Derivation of the Bistritzer MacDonald Hamiltonian

B. Andrei Bernevig[1,2,3,*]
[1] *Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*
[2] *Physics Department, Freie Universitat Berlin, Arnimallee 14, 14195 Berlin, Germany*
[3] *Max Planck Institute of Microstructure Physics, 06120 Halle, Germany*
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We present a step-by-step derivation of the BM Hamiltonian

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I. CONVENTIONS, LATTICE AND DEFINITIONS

A. Original Graphene Lattice and Brillouin Zone

The original graphene lattice has the lattice wavevectors, in vector and complex notation (x/y components are the real/imaginary part of the complex number):

$$a_1 = (a\sqrt{3}, 0) = a\sqrt{3}e^{i0}, \quad a_2 = a(\sqrt{3}/2, 3/2) = a\sqrt{3}(1/2, \sqrt{3}/2) = a\sqrt{3}e^{i\pi/6} \tag{1}$$

where a is the bond length. We now pick the unit cell. The origin of the unit cell (and by default the rotation of the axis of the Moire later) is in the center of the hexagon. This means that the A and B sites in the lattice are at position:

$$t_A = ae^{i\pi/6}, \quad t_B = ae^{-i\pi/6} \tag{2}$$

The BZ lattice vectors satisfy $G_i \cdot a_j = 2\pi\delta_{ij}$:

$$G_1 = \frac{2\pi}{a\sqrt{3}}(1, -1/\sqrt{3}) = \frac{4\pi}{3a}e^{-i\pi/6}, \quad G_2 = \frac{4\pi}{3a}e^{i\pi/2} \tag{3}$$

The K point is then defined as the C_3 symmetric point of the BZ:

$$K = (\frac{2}{3}G_{1x}, 0) = \frac{2}{3}(\vec{G}_1 + \frac{1}{2}\vec{G}_2) \tag{4}$$

We now move to the Moire BZ and to the Moire Lattice. Employing complex number notation, we define the difference in wavevectors between two layers

$$q_1 = 2|K|Sin(\theta/2)e^{i\pi/2}, \;\; q_2 = 2|K|Sin(\theta/2)e^{i7\pi/6}, \;\; q_3 = 2|K|Sin(\theta/2)e^{i11\pi/6} \tag{5}$$

shown in Fig[**??**], where θ is the rotation angle between two layesr.

B. Moire BZ for Bilayer

While the construction of the multi-layer BZ, where there are different angles is more complicated and will be addressed later, we find that the twisted bilayer Moire Brillouin zone wavevectors are:

$$G_{M1} = q_2 - q_1 = 2|K|\sin(\theta/2)\sqrt{3}e^{i4\pi/3}, \quad G_{M2} = q_3 - q_1 = 2|K|\sin(\theta/2)\sqrt{3}e^{i5\pi/3} \tag{6}$$

The bilayer Moire lattice vectors are then $\vec{M}_i \cdot \vec{G}_{M_j} = 2\pi\delta_{ij}$:

$$M_1 = \frac{4\pi}{3(2|K|\sin(\theta/2))}e^{i7\pi/6}; \quad M_2 = \frac{4\pi}{3(2|K|\sin(\theta/2))}e^{i11\pi/6} \tag{7}$$

From now on we will call $\Delta = 2|K|\sin(\theta/2)$.

* bernevig@princeton.edu

II. NOTATIONS ON SYMMETRIES AND REPRESENTATIONS

We first specify the notations about symmetry and representations. If the Hamiltonian is symmetric under a group operation, g, we have

$$H(g\mathbf{k}) = D_{\mathbf{k}}(g)H(\mathbf{k})D_{\mathbf{k}}(g^{-1}), \tag{8}$$

where $D_{\mathbf{k}}$, the representation matrix of symmetry operator, in general depends on $\mathbf{k}$. In general $H(\mathbf{k})$ is not periodic in $\mathbf{k}$: it may change through a unitary transformation after a translation of reciprocal lattice, *i.e.*,

$$H(\mathbf{k}+\mathbf{G}) = V^{\mathbf{G}}H(\mathbf{k})V^{\mathbf{G}\dagger}. \tag{9}$$

Here $V^{\mathbf{G}}$ is the "embedding matrix" [?] and it satisfies $V^{\mathbf{G}_1}V^{\mathbf{G}_2} = V^{\mathbf{G}_1+\mathbf{G}_2}$ and $V^0 = \mathbb{I}$. For *symmorphic* space groups, we can always make $D_{\mathbf{k}}$ independent on $\mathbf{k}$ by properly choosing the embedding matrices. To be specific, for tight-binding models we can define the Hamiltonian in momentum space as $H_{\alpha s,\beta s'}(\mathbf{k}) = \langle\phi_{\alpha s\mathbf{k}}|\hat{H}|\phi_{\beta s'\mathbf{k}}\rangle$, where the Blöch bases are $|\phi_{\alpha s\mathbf{k}}\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}\alpha s} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{t}_s)}|\alpha\mathbf{R}+\mathbf{t}_s\rangle$, such that the embedding matrices are $V^{\mathbf{G}}_{\alpha s,\beta s'} = \delta_{\alpha\beta}\delta_{s,s'}e^{-i\mathbf{G}\cdot\mathbf{t}_s}$ and the $D_{\mathbf{k}}$'s are independent on $\mathbf{k}$. Here α is the orbital label, $\mathbf{R}$ is the lattice vector, $\mathbf{t}_s$ is the sublattice vector (the position of the sites in the unit cell), and N is the number of unit cells in real space. In this gauge, adopted in the rest of the paper, we sometimes omit the notation $D_{\mathbf{k}}(g)$ and replace it directly with g. When we write g acting on Hamiltonian and wave function, *i.e.*, $gH(\mathbf{k})g^{-1}$ and $g|u\rangle$, we mean it shorthand for $D_{\mathbf{k}}(g)H(\mathbf{k})D_{\mathbf{k}}(g)^{-1}$ and $D_{\mathbf{k}}(g)|u\rangle$, respectively.

Substituting Eq. (9) to Eq. (8), we get the following the identity

$$gV^{\mathbf{G}}g^{-1} = V^{g\mathbf{G}}. \tag{10}$$

For a high symmetry momentum $\mathbf{k}$ on the Brillouin Zone (BZ) boundary, which satisfies $g\mathbf{k} = \mathbf{k}+\mathbf{G}$ with $\mathbf{G}$ some reciprocal lattice, we have

$$gH(\mathbf{k})g^{-1} = V^{g\mathbf{k}-\mathbf{k}}H(\mathbf{k})V^{g\mathbf{k}-\mathbf{k}\dagger}. \tag{11}$$

Using identity (10), it is direct to prove that the matrices $V^{\mathbf{k}-g\mathbf{k}}g$, with $g\mathbf{k} = \mathbf{k}$ (modulo a reciprocal lattice), form a group commutting with $H(\mathbf{k})$. Therefore, when we say the wave functions at $\mathbf{k}$, $|u_{n\mathbf{k}}\rangle$, form a representation of the symmetry g, we actually mean that

$$V^{\mathbf{k}-g\mathbf{k}}g|u_{n\mathbf{k}}\rangle = \sum_m |u_{m\mathbf{k}}\rangle S_{mn}(g). \tag{12}$$

Here $S_{mn}(g)$ is the corresponding representation matrix.

III. MOIRÉ BAND MODEL (MBM)

A. Twisted Layers of Graphene (TMLG): One-valley Moiré band model (MBM-1V)

We here present a detailed derivation of the band structure of the Moiré pattern in twisted M-layer ($M \in Z$) graphene, with emphasis on the symmetries of the system. When the twisting angle is small, a Moiré pattern is formed by the interference of lattices from the M layers. The Moiré pattern has a very large length scale (or unit cell, if commensurate). The low energy, close to half-filling band structure is formed only from the electron states around the Dirac cones in each layer. A Moiré band theory describing such a state is built by the authors of Ref. [?]. In the following, we refer to it as one-valley Moiré model (MBM-1V). Part of our analytical study, especially the topological study, is mainly based on this model. Thus in this section, we give a review of the one-valley Moiré model and extend it to M layers. In order to index the M layer angle, pick a reference layer, called layer 1 and index the angles of all layers a from that layer $\theta_{1a} = \theta_a,\ \ a \in (2\ldots M)$.

We define the Blöch bases in the layer a as

$$\left|\phi^{(a)}_{\mathbf{p}\alpha}\right\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}^a} e^{i(\mathbf{R^a}+\mathbf{t}^a_\alpha)\cdot\mathbf{p}}\,|\mathbf{R}^a+\mathbf{t}^a_\alpha\rangle \tag{13}$$

where $a = 1 \dots M$ is the layer index, $\alpha = 1,2$ is the sublattice index, $\mathbf{t}^a_\alpha$ is the sublattice vector in layer a, $\mathbf{R}^a$ is lattice vector in layer a, and $|\mathbf{R}^a + \mathbf{t}^a_\alpha\rangle$ is the Wannier state at site $\mathbf{t}^a_\alpha$ in lattice $\mathbf{R}^a$. The Blöch bases in any other layer $b = 1 \dots M$ can be obtained by rotating and shifting the Blöch basis in layer a

$$\left|\phi^{(b)}_{\mathbf{p}\beta}\right\rangle = \hat{P}_{\left\{M_{\theta_{ab}}|\mathbf{d}\right\}}\left|\phi^{(a)}_{\left(M^{-1}_{\theta_{ab}}\mathbf{p}\right)\beta}\right\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}^b} e^{i\left(\mathbf{R}^b+\mathbf{t}^b_\beta\right)\cdot\mathbf{p}}\left|\mathbf{R}^b + \mathbf{t}^b_\beta\right\rangle \tag{14}$$

Here $M_{\theta_{ab}}$ is a rotation (by an angle $\theta_{ab} = \theta_b - \theta_a$) along the z axis, $\mathbf{d}$ is the translation from top layer to bottom layer, $\hat{P}_{\{M_\theta|\mathbf{d}\}} = \sum_{R_a}|M_{\theta_{ab}}(\mathbf{R}^a + \mathbf{t}^a_\alpha)\rangle\langle\mathbf{R}^a + \mathbf{t}^a_\alpha|$ is the corresponding rotation operator on wave-functions, $\mathbf{R}^b$ is the lattice vector in the b layer, and $\mathbf{t}^b_\beta$ is the sublattice vector in the bottom layer. It is easy to show that the intra-layer single-particle first quantized Hamiltonians of the a and b layers are related by:

$$H^{(bb)}_{\alpha\beta}(\mathbf{p}) = H^{(aa)}_{\alpha\beta}\left(M^{-1}_{\theta_{ab}}\mathbf{p}\right) \tag{15}$$

Here $H^{(aa)}$ is the a layer Hamiltonian and $H^{(bb)}$ is the b layer Hamiltonian.

We now derive the inter-layer coupling. First we Fourier transform the inter-layer hopping to real space:

$$\begin{aligned} H^{(ab)}_{\alpha\beta}(\mathbf{p},\mathbf{p}') &= \left\langle\phi^{(a)}_{\mathbf{p}\alpha}\right|\hat{H}\left|\phi^{(b)}_{\mathbf{p}'\beta}\right\rangle \\ &= \frac{1}{N}\sum_{\mathbf{R}^a\mathbf{R}^b} e^{-i(\mathbf{R}^a+\mathbf{t}^a_\alpha)\cdot\mathbf{p}+i\left(\mathbf{R}^b+\mathbf{t}^b_\beta\right)\cdot\mathbf{p}'}\left\langle\mathbf{R}^a+\mathbf{t}^a_\alpha\right|\hat{H}\left|\mathbf{R}^b+\mathbf{t}^b_\beta\right\rangle \end{aligned} \tag{16}$$

We follow Ref. [?] to adopt the tight-binding, two-center approximation, for the inter-layer hopping, *i.e.*,

$$\begin{aligned} \left\langle\mathbf{R}^a+\mathbf{t}^a_\alpha\right|\hat{H}\left|\mathbf{R}^b+\mathbf{t}^b_\beta\right\rangle &= t\left(\mathbf{R}^a+\mathbf{t}^a_\alpha-\mathbf{R}^b-\mathbf{t}^b_\beta\right) \\ &\sim \exp\left(-\frac{1}{\lambda}\left(\mathbf{R}^a+\mathbf{t}^a_\alpha-\mathbf{R}^b-\mathbf{t}^b_\beta\right)^r\right) \end{aligned} \tag{17}$$

where r is a power, which for gaussian orbitals is 2. Other power-law terms can appear, but we here focus only on the exponetial, hence the $\sim$ equivalence. We now Fourier transform:

$$t\left(\mathbf{R}^a+\mathbf{t}^a_\alpha-\mathbf{R}^b-\mathbf{t}^b_\beta\right) = \frac{1}{N\Omega}\sum_{\mathbf{q}}\sum_{\mathbf{G}} t^{ab}_{\mathbf{q}+\mathbf{G}} e^{i(\mathbf{q}+\mathbf{G})\cdot\left(\mathbf{R}^a+\mathbf{t}^a_\alpha-\mathbf{R}^b-\mathbf{t}^b_\beta\right)} \tag{18}$$

Here $\mathbf{q}$ sums over all momenta in a chosen, reference layer BZ, $\mathbf{G}$ sums over all of that layer's reciprocal lattices. For reference, we can choose this layer to be layer 1, but this choice is of course arbitrary. and $t_{\mathbf{q}+\mathbf{G}}$ is the Fourier transformation of $t(\mathbf{r})$.

$$t^{ab}_q = \int d^2 r_\parallel e^{i\vec{q}\cdot\vec{r}_\parallel} e^{-\frac{1}{\lambda}\left(r^2_{ab}+r^2_\parallel\right)^{r/2}} \tag{19}$$

where the integral is over the in-plane distance $r_\parallel$ and $r_{ab} = |a-b|d$ is the perpendicular distance between the layers a and b.

Substituting this back into Eq. (20), we get

$$\begin{aligned} H^{(ab)}_{\alpha\beta}\left(\mathbf{p}^a,\mathbf{p}^b\right) &= \tfrac{1}{N^2\Omega}\textstyle\sum_{\mathbf{R}^a\mathbf{R}^b}\sum_{\mathbf{q}}\sum_{\mathbf{G}} t^{ab}_{\mathbf{q}+\mathbf{G}} e^{i(\mathbf{q}+\mathbf{G})\cdot\left(\mathbf{R}^a+\mathbf{t}^a_\alpha-\mathbf{R}^b-\mathbf{t}^b_\beta\right)} e^{-i(\mathbf{R}^a+\mathbf{t}^a_\alpha)\cdot\mathbf{p}^a+i\left(\mathbf{R}^b+\mathbf{t}^b_\beta\right)\cdot\mathbf{p}^b} = \\ &= \tfrac{1}{N^2\Omega}\textstyle\sum_{\mathbf{R}^a\mathbf{R}^b}\sum_{\mathbf{q}}\sum_{\mathbf{G}} t^{ab}_{\mathbf{q}+\mathbf{G}} e^{iR^b(p^b-q-G)} e^{-iR^a(p^a-q-G)} e^{i(t^b_\beta p^b - t^a_\alpha p^a + q(t^a_\alpha - t^b_\beta) + G(t^a_\alpha - t^a_\beta))} \end{aligned} \tag{20}$$

We use

$$\frac{1}{N}\sum_{R_b} e^{iR^b(p^b-q-G)} = \sum_{G^b}\delta_{q+G,p^b+G^b} \tag{21}$$

Where the second sum is over $\mathbf{G^b}$, the reciprocal lattice vector in the layer b which makes an angle θ_{1b} with layer 1. In other words $\mathbf{G^b} = \mathbf{M_{\theta_{1b}}G'}$ where $\mathbf{G'}$ is another vector in the reference layer BZ. Hence we can just sum over $\mathbf{G'}$ to obtain:

$$\frac{1}{N}\sum_{R_b} e^{iR^b(p^b-q-G)} = \sum_{\mathbf{G'}}\delta_{p^b-q-G+M_{1b}G',0} \tag{22}$$

Similarly:

$$\frac{1}{N}\sum_{R_a} e^{-iR^a(p^a-q-G)} = \sum_{\mathbf{G}''} \delta_{p^a-q-G+M_{1a}G'',0} \tag{23}$$

where $\mathbf{G}''$ is another vector in the reference layer BZ. We hence have:

$$\begin{aligned}
H^{(ab)}_{\alpha\beta}\left(\mathbf{p}^a,\mathbf{p}^b\right) &= \tfrac{1}{\Omega}\textstyle\sum_q \sum_{G,G',G''} t^{ab}_{\mathbf{q}+\mathbf{G}} \delta_{p^a-q-G+M_{1a}G'',0}\delta_{p^b-q-G+M_{1b}G',0} e^{i(t^b_\beta p^b - t^a_\alpha p^a + q(t^a_\alpha - t^b_\beta)+G(t^a_\alpha - t^a_\beta))} = \\
&= \textstyle\sum_{G',G''} t^{ab}_{p^b+M_{1b}G'} \delta_{p^a+M_{1a}G'',p^b+M_{1b}G'} e^{i(t^b_\beta p^b - t^a_\alpha p^a + (p^b+M_{1b}G'-G)(t^a_\alpha - t^b_\beta)+G(t^a_\alpha - t^a_\beta))} = \\
&= \textstyle\sum_{G',G''} t^{ab}_{p^b+M_{1b}G'} \delta_{p^a+M_{1a}G'',p^b+M_{1b}G'} e^{i(t^b_\beta p^b - t^a_\alpha p^a + (p^b+M_{1b}G')(t^a_\alpha - t^b_\beta))} = \\
&= \textstyle\sum_{G',G''} t^{ab}_{p^b+M_{1b}G'} \delta_{p^a+M_{1a}G'',p^b+M_{1b}G'} e^{i(t^a_\alpha p^b - t^a_\alpha p^a + M_{1b}G'(t^a_\alpha - t^b_\beta))} = \\
&= \textstyle\sum_{G',G''} t^{ab}_{p^b+M_{1b}G'} \delta_{p^a+M_{1a}G'',p^b+M_{1b}G'} e^{i(t^a_\alpha (p^a+M_{1a}G''-M_{1b}G') - t^a_\alpha p^a + M_{1b}G'(t^a_\alpha - t^b_\beta))} = \\
&= \textstyle\sum_{G',G''} t^{ab}_{p^b+M_{1b}G'} \delta_{p^a+M_{1a}G'',p^b+M_{1b}G'} e^{i(t^a_\alpha (M_{1a}G''-M_{1b}G') + M_{1b}G'(t^a_\alpha - t^b_\beta))} = \\
&= \textstyle\sum_{G',G''} t^{ab}_{p^b+M_{1b}G'} \delta_{p^a+M_{1a}G'',p^b+M_{1b}G'} e^{i(t^a_\alpha M_{1a}G'' - t^b_\beta M_{1b}G')} = \\
&= \textstyle\sum_{G',G''} t^{ab}_{p^b+M_{1b}G'} \delta_{p^a+M_{1a}G'',p^b+M_{1b}G'} e^{i(t_\alpha G'' - t_\beta G')}
\end{aligned} \tag{24}$$

where t_α, t_β are the hoppings in the reference layer (we have used $t^a_\alpha M_{1a}G'' = (M_{1a})^{-1} t^a_\alpha G'' = t_\alpha G''$). We hence find:

$$H^{(ab)}_{\alpha\beta}\left(\mathbf{p}^a,\mathbf{p}^b\right) = \sum_{G',G''} t^{ab}_{p^a+M_{1a}G''} \delta_{p^a+M_{1a}G'',p^b+M_{1b}G'} e^{i(\mathbf{t}_\alpha \mathbf{G}'' - \mathbf{t}_\beta \mathbf{G}')} \tag{25}$$

where both $\mathbf{G}'$ and $\mathbf{G}''$ are reciprocal lattice vectors in the reference layer. Since the hopping between layers decays exponentially, we will only consider t^{ab} amplitudes between consecutive layers $a = b \pm 1$ and we will call this t_q.

In the MBM-1V, only the low energy electron states around Dirac cones are considered. Thus we approximate the intra-layer Hamiltonian in the reference layer 1 as

$$H^{(11)}\left(\mathbf{K}+\delta\mathbf{p}\right) \approx v_F \delta\mathbf{p}\cdot\boldsymbol{\sigma} \tag{26}$$

$$H^{(bb)}\left(M_\theta\mathbf{K}+\delta\mathbf{p}\right) \approx v_F\left(M^{-1}_{\theta_{1b}}\delta\mathbf{p}\right)\cdot\boldsymbol{\sigma} \approx v_F\delta\mathbf{p}\cdot\boldsymbol{\sigma} \tag{27}$$

Here $\delta\mathbf{p}$ is a small momentum deviation from the K point. In the bottom layer Hamiltonian, we perform a second approximation and neglect the θ-dependence of $H^{(bb)}$. We leave the discussion of the effect of this approximation for appendix **??**.

The computations and approximations involved in $H^{(ab)}$ are not so direct and need more discussion. First, in Eq. (25), for small θ_{1a}, we only need to consider the electron states around the Dirac cone in each layer, *i.e.*, states with momenta $\mathbf{p}_a = M_{1a}\mathbf{K}+\delta\mathbf{p}_a$ and $\mathbf{p}_b = M_{1b}\mathbf{K}+\delta\mathbf{p}_b$ (modulo a reciprocal lattice vector). $t_\mathbf{q}$ depends only on the magnitude of $\mathbf{q}$ and decays exponentially when $|\mathbf{q}|$ becomes larger than $1/d_\perp$: $t_\mathbf{q} \propto \exp(-\alpha(|\mathbf{q}|d_\perp)^\gamma)$, here $d_\perp$ is the distance between two layers,. Fitting to data gives $\alpha \approx 0.13$, and $\gamma \approx 1.25$ [**?**]. Therefore we keep the three largest relevant $t_{p^a+M_{1a}G''}$ terms as $t_{M_{1a}\mathbf{K}+\delta\mathbf{p}_a}$, $t_{C_{3z}M_{1a}\mathbf{K}+\delta\mathbf{p}_a}$, and $t_{C^2_{3z}M_{1a}\mathbf{K}+\delta\mathbf{p}_a}$, corresponding in Eq. (25) to $\mathbf{p} = \mathbf{M_{1a}K}+\delta\mathbf{p_a}$ and $\mathbf{G}''=0$, $\mathbf{G}'' = C_{3z}\mathbf{K}-\mathbf{K}$, and $\mathbf{G}'' = C^2_{3z}\mathbf{K}-\mathbf{K}$ in Eq. (25), respectively (notice all these vectors are in reference layer 1). With C_3 symmetry, all these three terms are equal to $w\Omega$, and the inter-layer coupling can be reformulated as

$$\begin{aligned}
H^{(aa+1)}_{\alpha\beta}\left(M_{1a}\mathbf{K}+\delta\mathbf{p}_a, M_{1a+1}\mathbf{K}+\delta\mathbf{p}_{a+1}\right) \approx w\sum_{\mathbf{G}'}\Big\{&\delta_{M_{1a}\mathbf{K}+\delta\mathbf{p}_a,\ M_{1a+1}\mathbf{K}+\delta\mathbf{p}_{a+1}+M_{1a+1}\mathbf{G}'} e^{-i\mathbf{t}_\beta\cdot\mathbf{G}'} \\
&+\delta_{C_{3z}M_{1a}\mathbf{K}+\delta\mathbf{p}_a,\ M_{1a+1}\mathbf{K}+\delta\mathbf{p}_{a+1}+M_{1a+1}\mathbf{G}'} e^{i\mathbf{t}_\alpha\cdot(C_{3z}\mathbf{K}-\mathbf{K})-i\mathbf{t}_\beta\cdot\mathbf{G}'} \\
&+\delta_{C^2_{3z}M_{1a}\mathbf{K}+\delta\mathbf{p}_a,\ M_{1a+1}\mathbf{K}+\delta\mathbf{p}_{a+1}+M_{1a+1}\mathbf{G}'} e^{i\mathbf{t}_\alpha\cdot\left(C^2_{3z}\mathbf{K}-\mathbf{K}\right)-i\mathbf{t}_\beta\cdot\mathbf{G}'}\Big\}
\end{aligned} \tag{28}$$

Since $\delta\mathbf{p}_a$, $\delta\mathbf{p}_{a+1}$, and $M_{1a+1}\mathbf{K}-M_{1,a}\mathbf{K}$ $(\forall a)$ are all small quantities compared with reciprocal lattice vector, only the $\mathbf{G}'' = 0, C_{3z}K-K, C^2_{3z}K-K$ terms are nonzero in the first, second, and third term. We have also assumed that only $a, a+1$ layer coupling takes place - the coupling between other layers is considered irrelevant. Therefore the inter-layer Hamiltonian is:

$$\begin{aligned}
H^{(aa+1)}_{\alpha\beta}\left(M_{1a}\mathbf{K}+\delta\mathbf{p}_a, M_{1a+1}\mathbf{K}+\delta\mathbf{p}_{a+1}\right) \approx w\Big\{&\delta_{M_{1a}\mathbf{K}+\delta\mathbf{p}_a,\ M_{1a+1}\mathbf{K}+\delta\mathbf{p}_{a+1}} + \\
+\delta_{C_{3z}M_{1a}\mathbf{K}+\delta\mathbf{p}_a,\ M_{1a+1}C_{3z}\mathbf{K}+\delta\mathbf{p}_{a+1}} e^{i(\mathbf{t}_\alpha-\mathbf{t}_\beta)\cdot(C_{3z}\mathbf{K}-\mathbf{K})} &+ \delta_{C^2_{3z}M_{1a}\mathbf{K}+\delta\mathbf{p}_a,\ M_{1a+1}C^2_{3z}\mathbf{K}+\delta\mathbf{p}_{a+1}} e^{i(\mathbf{t}_\alpha-\mathbf{t}_\beta)\cdot\left(C^2_{3z}\mathbf{K}-\mathbf{K}\right)}\Big\}
\end{aligned} \tag{29}$$

Since C_{3z} commutes with any axis rotation, we can write:

$$H_{\alpha\beta}^{(aa+1)}\left(M_{1a}\mathbf{K}+\delta\mathbf{p}_a, M_{1a+1}\mathbf{K}+\delta\mathbf{p}_{a+1}\right)\approx w\Big\{\delta_{\delta\mathbf{p}_a,\ \delta\mathbf{p}_{a+1}+(M_{1a+1}-M_{1a})\mathbf{K}}$$

$$+\,\delta_{\delta\mathbf{p}_a,\ \delta\mathbf{p}_{a+1}+C_{3z}(M_{1a+1}-M_{1a})\mathbf{K}}e^{i(\mathbf{t}_\alpha-\mathbf{t}_\beta)\cdot(C_{3z}\mathbf{K}-\mathbf{K})}+\delta_{\delta\mathbf{p}_a,\ \delta\mathbf{p}_{a+1}+C_{3z}^2(M_{1a+1}-M_{1a})\mathbf{K}}e^{i(\mathbf{t}_\alpha-\mathbf{t}_\beta)\cdot\left(C_{3z}^2\mathbf{K}-\mathbf{K}\right)}\Big\} \tag{30}$$

In order to restore the general hopping between two layers (not only consecutive layer hopping, all one needs to do is make the substitution $a+1\to b$ $w\to t^{ab}$).

We now make one further approximation

1. Small angle approximation $(M_{1a+1}-M_{1a})=M_{a+1,a}$

We hence have that the Hamiltonian can be finally written as

$$H_{\alpha\beta}^{(aa+1)}\left(M_{1a}\mathbf{K}+\delta\mathbf{p}_a, M_{1a+1}\mathbf{K}+\delta\mathbf{p}_{a+1}\right)\approx w\Big\{\delta_{\delta\mathbf{p}_a,\ \delta\mathbf{p}_{a+1}+M_{a+1,a}\mathbf{K}}$$

$$+\,\delta_{\delta\mathbf{p}_a,\ \delta\mathbf{p}_{a+1}+C_{3z}(M_{a+1,a})\mathbf{K}}e^{i(\mathbf{t}_\alpha-\mathbf{t}_\beta)\cdot(C_{3z}\mathbf{K}-\mathbf{K})}+\delta_{\delta\mathbf{p}_a,\ \delta\mathbf{p}_{a+1}+C_{3z}^2(M_{a+1,a})\mathbf{K}}e^{i(\mathbf{t}_\alpha-\mathbf{t}_\beta)\cdot\left(C_{3z}^2\mathbf{K}-\mathbf{K}\right)}\Big\} \tag{31}$$

$$H_{\alpha\beta}^{(aa+1)}\approx w\sum_{j=1}^{3}\delta_{\delta\mathbf{p}_a,\delta\mathbf{p}_{a+1}+\mathbf{q}_j^{a,a+1}}T_{\alpha\beta}^{j} \tag{32}$$

where $\mathbf{q}_1^{a,a+1}=M_{aa+1}\mathbf{K}$, $\mathbf{q}_2^{a,a+1}=C_{3z}\mathbf{q}_1^{a,a+1}$, $\mathbf{q}_3^{a,a+1}=C_{3z}\mathbf{q}_2^{a,a+1}$ (Fig. **??**), and

$$T_1=\sigma_0+\sigma_x \tag{33}$$

$$T_2=\sigma_0+\cos\left(\frac{2\pi}{3}\right)\sigma_x+\sin\left(\frac{2\pi}{3}\right)\sigma_y \tag{34}$$

$$T_3=\sigma_0+\cos\left(\frac{2\pi}{3}\right)\sigma_x-\sin\left(\frac{2\pi}{3}\right)\sigma_y \tag{35}$$

The general form of this expression, for layers ab is

$$H_{\alpha\beta}^{(ab)}\approx w^{ab}\sum_{j=1}^{3}\delta_{\delta\mathbf{p}_a,\delta\mathbf{p}_b+\mathbf{q}_j^{a,b}}T_{\alpha\beta}^{j} \tag{36}$$

where $\mathbf{q}_1^{a,b}=M_{ab}\mathbf{K}$, $\mathbf{q}_2^{a,b}=C_{3z}\mathbf{q}_1^{a,b}$, $\mathbf{q}_3^{a,b}=C_{3z}\mathbf{q}_2^{a,b}$. The full Hamiltonian can be written as:

$$H_{\alpha,\beta}^{(ab)}(\delta p_a,\delta p_b)\approx v_F\delta\mathbf{p}\cdot\boldsymbol{\sigma}\delta_{p_ap_b}+w^{ab}\sum_{j=1}^{3}\delta_{\delta\mathbf{p}_a,\delta\mathbf{p}_b+\mathbf{q}_j^{a,b}}T_{\alpha\beta}^{j} \tag{37}$$

Notice that while we have the Hamiltonian, we have not yet worked out its symmetry properties, nor the Bloch translation properties.

B. Two Layers in 2D

We review here the two-layer example, where there is only one set of q_j. To write the Hamiltonian in more compact form, hereafter we re-label $\delta\mathbf{p}_a$ as $\mathbf{k}-\mathbf{Q}$, and $\delta\mathbf{p}_b$ as $\mathbf{k}-\mathbf{Q}'$. $\mathbf{Q}$ and $\mathbf{Q}'$ take value in the hexagonal lattice formed by adding $\mathbf{q}_{1,2,3}$ iteratively (Fig. **??**(b)) with integer coefficients. There are two types of $\mathbf{Q}$'s, denoted as black and red circles respectively, one for the top layer states and the other for the bottom layer states. Then, the Moiré Hamiltonian can be written as

$$H_{\mathbf{Q},\mathbf{Q}'}^{(MBM-1V)}(\mathbf{k})=\delta_{\mathbf{Q}\mathbf{Q}'}v_F\left(\mathbf{k}-\mathbf{Q}\right)\cdot\boldsymbol{\sigma}+w\sum_{j=1}^{3}\left(\delta_{\mathbf{Q}'-\mathbf{Q},\mathbf{q}_j}+\delta_{\mathbf{Q}-\mathbf{Q}',\mathbf{q}_j}\right)T^j \tag{38}$$

Such a Hamiltonian, when an infinite number of $\mathbf{Q},\mathbf{Q}'$ are included, is periodic in momentum space: it keeps invariant (up to a unitary transformation) under a translation of $\mathbf{b}_1=\mathbf{q}_1-\mathbf{q}_3$ or $\mathbf{b}_2=\mathbf{q}_2-\mathbf{q}_3$:

$$H^{MBM-1V}(\mathbf{k}+\mathbf{b}_i)=V^{\mathbf{b}_i}H^{MBM-1V}(\mathbf{k})V^{\mathbf{b}_i\dagger}, \tag{39}$$

where $i=1,2$, and $V^{\mathbf{G}}_{\mathbf{Q},\mathbf{Q}'}=\delta_{\mathbf{Q},\mathbf{Q}+\mathbf{G}}$ is the embedding matrix. Thus $\mathbf{b}_{i=1,2}$ can be thought as Moiré reciprocal bases, and a Moiré BZ can then be defined, as shown Fig. **??**(b). An important property of this Hamiltonian is that, up to a scaling constant, it depends on a single parameter

$$H^{(MBM-1V)}_{\mathbf{Q},\mathbf{Q}'}(\mathbf{k})=v_F k_D\left\{\delta_{\mathbf{Q}\mathbf{Q}'}\left(\bar{\mathbf{k}}-\bar{\mathbf{Q}}\right)\cdot\boldsymbol{\sigma}+\alpha\sum_{j=1}^{3}\left(\delta_{\bar{\mathbf{Q}}'-\bar{\mathbf{Q}},\bar{\mathbf{q}}_j}+\delta_{\bar{\mathbf{Q}}-\bar{\mathbf{Q}}',\bar{\mathbf{q}}_j}\right)T^j\right\} \tag{40}$$

Here $k_D=|M_\theta\mathbf{K}-\mathbf{K}|=2|\mathbf{K}|\sin\frac{\theta}{2}$ is the distance between the top layer Dirac cone and the bottom layer Dirac cone (Fig. **??**(a)), $\bar{\mathbf{k}}=\mathbf{k}/k_D$, $\bar{\mathbf{Q}}=\mathbf{Q}/k_D$, $\bar{\mathbf{q}}_j=\mathbf{q}_j/k_D$ are dimensionless momenta, and $\alpha=\frac{w}{v_F k_D}$ is the single parameter that the Hamiltonian depends on.

C. Symmetries

Then the momentum lattice in the layers is given by Q_1,Q_2 which run over (the origin of our system of coordinates is in layer 1)

$$Q_1: n_1b_1+n_2b_2;\quad Q_2: n_1b_1+n_2b_2+q_1,\quad n_1,n_2\in Z \tag{41}$$

With these vectors, we can write the momentum in the 3 layers:

$$\delta p_1=k-Q_1;\qquad \delta p_2=k-Q_2;\qquad \delta p_3=k-Q_3 \tag{42}$$

We now derive the important equations

- Hamiltonian:

$$\boxed{H^{\alpha\beta}_{Q_mQ_n}(k)=(\vec{k}-\vec{Q}_m)\cdot\vec{\sigma}_{\alpha\beta}\delta_{mn}+w^{mn}\sum_j T^j_{\alpha,\beta}\delta_{Q_m,Q_n-q^{mn}_j}} \tag{43}$$

- Bloch Periodicity

$$\boxed{H(k-b_i)=V^{b_i}H(k)V^{b_i\dagger},\qquad V^G_{Q_m,Q_n}=\delta_{Q_n,Q_m+G}} \tag{44}$$

  . b_1,b_2 can be thought of as reciprocal lattice vectors. We hence have a Bloch periodicity and a Brillouin Zone with reciprocal lattice vectors b_1,b_2

- C_{3z} symmetry:

  Using the properties (our rotations are counter-clockwise) in both spin and lattice coordinates

$$\boxed{\mathcal{C}_{3z}=\exp(i2\pi/3s_z)\delta_{Q_m,C_{3z}Q_n}} \tag{45}$$

  where we notice that if Q_m belongs to one layer, $C_{3z}Q_m$ belongs to the same layer (C_{3z} rotation does not change layer. We clearly notice the defining group properties.)

$$C^3_{3z}=1;\qquad C_{3z}C^\dagger_{3z}=1 \tag{46}$$

$$\mathcal{C}_{3z}T_j\mathcal{C}^\dagger_{3z}=T_{j+1};\quad (T_4=T_1);\quad \mathcal{C}_{3z}(\vec{k}\cdot\vec{\sigma})\mathcal{C}^\dagger_{3z}=(\vec{C_{3z}k})\cdot\sigma;\quad C_{3z}q_j=q_{j+1} \tag{47}$$

We are ready to obtain the Hamiltonian transformation:

$$
\begin{gathered}
\boxed{\mathcal{C}_{3z} H(k) \mathcal{C}_{3z}^{\dagger}} = (\mathcal{C}_{3z} H(k) \mathcal{C}_{3z}^{\dagger})^{\alpha\beta}_{Q_r Q_p} = \\
= \delta_{Q_r, C_3 Q_m} (C_{3z}\vec{k} - C_{3z}\vec{Q}_m) \cdot \vec{\sigma}_{\alpha\beta} \delta_{mn} \delta_{Q_p, C_{3z} Q_n} + \delta_{Q_r, C_{3z} Q_m} w^{mn} \sum_j T^{j+1}_{\alpha,\beta} \delta_{Q_m, Q_n - q_j^{mn}} \delta_{Q_p, C_{3z} Q_n} = \\
= (C_{3z}\vec{k} - \vec{Q}_r) \cdot \vec{\sigma}_{\alpha\beta} \delta_{rp} + w^{rp} \sum_j T^{j+1}_{\alpha,\beta} \delta_{C_{3z}^{-1} Q_r, C_{3z}^{-1} Q_p - q_j^{rp}} = \\
= (C_{3z}\vec{k} - \vec{Q}_r) \cdot \vec{\sigma}_{\alpha\beta} \delta_{rp} + w^{rp} \sum_j T^{j}_{\alpha,\beta} \delta_{C_{3z}^{-1} Q_r, C_{3z}^{-1} Q_p - q_{j-1}^{rp}} = \\
= (C_{3z}\vec{k} - \vec{Q}_r) \cdot \vec{\sigma}_{\alpha\beta} \delta_{rp} + w^{rp} \sum_j T^{j}_{\alpha,\beta} \delta_{C_{3z}^{-1} Q_r, C_{3z}^{-1} Q_p - C_{3j}^{-1} q_j^{rp}} = \\
= (C_{3z}\vec{k} - \vec{Q}_r) \cdot \vec{\sigma}_{\alpha\beta} \delta_{rp} + w^{rp} \sum_j T^{j}_{\alpha,\beta} \delta_{Q_r, Q_p - q_j^{rp}} = H(C_{3z} k)^{\alpha\beta}_{Q_r Q_p} = \boxed{H(C_{3z} k)}
\end{gathered}
\tag{48}
$$

In going from the first to second layer we used the fact that if Q_m is in a certain layer, so is $C_{3z} Q_m$ and hence Q_r

- C_{2x} symmetry:

  We pick a center of rotation that runs between the two layers. As such, the rotation sends layer 1 into 2 and viceversa

$$
C_{2x} : Q_1 \leftrightarrow Q_3, \quad Q_2 \leftrightarrow Q_2 \tag{49}
$$

$$
C_{2x} : q_1 \to -q_1, \quad q_2 \to -q_3, \quad q_3 \to -q_2 \tag{50}
$$

The symmetry operator is:

$$
\boxed{\mathcal{C}_{2x} = \sigma_x \delta_{Q_m, C_{2x} Q_n}}, \quad \mathcal{C}_{2x}^2 = \mathcal{C}_{2x} \mathcal{C}_{2x}^{\dagger} = 1 \tag{51}
$$

The σ_x acts on the T matrices as:

$$
\mathcal{C}_{2x} T_1 \mathcal{C}_{2x}^{\dagger} = T_1, \quad \mathcal{C}_{2x} T_2 \mathcal{C}_{2x}^{\dagger} = T_3, \quad \mathcal{C}_{2x} T_3 \mathcal{C}_{2x}^{\dagger} = T_2, \tag{52}
$$

We are ready to obtain the Hamiltonian transformation:

$$
\begin{gathered}
\boxed{\mathcal{C}_{2x} H(k) \mathcal{C}_{2x}^{\dagger}} = (\mathcal{C}_{2x} H(k) \mathcal{C}_{2x}^{\dagger})^{\alpha\beta}_{Q_r Q_p} = \\
= \delta_{Q_r, C_{2x} Q_m} (C_{2x}\vec{k} - C_{2x}\vec{Q}_m) \cdot \vec{\sigma}_{\alpha\beta} \delta_{mn} \delta_{Q_p, C_{2x} Q_n} + \\
+ \delta_{Q_r, C_{2x} Q_m} w^{mn} (T^1_{\alpha,\beta} \delta_{Q_m, Q_n - q_1^{mn}} + T^3_{\alpha,\beta} \delta_{Q_m, Q_n - q_2^{mn}} + T^2_{\alpha,\beta} \delta_{Q_m, Q_n - q_3^{mn}}) \delta_{Q_p, C_{2x} Q_n} = \\
= (C_{2x}\vec{k} - \vec{Q}_r) \cdot \vec{\sigma}_{\alpha\beta} \delta_{rp} + \\
+ \delta_{Q_r, C_{2x} Q_m} w^{mn} (T^1_{\alpha,\beta} \delta_{C_{2x}^{-1} Q_r, C_{2x}^{-1} Q_p - q_1^{mn}} + T^3_{\alpha,\beta} \delta_{C_{2x}^{-1} Q_r, C_{2x}^{-1} Q_p - q_2^{mn}} + T^2_{\alpha,\beta} \delta_{C_{2x}^{-1} Q_r, C_{2x}^{-1} Q_p - q_3^{mn}}) \delta_{Q_p, C_{2x} Q_n} = \\
= H(C_{2x} k)^{\alpha\beta}_{Q_r Q_p} = \boxed{H(C_{2x} k)}
\end{gathered}
\tag{53}
$$

In order to check that this is true (and it is) we will need to check the above equation term by term. The diagonal part is obviously true, we only need to check the hopping part; We introduce the notation $m = C_{2x}^{-1} r$ for the indices of Q_r, Q_m etc:

$$
\begin{gathered}
\delta_{Q_r, C_{2x} Q_m} w^{mn} (T^1_{\alpha,\beta} \delta_{C_{2x}^{-1} Q_r, C_{2x}^{-1} Q_p - q_1^{mn}} + T^3_{\alpha,\beta} \delta_{C_{2x}^{-1} Q_r, C_{2x}^{-1} Q_p - q_2^{mn}} + T^2_{\alpha,\beta} \delta_{C_{2x}^{-1} Q_r, C_{2x}^{-1} Q_p - q_3^{mn}}) \delta_{Q_p, C_{2x} Q_n} = \\
= w^{C_{2x}^{-1} r, C_{2x}^{-1} p} (T^1_{\alpha,\beta} \delta_{C_{2x}^{-1} Q_r, C_{2x}^{-1} Q_p - q_1^{C_{2x}^{-1} r, C_{2x}^{-1} p}} + T^3_{\alpha,\beta} \delta_{C_{2x}^{-1} Q_r, C_{2x}^{-1} Q_p - q_2^{C_{2x}^{-1} r, C_{2x}^{-1} p}} + T^2_{\alpha,\beta} \delta_{C_{2x}^{-1} Q_r, C_{2x}^{-1} Q_p - q_3^{C_{2x}^{-1} r, C_{2x}^{-1} p}})
\end{gathered}
\tag{54}
$$

- $C_{2z}T$ Symmetry.

  This symmetry does nothing to the wavevectors q_i or lattices Q, and hence is represented diagonally in Q space. In spin space, it takes Complex conjugates, but then acts with another spin matrix so as to get back to the same Hamiltonian. This pins the summetry to be

$$\boxed{\mathcal{C}_{2z}\mathcal{T} = \sigma_x \delta_{Q_m,Q_n} K} \tag{55}$$

where K is the complex conjugation. We find that

$$\mathcal{C}_{2z}\mathcal{T}T_1\mathcal{T}^\dagger\mathcal{C}_{2z}^\dagger = T_1, \quad \mathcal{C}_{2z}\mathcal{T}T_2\mathcal{T}^\dagger\mathcal{C}_{2z}^\dagger = T_2, \quad \mathcal{C}_{2z}\mathcal{T}T_3\mathcal{T}^\dagger\mathcal{C}_{2z}^\dagger = T_3 \tag{56}$$

and

$$(C_{2z}T)^2 = 1 \tag{57}$$

The proof is:

$$\begin{aligned} \boxed{\mathcal{C}_{2z}\mathcal{T}H(k)\mathcal{T}^\dagger\mathcal{C}_{2z}^\dagger} = (\mathcal{C}_{2z}\mathcal{T}H(k)\mathcal{T}^\dagger\mathcal{C}_{2z}^\dagger)^{\alpha\beta}_{Q_rQ_p} = \\ = \delta_{Q_r,Q_m}(\vec{k}-\vec{Q}_m)\cdot\vec{\sigma}_{\alpha\beta}\delta_{mn}\delta_{Q_p,Q_n} + \delta_{Q_r,Q_m} w^{mn\star}\sum_j T^j_{\alpha,\beta}\delta_{Q_m,Q_n-q_j^{mn}}\delta_{Q_p,Q_n} = \\ = H(k)^{\alpha\beta}_{Q_rQ_p} = \boxed{H(k)} \end{aligned} \tag{58}$$

iff

$$\boxed{w^{mn} = w^{mn\star}} \tag{59}$$

Remember that $\mathcal{T}$ acts only as complex conjugation on $H(k)$ in the above. All rotations of momenta here are with respect to the Γ point of the Moire BZ.