau}(k, k+q+G)\left(c_{k,m,\tau}^\dagger c_{k+q,n,\tau} - \frac{1}{2}\delta_{q,0}\delta_{m,n}\right) = \rho_{-q-G}^\dagger$$

Here $\lambda_{m,n,\tau}(k, k+q+G) \equiv \sum_{G'} u_{m,\tau,G'}^*(k) u_{n,\tau,G'}(k+q+G)$, $u_{n,\tau,G'}(k+q+G)$ is the eigenvector of band n at momentum point $k+q+G$ and valley τ. $\frac{V(q+G)}{\Omega} \approx \frac{\theta}{\epsilon_r N_k} \frac{4\pi}{\sqrt{3}} \frac{\tanh(q\cdot d)}{q\cdot a_M}$, 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)



By noticing a particle-hole symmetry, we can rewrite particle operator at valley $-\tau$ as hole operator

$$\rho_{q+G,-\tau} = \sum_{k,m,n} \lambda_{m,n,-\tau}(k,k+q+G)\left(c^{\dagger}_{k,m,-\tau}c_{k+q,n,-\tau} - \frac{1}{2}\delta_{q,0}\delta_{m,n}\right)$$
$$= -\sum_{k,m,n} \lambda_{n,m,\tau}(k,k+q+G)\left(c_{-k,n,-\tau}c^{\dagger}_{-k-q,m,-\tau} - \frac{1}{2}\delta_{q,0}\delta_{m,n}\right)$$
$$= -\sum_{k,m,n} \lambda_{n,m,\tau}(k,k+q+G)\left(\tilde{c}^{\dagger}_{k,n,-\tau}\tilde{c}_{k+q,m,-\tau} - \frac{1}{2}\delta_{q,0}\delta_{m,n}\right)$$

Here we redefine $\tilde{c}^{\dagger}_{k,n,-\tau} = c_{-k,n,-\tau}$ so that

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

Ground states, Single-particle excitations and correlations

Contrast with the case for Gamma valley, where there is a spin SU(2) symmetry, K valley freedom form a σ_z not σ_0 so that there is only a Z_2 symmetry. From $\rho_{q+G} = \sum_{k,m,n} \lambda_{m,n,\tau}(k,k+q+G)\left(c^{\dagger}_{k,m,\tau}c_{k+q,n,\tau} - \tilde{c}^{\dagger}_{k,m,-\tau}\tilde{c}_{k+q,n,-\tau}\right)$, we can easily find these two degenerate states $|\psi^{Full}_{\tau}\rangle \otimes |\tilde{\psi}^{Full}_{-\tau}\rangle$ and $|\psi^{Empty}_{\tau}\rangle \otimes |\tilde{\psi}^{Empty}_{-\tau}\rangle$. If one interprets $\tilde{c}^{\dagger}_{k,n,-\tau}$ back to $c_{-k,n,-\tau}$, these are two valley-polarized (spin-polarized) ground states $|\psi^{Full}_{\tau}\rangle \otimes |\psi^{Empty}_{-\tau}\rangle$ and $|\psi^{Empty}_{\tau}\rangle \otimes |\psi^{Full}_{-\tau}\rangle$.

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

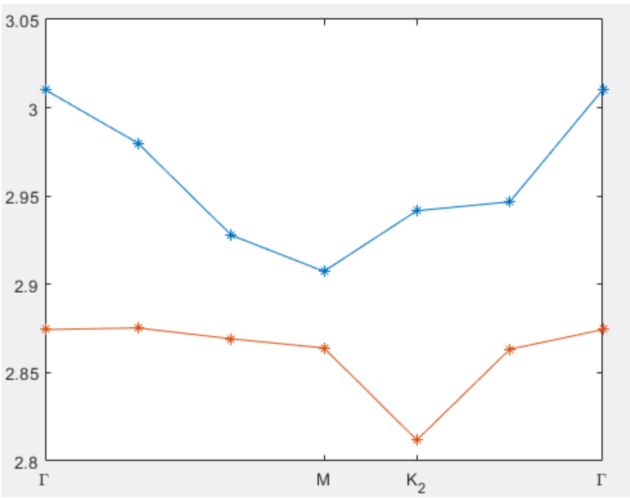
$$H_{\tau} = \frac{1}{2\Omega}\sum_{q+G\neq 0} V(q+G) \sum_{k,m,n,n'} \lambda_{m,n',\tau}(k,k+q+G)\lambda_{n',n,\tau}(k+q+G,k)c^{\dagger}_{k,m,\tau}c_{k,n,\tau}$$

While excite a particle at valley $-\tau$ on state $|\psi^{Full}_{\tau}\rangle \otimes |\psi^{Empty}_{-\tau}\rangle$ can be achieved by diagonalizing $H_{-\tau}$

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

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

This means single particle excitation $\varepsilon_{k,\tau,1} = \varepsilon_{-k,-\tau,1}$. Besides, one should notice there is another local C_{2z} rotation symmetry for $H_+(k,r)$. This rotation center is at middle point between K_b and K_t and can interchange two layers $H_+(k,r) = \sigma_x H_+(-k,-r)\sigma_x$. According to this rotation, $\lambda_{m,n,\tau}(k,k+q+G) = \lambda_{m,n,\tau}(-k,-k-q-G)$ after choosing a homogenous gauge. Finally, single particle excitation energy $\varepsilon_{k,\tau,1} = \varepsilon_{-k,\tau,1} = \varepsilon_{k,-\tau,1} = \varepsilon_{-k,-\tau,1} \equiv \varepsilon_{k,1}$. We plot $\varepsilon_{k,1}$ $\varepsilon_{k,2}$ for different momentum point k below



Single particle correlation (Green's function) at low temperature is easy to achieve

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

$$\lim_{\beta\to\infty} \frac{1}{2}\left[e^{-t\varepsilon_{k,1}}\left|\langle c_{k,1,\tau}^{\dagger}\psi_{\tau}^{Empty}|\psi_{\tau,k,1}\rangle\right|^2 + e^{-(\beta-t)\varepsilon_{k,1}}\left|\langle\psi_{\tau,k,-1}|c_{k,1,s}\psi_{\tau}^{Full}\rangle\right|^2\right]$$

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

This form is the same with the Gamma valley case.

Order parameter, gapped exciton excitations

Different with Gamma valley, this Z_2 symmetry can be broken with finite temperature fluctuation. And $O_{x,q}, O_{z,q}$ defined below will give totally different results because of lacking SU(2).

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

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

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

When $q = 0$, $[O_{z,0}, \rho_{q+G}] = 0$ so that

$$\langle O_{z,0}(t)O_{z,0}(0)\rangle = \langle O_{z,0}(0)O_{z,0}(0)\rangle$$

$$= \frac{Tr\left(e^{-\beta H}O_{z,0}O_{z,0}\right)}{Tr(e^{-\beta H})}$$

$$\lim_{\beta\to\infty}\frac{1}{2}\,2(2N)^2$$

$$= 4N^2$$

This means spectrum should have at least one zero point at momentum $p = 0$. While $[O_{x,0}, \rho_{q+G}] \neq 0$ and $\langle O_{x,0}(t)O_{x,0}(0)\rangle$ will decay exponentially with t or $\beta - t$.

When $q \neq 0$, $[O_{z,0}, \rho_{q+G}] \neq 0$. For computing exciton excitations, one need

$$[H_I, c_{k,m_1,\tau}^{\dagger}c_{k+p,n_1,-\tau}]|\psi_{\tau}^{Empty}\rangle\otimes|\psi_{-\tau}^{Full}\rangle$$

$$= \sum_{q+G\neq 0}V(q+G)\sum_{m,n}\Big[\lambda_{n,m,\tau}(k,k+q+G)\lambda_{m,m_1,\tau}(k+q+G,k)c_{k,n,\tau}^{\dagger}c_{k+p,n_1,-\tau}$$

$$- 2\lambda_{n_1,n,-\tau}(k+p,k+p+q+G)\lambda_{m,m_1,\tau}(k+q+G,k)c_{k+q,m,\tau}^{\dagger}c_{k+q+p,n,-\tau}$$

$$+ \lambda_{n,m,-\tau}(k+p+q+G,k+p)\lambda_{n_1,n,-\tau}(k+p,k+p+q+G)c_{k,m_1,\tau}^{\dagger}c_{k+p,m,-\tau}\Big]|\psi_{\tau}^{Empty}\rangle\otimes|\psi_{-\tau}^{Full}\rangle$$

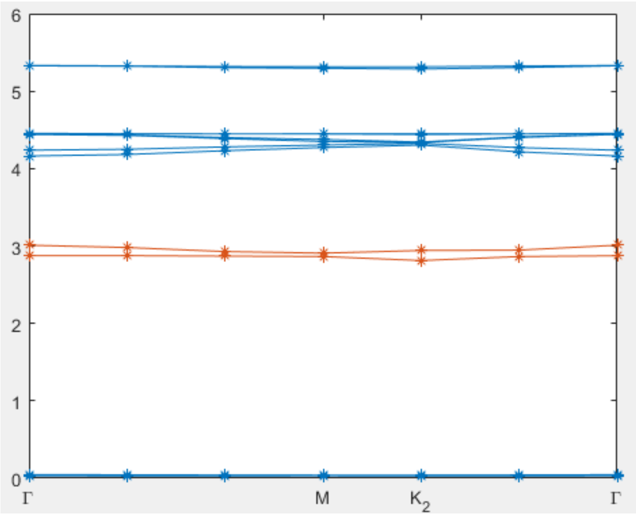
$$= \sum_{q+G\neq 0}V(q+G)\sum_{m,n}\Big[\lambda_{n,m,\tau}(k,k+q+G)\lambda_{m,m_1,\tau}(k+q+G,k)c_{k,n,\tau}^{\dagger}c_{k+p,n_1,-\tau}$$

$$- 2\lambda_{n_1,n,\tau}^{*}(k+p,k+p+q+G)\lambda_{m,m_1,\tau}(k+q+G,k)c_{k+q,m,\tau}^{\dagger}c_{k+q+p,n,-\tau}$$

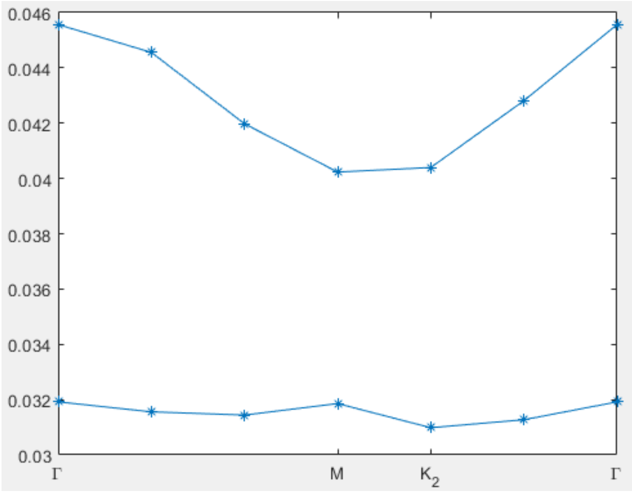
$$+ \lambda_{n,m,\tau}^{*}(k+p+q+G,k+p)\lambda_{n_1,n,\tau}^{*}(k+p,k+p+q+G)c_{k,m_1,\tau}^{\dagger}c_{k+p,m,-\tau}\Big]|\psi_{\tau}^{Empty}\rangle\otimes|\psi_{-\tau}^{Full}\rangle$$

By noticing $c_{k,m_1,\tau}^{\dagger}c_{k+p,n_1,\tau}|\psi_{\tau}^{Empty}\rangle\otimes|\psi_{-\tau}^{Full}\rangle$ always be zero if $q \neq 0$, we only diagonalize

$[H_I, c_{k,m_1,\tau}^{\dagger}c_{k+p,n_1,-\tau}]|\psi_{\tau}^{Empty}\rangle\otimes|\psi_{-\tau}^{Full}\rangle$ and the result is shown below



Here the blue line represents the lowest 10 $c^{\dagger}_{k,m_1,\tau}c_{k+p,n_1,-\tau}$ 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



One can see exciton excitation is gapped (only two lowest excitations are plotted), though the gap is much smaller than single particle's gap.