NUMERICAL COMPUTATIONS FOR AN EFFECTIVE MODEL OF TWISTED BILAYER GRAPHENE

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1. Standard monolayer

We recall that

$$a_1 = a \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \qquad a_2 = a \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix}$$

$$a_1^* = \frac{2\pi}{a} \begin{pmatrix} \frac{1}{\sqrt{3}} \\ 1 \end{pmatrix} = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \qquad a_2^* = \frac{2\pi}{a} \begin{pmatrix} \frac{1}{\sqrt{3}} \\ -1 \end{pmatrix} = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix}$$

In reduced coordinates, with

$\mathcal{M} : \mathbb{T}^2 \simeq [0,1]^2 \to \Omega$,

$$\mathcal{M} := \frac{a}{2} \begin{pmatrix} \sqrt{3} & \sqrt{3} \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} a_1 & a_2 \end{pmatrix}, \qquad \mathcal{M}^{-1} = \frac{1}{a} \begin{pmatrix} \frac{1}{\sqrt{3}} & 1 \\ \frac{1}{\sqrt{3}} & -1 \end{pmatrix}$$

and

$$2\pi \left(\mathcal{M}^{-1}\right)^* = \begin{pmatrix} a_1^* & a_2^* \end{pmatrix} = \frac{2\pi}{a} \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 1 & -1 \end{pmatrix} =: S$$

1.1. Fourier conventions.

We will manipulate functions which are Ω-periodic in $\mathbf{x}$, but not in z, our Fourier transform conventions will be

$$\left(\mathcal{F}f\right)_G(k_z) := \frac{1}{2\pi\,|\Omega|} \int_{\Omega\times\mathbb{R}} e^{-i(k\mathbf{x}+k_z z)} f(\mathbf{x},z)\mathrm{d}\mathbf{x}\mathrm{d}z$$

hence any function can be decomposed as

$$f(\mathbf{x},z) = \sum_{\mathbf{G}\in\mathbb{L}^*} \int_{\mathbb{R}} e^{i(\mathbf{G}\mathbf{x}+k_z z)} f_{\mathbf{G}}(k_z)\mathrm{d}k_z$$

We also recall that $\int_{\mathbb{R}} e^{ipz}\mathrm{d}z = 2\pi\delta(p)$.

Now we consider that f and g are L-periodic in z,

$$f(\mathbf{x},z) = \sum_{\mathbf{G},G_z} e^{i(\mathbf{G}\mathbf{x}+G_z z)} \widehat{f}_{\mathbf{G},G_z}$$

or, in reduced coordinates,

$$\boxed{f(\mathbf{x},z) = \sum_{\substack{\mathbf{m}\in\mathbb{Z}^2 \\ m_z\in\mathbb{Z}}} e^{i\left(\mathbf{m}\mathbf{a}^*\cdot\mathbf{x}+m_z\frac{2\pi}{L}z\right)} \widehat{f}_{\mathbf{m},m_z}} \tag{1}$$

We define the scalar product

$$\langle f,g\rangle := \int_{\Omega\times[0,L]} \overline{f}g$$

and compute Plancherel's formula

$$\langle f, g\rangle = L\,|\Omega| \sum_{\substack{\mathbf{m}\in\mathbb{Z}^2 \\ m_z\in\mathbb{Z}}} \overline{\widehat{f}_{\mathbf{m},m_z}}\,\widehat{g}_{\mathbf{m},m_z}. \tag{2}$$

Hence, as a verification, we test that the normalization of the $\widehat{u_j}$'s is the right one by checking that $\|u_j\|^2_{L^2} = 1$ via (2).

1.2. **Rotation action.** We know that $R_{\frac{2\pi}{3}}(ma^*) = \left(R^{\mathrm{red}}_{\frac{2\pi}{3}} m\right) a^*$ where

$$R^{\mathrm{red}}_{\frac{2\pi}{3}} = S^{-1} R_{\frac{2\pi}{3}} S = \mathcal{M}^* R_{\frac{2\pi}{3}} (\mathcal{M}^*)^{-1} = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}, \qquad R^{\mathrm{red}}_{-\frac{2\pi}{3}} = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$$

and

$$\mathcal{R}_{\frac{2\pi}{3}} f(x) = \sum_m f_m e^{i\left(R^{\mathrm{red}}_{\frac{2\pi}{3}} m\right) a^*\cdot x} = \sum_m f_{R^{\mathrm{red}}_{-\frac{2\pi}{3}} m} e^{ima^*\cdot x}$$

2. Computation of V_{int}

For $\mathbf{s} \in \Omega := [0,1]\mathbf{a}_1 + [0,1]\mathbf{a}_2$, we denote by $V^{(2)}_{\mathbf{s}}$ the true Kohn-Sham mean-field potential for the configuration where the two sheets are aligned (no angle), but with the upper one shifted by a vector $\mathbf{s}$. We set

$$\begin{aligned}
V_{\mathrm{int},\mathbf{s}}(z) &:= \frac{1}{|\Omega|}\int_\Omega \left(V^{(2)}_{\mathbf{s}}(\mathbf{x},z) - V(\mathbf{x}, z+\tfrac{d}{2}) - V(\mathbf{x}-\mathbf{s}, z-\tfrac{d}{2})\right)\mathrm{d}\mathbf{x} \\
&= \frac{1}{|\Omega|}\int_\Omega \left(V^{(2)}_{\mathbf{s}}(\mathbf{x},z) - V(\mathbf{x}, z+\tfrac{d}{2}) - V(\mathbf{x}, z-\tfrac{d}{2})\right)\mathrm{d}\mathbf{x} \\
&= \frac{1}{|\Omega|}\sum_{\substack{\mathbf{m}\in\mathbb{Z}^2 \\ m_z\in\mathbb{Z}}} \left(\widehat{\left(V^{(2)}_{\mathbf{s}}\right)}_{\mathbf{m},m_z} - \widehat{V}_{\mathbf{m},m_z} e^{im_z\frac{2\pi}{L}\frac{d}{2}} - \widehat{V}_{\mathbf{m},m_z} e^{-im_z\frac{2\pi}{L}\frac{d}{2}}\right) \\
&\qquad\qquad \times \int_\Omega e^{i\left(\mathbf{m}a^*\cdot\mathbf{x} + m_z\frac{2\pi}{L}z\right)}\mathrm{d}\mathbf{x} \\
&= \sum_{m_z\in\mathbb{Z}} e^{im_z\frac{2\pi}{L}z}\left(\widehat{\left(V^{(2)}_{\mathbf{s}}\right)}_{0,m_z} - 2\widehat{V}_{0,m_z}\cos\left(m_z\tfrac{\pi d}{L}\right)\right)
\end{aligned}$$

and we obtain the Fourier coefficients

$$\left(\widehat{V_{\mathrm{int},\mathbf{s}}}\right)_{m_z} = \widehat{\left(V^{(2)}_{\mathbf{s}}\right)}_{0,m_z} - 2\widehat{V}_{0,m_z}\cos\left(m_z\tfrac{\pi d}{L}\right)$$

We then compute

$$V_{\mathrm{int}}(z) := \frac{1}{|\Omega|}\int_\Omega V_{\mathrm{int},\mathbf{s}}(z)\mathrm{d}\mathbf{s} = \frac{1}{N^2}\sum_{s_x,s_y\in[\![1,N]\!]} V^{\mathrm{array}}_{\mathrm{int},(\mathrm{s_x},\mathrm{s_y})}(z)$$

and finally obtain the Fourier coefficients

$$\boxed{\left(\widehat{V_{\mathrm{int}}}\right)_{m_z} = \frac{1}{N^2}\sum_{s_x,s_y\in[\![1,N]\!]}\left(\widehat{V_{\mathrm{int},\mathbf{s}}}\right)_{m_z}}$$

and we expect $V_{\text{int},\mathbf{s}}$ not to depend too much on $\mathbf{s}$, that is we expect that

$$\begin{aligned}\delta_{V_{\text{int}}} &:= \frac{\int_{\Omega\times\mathbb{R}} |V_{\text{int},\mathbf{s}}(z) - V_{\text{int}}(z)|^2 \,\mathrm{d}\mathbf{s}\mathrm{d}z}{|\Omega| \int_{\mathbb{R}} V_{\text{int}}(z)^2 \mathrm{d}z} \\ &= \frac{\sum_{m_z} \int_\Omega \left| \left(\widehat{V_{\text{int},\mathbf{s}}}\right)_{m_z} - \left(\widehat{V_{\text{int}}}\right)_{m_z} \right|^2 \mathrm{d}\mathbf{s}}{|\Omega| \sum_{m_z} \left(\widehat{V_{\text{int}}}\right)_{m_z}^2} \\ &= \frac{\sum_{s_x,s_y,m_z} \left| \left(\widehat{V}_{\text{int},(\text{s}_\text{x},\text{s}_\text{y})}\right)_{m_z} - \left(\widehat{V_{\text{int}}}\right)_{m_z} \right|^2}{N^2 \sum_{m_z} \left(\widehat{V_{\text{int}}}\right)_{m_z}^2}\end{aligned}$$

is small. We also verify that $V_{\text{int}}(-z) = V_{\text{int}}(z)$.

3. Effective potentials

We defined

$$(\!(f, g)\!)^{\eta,\eta'}(\mathbf{X}) := \frac{1}{|\Omega|} \int_{\Omega\times\mathbb{R}} \overline{f}\left(x - \eta J\mathbf{X}, z - \eta\tfrac{d}{2}\right) g\left(x - \eta' J\mathbf{X}, z - \eta'\tfrac{d}{2}\right) \mathrm{d}\mathbf{x}\mathrm{d}z$$

and

$$\begin{aligned}&\langle\!\langle f, g\rangle\!\rangle^{\eta,\eta'}(\mathbf{X}) \\ &:= \frac{e^{i(\eta-\eta')\mathbf{K}\cdot J\mathbf{X}}}{|\Omega|} \int_{\Omega\times\mathbb{R}} \overline{f}\left(x - \eta J\mathbf{X}, z - \eta\tfrac{d}{2}\right) g\left(x - \eta' J\mathbf{X}, z - \eta'\tfrac{d}{2}\right) \mathrm{d}\mathbf{x}\mathrm{d}z\end{aligned}$$

so $\langle\!\langle f, g\rangle\!\rangle^{\eta,\eta'} = e^{i(\eta-\eta')\mathbf{K}\cdot J\mathbf{X}} (\!(f, g)\!)^{\eta,\eta'}$. Now we make the approximation

$$\int_{\Omega\times\mathbb{R}} \simeq \int_{\Omega\times[0,L]}$$

The situation is drawn on Figure 3. The functions are defined on $[-L/2, L/2]$ but we need to integrate on the common segment, which is $[-\frac{L-d}{2}, \frac{L-d}{2}]$, so on $[-L/2, L/2]$ to recover the initial domain.

Firstly, using the Fourier decomposition (1),

$$\begin{aligned}(\!(f, g)\!)^{\eta,\eta'} &= L \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{i(\eta-\eta')ma^*\cdot J\mathbf{X}} \sum_{m_z\in\mathbb{Z}} e^{i(\eta-\eta')\frac{2\pi}{L}m_z\frac{d}{2}} \overline{\widehat{f}_{m,m_z}} \widehat{g}_{m,m_z} \\ &= \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{i(\eta-\eta')ma^*\cdot J\mathbf{X}} C_{\mathbf{m}}\end{aligned}$$

where

$$\boxed{C_{\mathbf{m}} := L \sum_{m_z\in\mathbb{Z}} e^{i(\eta-\eta')\frac{d\pi}{L}m_z} \overline{\widehat{f}_{m,m_z}} \widehat{g}_{m,m_z}}$$

and we also define

$$C_{\mathbf{m}}^{\pm} := L \sum_{m_z\in\mathbb{Z}} e^{\pm i2\frac{d\pi}{L}m_z} \overline{\widehat{f}_{m,m_z}} \widehat{g}_{m,m_z}$$

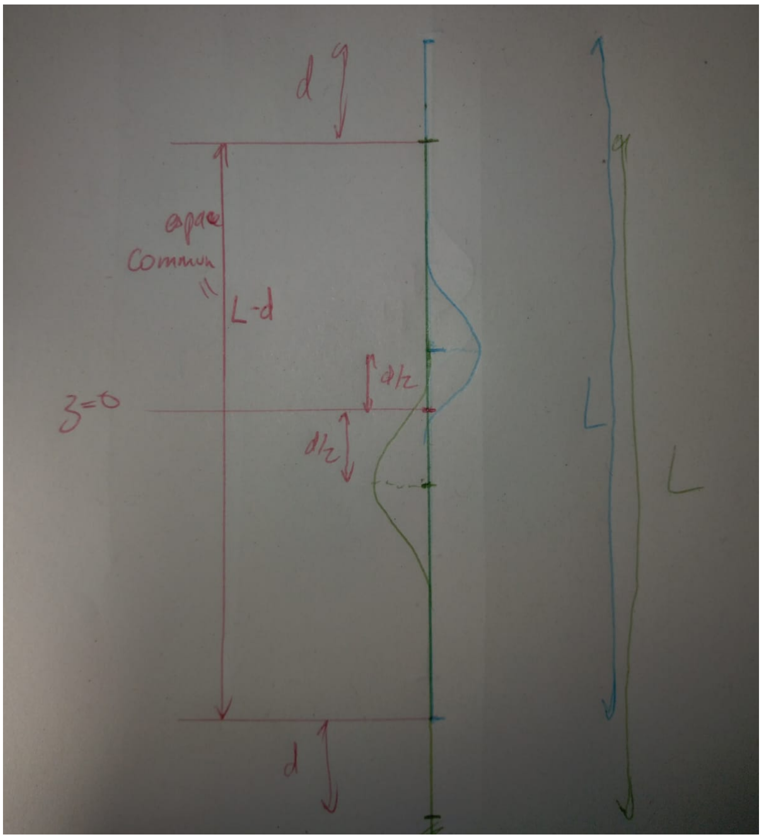

FIGURE 1. Situation on the z coordinate

Then,

$$\langle\!\langle f, g\rangle\!\rangle^{\eta,\eta'} = e^{i(\eta-\eta')\mathbf{K}\cdot J\mathbf{X}} \left(\!\left(f, g\right)\!\right)^{\eta,\eta'} = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{i(\eta-\eta')(m+m_K)a^*\cdot J\mathbf{X}} C_{\mathbf{m}}$$

Hence

$$\boxed{\left(\!\left(f, g\right)\!\right)^{+-}\left(-\tfrac{3}{2}J\mathbf{X}\right) = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{i3ma^*\cdot\mathbf{X}} C^+_{\mathbf{m}} = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{ima^*\cdot\mathbf{X}} C^+_{\frac{\mathbf{m}}{3}},}$$

and

$$\boxed{\langle\!\langle f, g\rangle\!\rangle^{+-}\left(-\tfrac{3}{2}J\mathbf{X}\right) = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{i3(m+m_k)a^*\cdot\mathbf{X}} C^+_{\mathbf{m}} = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{ima^*\cdot\mathbf{X}} C^+_{\frac{\mathbf{m}-3\mathbf{m}_K}{3}}}$$

where $C_{\frac{\mathbf{m}}{n}} := 0$ if n does not divide m_1 and m_2.

Similarly

$$\left(\!\left(f, g\right)\!\right)^{-+}\left(-\tfrac{3}{2}J\mathbf{X}\right) = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{-i3ma^*\cdot\mathbf{X}} C^-_{\mathbf{m}} = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{ima^*\cdot\mathbf{X}} C^-_{-\frac{\mathbf{m}}{3}},$$

For the potentials, we finally need to implement

$$\mathbb{W}^+_{j,j'} = \left(\!\left(\overline{u}_j u_{j'}, V\right)\!\right)^{+-}, \qquad \mathbb{W}^-_{j,j'} = \left(\!\left(\overline{u}_j u_{j'}, V\right)\!\right)^{-+},$$

$$\mathbb{V}_{j,j'} = \langle\!\langle (V + V_{\text{int}})\, u_j, u_{j'}\rangle\!\rangle^{+-}$$

If $f(z) = \varepsilon f(-z)$, then $\widehat{f}_{-m_z} = \varepsilon \widehat{f}_{m_z}$, from this we see that $\overline{C_{\mathbf{m}}^{u_{j'},u_j}} = C_{\mathbf{m}}^{u_j,u_{j'}}$ and hence $\mathbb{V}(-X)^* = \mathbb{V}(X)$

3.1. **Magnetic term.** As for the magnetic term, we have

$$(-i\nabla_{\mathbf{x}} + \mathbf{K})\, g = \sum_{\mathbf{m},m_z} (\mathbf{m} + \mathbf{m}_K)\, \mathbf{a}^* e^{i\left(\mathbf{m}\mathbf{a}^*\cdot\mathbf{x} + m_z \frac{2\pi}{L} z\right)} \widehat{f}_{\mathbf{m},m_z}$$

so

$$\langle\!\langle f, (-i\nabla_{\mathbf{x}} + \mathbf{K}) g\rangle\!\rangle^{+-}(\mathbf{X}) = \sum_{\mathbf{m}\in\mathbb{Z}^2} (\mathbf{m} + \mathbf{m}_K)\, \mathbf{a}^*\, C_{\mathbf{m}} e^{2i(\mathbf{m}+\mathbf{m}_K)\mathbf{a}^*\cdot J\mathbf{X}}$$

and

$$\langle\!\langle f, (-i\nabla_{\mathbf{x}} + \mathbf{K}) g\rangle\!\rangle^{+-}\left(-\tfrac{3}{2} J\mathbf{X}\right) = \sum_{\mathbf{m}\in\mathbb{Z}^2} (\mathbf{m} + \mathbf{m}_K)\, \mathbf{a}^*\, C_{\mathbf{m}} e^{i3(\mathbf{m}+\mathbf{m}_K)\mathbf{a}^*\cdot \mathbf{X}}$$

so

$$\boxed{\langle\!\langle f, (-i\nabla_{\mathbf{x}} + \mathbf{K}) g\rangle\!\rangle^{+-}\left(-\tfrac{3}{2} J\mathbf{X}\right) = \frac{1}{3} \sum_{\mathbf{m}\in\mathbb{Z}^2} \mathbf{m}\mathbf{a}^*\, C_{\frac{\mathbf{m}-3\mathbf{m}_K}{3}}\, e^{i\mathbf{m}\mathbf{a}^*\cdot\mathbf{X}}}$$

so we can implement

$$\boldsymbol{\mathcal{A}}_{j,j'}\left(-\tfrac{3}{2} J\mathbf{X}\right) = \langle\!\langle u_j, (-i\nabla_{\mathbf{x}} + \mathbf{K}) u_{j'}\rangle\!\rangle^{+-}\left(-\tfrac{3}{2} J\mathbf{X}\right)$$

3.2. **$\mathbb{W}$'s V_{int} term.** We write $V_{\text{int}}(z) = \sum_{m_z\in\mathbb{Z}} \widehat{V}_{\text{int}}^{m_z} e^{i\frac{2\pi}{L} m_z z}$ hence

$$\begin{aligned}\left\langle u_j, V_{\text{int}} u_{j'}\right\rangle &= \sum_{\substack{\mathbf{m}\in\mathbb{Z}^2\\ m_z,m_z',M_z\in\mathbb{Z}}} \left(\overline{\widehat{u}_j}\right)_{\mathbf{m},m_z} \left(\widehat{u}_{j'}\right)_{\mathbf{m},m_z'} \left(\widehat{V_{\text{int}}}\right)_{M_z} \int_z e^{iz\frac{2\pi}{L}(M_z + m_z' - m_z)} \\ &= L \sum_{\substack{\mathbf{m}\in\mathbb{Z}^2\\ m_z,m_z'\in\mathbb{Z}}} \left(\overline{\widehat{u}_j}\right)_{\mathbf{m},m_z} \left(\widehat{u}_{j'}\right)_{\mathbf{m},m_z'} \left(\widehat{V_{\text{int}}}\right)_{m_z - m_z'}\end{aligned}$$

and the matrix $M_{j,j'} := \left\langle u_j, V_{\text{int}} u_{j'}\right\rangle$ is such that $M^* = M$ and $M_{11} = M_{22}$.

4. BM configuration

From [1], the BM Hamiltonian is

$$H = \begin{pmatrix} -i\sigma\nabla & T^c(x) \\ T^c(x)^* & -i\sigma\nabla \end{pmatrix},$$

where

$$\boxed{T_1 = \begin{pmatrix} w_0 & w_1 \\ w_1 & w_0 \end{pmatrix}, \quad T_2 = \begin{pmatrix} w_0 & w_1 e^{-i\phi} \\ w_1 e^{i\phi} & w_0 \end{pmatrix}, \quad T_3 = \begin{pmatrix} w_0 & w_1 e^{i\phi} \\ w_1 e^{-i\phi} & w_0 \end{pmatrix}}$$

and where, for $x \in \mathbb{R}^2$,

$$T^c(x) := \sum_{j=1}^{3} T_j e^{-iq_j^c\cdot x} = \sum_{j=1}^{3} T_j e^{iq_j a^*\cdot x}, \qquad \widehat{T}_p = \sum_{j=1}^{3} T_j \delta_{p,q_j^c}$$

and

$$q_1^c = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = a_1^* + a_2^*,$$

$$q_2^c = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} = -a_2^*, \qquad q_3^c = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} = -a_1^*,$$

where we took rotated q_j^c's by J with respect to [1], and with a rescaling of $\frac{4\pi}{a\sqrt{3}}$.

We define the reduced dual vectors $q_j := -\mathcal{M}^* q_j^c / 2\pi$ so

$$T(x) = T^c(\mathcal{M}x) = \sum_{j=1}^{3} T_j e^{-ix\cdot\mathcal{M}^* q_j^c} = \sum_{j=1}^{3} T_j e^{i2\pi x\cdot q_j}$$

and we compute

$$\boxed{q_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad q_2 = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \qquad q_3 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}}$$

Or

$$\boxed{T(x) = \sum_{j=1}^{3} T_j e^{iq_j a^*\cdot x}}$$

Since $T_j^* = T_j$, then $T(-x)^* = T(x)$

5. Operators in basis

5.1. **Goal.** Our goal is to study the eigenvalue equation

$$\mathcal{H}\psi = \mathcal{S}\psi$$

where $\mathcal{S}$ is Hermitian and positive and

$$\mathcal{H} := \frac{1}{\varepsilon_\theta}\mathcal{V} + c_\theta T + \varepsilon_\theta T^{(1)}$$

where

$$T := v_{\mathrm{F}} \begin{pmatrix} \boldsymbol{\sigma}\cdot(-i\nabla) & \boldsymbol{\mathcal{A}}\cdot(-i\nabla) \\ \boldsymbol{\mathcal{A}}^*\cdot(-i\nabla) & \boldsymbol{\sigma}\cdot(-i\nabla) \end{pmatrix},$$

$$T^{(1)} := v_{\mathrm{F}} \begin{pmatrix} -\boldsymbol{\sigma}\cdot J(-i\nabla) - \frac{1}{2}\Delta & \boldsymbol{\mathcal{A}}\cdot J(-i\nabla) - \frac{1}{2}\Sigma\Delta \\ \boldsymbol{\mathcal{A}}^*\cdot J(-i\nabla) - \frac{1}{2}\Sigma^*\Delta & \boldsymbol{\sigma}\cdot J(-i\nabla) - \frac{1}{2}\Delta \end{pmatrix},$$

$$\mathcal{V} := \begin{pmatrix} \mathbb{W} & \mathbb{V} \\ \mathbb{V}^* & \mathbb{W} \end{pmatrix},$$

and their Bloch transform becomes

$$T_k := v_{\mathrm{F}} \begin{pmatrix} \boldsymbol{\sigma}\cdot(-i\nabla+k) & \boldsymbol{\mathcal{A}}\cdot(-i\nabla+k) \\ \boldsymbol{\mathcal{A}}^*\cdot(-i\nabla+k) & \boldsymbol{\sigma}\cdot(-i\nabla+k) \end{pmatrix},$$

$$T_k^{(1)} := v_{\mathrm{F}} \begin{pmatrix} -\boldsymbol{\sigma}\cdot J(-i\nabla+k) + \frac{1}{2}(-i\nabla+k)^2 & \boldsymbol{\mathcal{A}}\cdot J(-i\nabla+k) + \frac{1}{2}\Sigma(-i\nabla+k)^2 \\ \boldsymbol{\mathcal{A}}^*\cdot J(-i\nabla+k) + \frac{1}{2}\Sigma^*(-i\nabla+k)^2 & \boldsymbol{\sigma}\cdot J(-i\nabla+k) + \frac{1}{2}(-i\nabla+k)^2 \end{pmatrix}$$

and we want the middle of the spectrum of

$$\mathcal{H}_k := \mathcal{S}^{-\frac{1}{2}} \left(\frac{1}{\varepsilon_\theta} \mathcal{V} + c_\theta T_k + \varepsilon_\theta T_k^{(1)} \right) \mathcal{S}^{-\frac{1}{2}}$$

5.2. **Basis.** We define $e_m := \frac{1}{\sqrt{|\Omega|}} e^{ima^* \cdot x}$, and

$$e_{\alpha,m} := e_\alpha \otimes e_m = e_\alpha \frac{e^{ima^* \cdot x}}{\sqrt{|\Omega|}}, \qquad \text{where } e_1 := \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \dots$$

5.3. **Multiplication-derivation operators.** For $A = (A_1, A_2)$ and $A_j = \sum_\ell \left(\widehat{A_j} \right)_\ell e^{i\ell a^* \cdot x}$, we have

$$\begin{aligned}
\langle e_n, A \cdot (-i\nabla + k) e_m \rangle = \sum_\ell \left(\widehat{A_1} \right)_\ell (ma^* + k)_1 \left\langle e_n, e^{i\ell a^* \cdot x} e_m \right\rangle \\
+ \left(\widehat{A_2} \right)_\ell (ma^* + k)_2 \left\langle e_n, e^{i\ell a^* \cdot x} e_m \right\rangle \\
= \left(\widehat{A_1} \right)_{n-m} (ma^* + k)_1 + \left(\widehat{A_2} \right)_{n-m} (ma^* + k)_2 = \widehat{A}_{n-m} \cdot (ma^* + k)
\end{aligned}$$

For $V = \sum_\ell \widehat{V}_\ell e^{i\ell a^* x}$, we have

$$\left\langle e_n, V(-i\nabla + k)^2 e_m \right\rangle = (ma^* + k)^2 \, \widehat{V}_{n-m}$$

5.4. **On-diagonal potential.** For a general $W^\pm = \sum_m W_m^\pm e^{ima^* \cdot x}$, we have

$$\left\langle e_{\alpha,n}, \begin{pmatrix} W^+ & 0 \\ 0 & W^- \end{pmatrix} e_{\beta,m} \right\rangle = \delta_{\alpha \in \{1,2\}}^{\beta \in \{1,2\}} \left(W_{n-m}^+ \right)_{\alpha_1 \beta_1} + \delta_{\alpha \in \{3,4\}}^{\beta \in \{3,4\}} \left(W_{n-m}^- \right)_{\alpha_2 \beta_2}$$

5.5. **Off-diagonal potential.** For a general $V = \sum_m V_m e^{ima^* \cdot x}$, we have $V^* = \sum_m V_m^* e^{-ima^* \cdot x}$ and

$$\begin{aligned}
M_{IJ} &:= \left\langle e_{\alpha,n}, \begin{pmatrix} 0 & V \\ V^* & 0 \end{pmatrix} e_{\beta,m} \right\rangle \\
&= \sum_k \left(\delta_{\alpha \in \{1,2\}}^{\beta \in \{3,4\}} \delta_{m+k-n} \langle e_{\alpha_1}, V_k e_{\beta_2} \rangle + \delta_{\alpha \in \{3,4\}}^{\beta \in \{1,2\}} \delta_{m-k-n} \langle e_{\alpha_2}, V_k^* e_{\beta_1} \rangle \right) \\
&= \delta_{\alpha \in \{1,2\}}^{\beta \in \{3,4\}} \langle e_{\alpha_1}, V_{n-m} e_{\beta_2} \rangle + \delta_{\alpha \in \{3,4\}}^{\beta \in \{1,2\}} \left\langle e_{\alpha_2}, V_{m-n}^* e_{\beta_1} \right\rangle \\
&= \delta_{\alpha \in \{1,2\}}^{\beta \in \{3,4\}} \left(V_{n-m} \right)_{\alpha_1 \beta_2} + \delta_{\alpha \in \{3,4\}}^{\beta \in \{1,2\}} \overline{\left(V_{m-n} \right)_{\beta_1 \alpha_2}}
\end{aligned}$$

and M is also Hermitian.

5.6. **Off-diagonal magnetic term.** For a general $A = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}$, $A_j = \sum_\ell (A_j)_\ell \, e^{i\ell a^* \cdot x}$, we have $A_j^* = \sum_\ell (A_j)_\ell^* \, e^{-i\ell a^* \cdot x}$ and we compute

$$\left\langle e_{\alpha,n}, \begin{pmatrix} 0 & A \cdot (-i\nabla + k) \\ A^* \cdot (-i\nabla + k) & 0 \end{pmatrix} e_{\beta,m} \right\rangle$$
$$= \delta_{\alpha \in \{1,2\}}^{\beta \in \{3,4\}} \Big((ma^* + k)_1 \left((A_1)_{n-m} \right)_{\alpha_1 \beta_2} + (ma^* + k)_2 \left((A_2)_{n-m} \right)_{\alpha_1 \beta_2} \Big)$$
$$+ \delta_{\alpha \in \{3,4\}}^{\beta \in \{1,2\}} \Big((ma^* + k)_1 \overline{\left((A_1)_{m-n} \right)_{\beta_1 \alpha_2}} + (ma^* + k)_2 \overline{\left((A_2)_{m-n} \right)_{\beta_1 \alpha_2}} \Big)$$

5.7. **Dirac operator.** We have

$$\begin{aligned} \sigma \cdot (-i\nabla + k) &= \sigma_1 (-i\partial_1 + k_1) + \sigma_2 (-i\partial_2 + k_2) \\ &= \begin{pmatrix} 0 & -i(\partial_1 - i\partial_2) + \overline{k_{\mathbb{C}}} \\ -i(\partial_1 + i\partial_2) + k_{\mathbb{C}} & 0 \end{pmatrix} \end{aligned}$$

where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

so, with $k_{\mathbb{C}} := k_1 + ik_2$,

$$\sigma \cdot (-i\nabla + k) \begin{pmatrix} 1 \\ 0 \end{pmatrix} e_m = (ma^* + k)_{\mathbb{C}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e_m$$
$$\sigma \cdot (-i\nabla + k) \begin{pmatrix} 0 \\ 1 \end{pmatrix} e_m = \overline{(ma^* + k)_{\mathbb{C}}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e_m$$

Then

$$\begin{pmatrix} \sigma \cdot (-i\nabla + k) & 0 \\ 0 & \sigma \cdot (-i\nabla + k) \end{pmatrix} e_{1,m} = (ma^* + k)_{\mathbb{C}} \, e_{2,m}$$
$$\begin{pmatrix} \sigma \cdot (-i\nabla + k) & 0 \\ 0 & \sigma \cdot (-i\nabla + k) \end{pmatrix} e_{2,m} = \overline{(ma^* + k)_{\mathbb{C}}} e_{1,m}$$
$$\begin{pmatrix} \sigma \cdot (-i\nabla + k) & 0 \\ 0 & \sigma \cdot (-i\nabla + k) \end{pmatrix} e_{3,m} = (ma^* + k)_{\mathbb{C}} \, e_{4,m}$$
$$\begin{pmatrix} \sigma \cdot (-i\nabla + k) & 0 \\ 0 & \sigma \cdot (-i\nabla + k) \end{pmatrix} e_{4,m} = \overline{(ma^* + k)_{\mathbb{C}}} e_{3,m}$$

We know that $e^{-ikx} (-i\nabla) \, e^{ikx} \cdot = -i\nabla + k$ hence

$$e^{-ikx} \left(-\frac{1}{2} \Delta \right) e^{ikx} \cdot = \frac{1}{2} (-i\nabla + k)^2$$

and with $f(x) = \sum_m \widehat{f}_m e^{ima^* x}$

$$(-i\nabla + k) \, f = \sum_m (ma^* + k) \, \widehat{f}_m e^{ima^* x},$$

so

$$\frac{1}{2} (-i\nabla + k)^2 \, f = \sum_m \frac{1}{2} (ma^* + k)^2 \, \widehat{f}_m e^{ima^* x}$$

We have

$$\left\langle e_{\alpha,n}, \frac{1}{2}\left(-i\nabla+k\right)^2 e_{\beta,m}\right\rangle = \frac{1}{2}\left(ma^*+k\right)^2 \delta_{\alpha,\beta}\delta_{m-n}$$

We have

$$\sigma\cdot k = \begin{pmatrix} 0 & \overline{k_{\mathbb{C}}} \\ k_{\mathbb{C}} & 0 \end{pmatrix}, \qquad (Jk)_{\mathbb{C}} = ik_{\mathbb{C}}, \qquad \sigma\cdot Jk = \begin{pmatrix} 0 & -i\overline{k_{\mathbb{C}}} \\ ik_{\mathbb{C}} & 0 \end{pmatrix}$$

so

$$\begin{pmatrix} -\sigma\cdot J\left(-i\nabla+k\right) & 0 \\ 0 & \sigma\cdot J\left(-i\nabla+k\right) \end{pmatrix} e_{1,m} = -i\left(ma^*+k\right)_{\mathbb{C}} e_{2,m}$$
$$\begin{pmatrix} -\sigma\cdot J\left(-i\nabla+k\right) & 0 \\ 0 & \sigma\cdot J\left(-i\nabla+k\right) \end{pmatrix} e_{2,m} = i\,\overline{\left(ma^*+k\right)_{\mathbb{C}}}\, e_{1,m}$$
$$\begin{pmatrix} -\sigma\cdot J\left(-i\nabla+k\right) & 0 \\ 0 & \sigma\cdot J\left(-i\nabla+k\right) \end{pmatrix} e_{3,m} = i\left(ma^*+k\right)_{\mathbb{C}} e_{4,m}$$
$$\begin{pmatrix} -\sigma\cdot J\left(-i\nabla+k\right) & 0 \\ 0 & \sigma\cdot J\left(-i\nabla+k\right) \end{pmatrix} e_{4,m} = -i\,\overline{\left(ma^*+k\right)_{\mathbb{C}}}\, e_{3,m}$$

For a general $V=\sum_m \widehat{V}_m e^{ima^*\cdot x}$, we have $V^*=\sum_m \widehat{V}_m^* e^{-ima^*\cdot x}$ and we compute

$$\begin{aligned}
&\left\langle e_{\alpha,n}, \begin{pmatrix} 0 & V\left(-i\nabla+k\right)^2 \\ V^*\left(-i\nabla+k\right)^2 & 0 \end{pmatrix} e_{\beta,m}\right\rangle \\
&\qquad = \left(ma^*+k\right)^2\left(\delta^{\beta\in\{3,4\}}_{\alpha\in\{1,2\}}\left(\widehat{V}_{n-m}\right)_{\alpha_1\beta_2} + \delta^{\beta\in\{1,2\}}_{\alpha\in\{3,4\}}\overline{\left(\widehat{V}_{m-n}\right)_{\beta_1\alpha_2}}\right)
\end{aligned}$$

6. Symmetries

6.1. **Particle-hole.** We define

$$\mathcal{S}u(x) := i\begin{pmatrix} 0 & -\mathbb{1}_{2\times 2} \\ \mathbb{1}_{2\times 2} & 0 \end{pmatrix} u(-x)$$

We have

$$\mathcal{S}\begin{pmatrix} 0 & B \\ B^* & 0 \end{pmatrix}\mathcal{S} = -\begin{pmatrix} 0 & B^*(-x) \\ B(-x) & 0 \end{pmatrix}$$

We have $T(-x)^* = T(x)$ hence we should have that

$$\mathcal{S}H\mathcal{S} = -H$$

We compute

$$\begin{aligned}
\mathcal{S}_{IJ} = \langle e_{\alpha,n}, \mathcal{S}e_{\beta,m}\rangle &= i\left\langle e_{\alpha,n}, \begin{pmatrix} -e_{\beta_2,-m} \\ e_{\beta_1,-m} \end{pmatrix}\right\rangle \\
&= i\delta_{m+n}\left(\delta^{\beta\in\{1,2\}}_{\alpha\in\{3,4\}}\delta_{\beta_1-\alpha_2} - \delta^{\beta\in\{3,4\}}_{\alpha\in\{1,2\}}\delta_{\beta_2-\alpha_1}\right)
\end{aligned}$$

6.2. **Mirror.** First, for any function B, we have $\sigma_1 B^* \sigma_1 = \begin{pmatrix} \overline{B_{22}} & \overline{B_{12}} \\ \overline{B_{21}} & \overline{B_{11}} \end{pmatrix}$.

The mirror operator for the BM Hamiltonian is

$$\mathcal{M}u(\mathbf{X}) := \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix} u(\overline{\mathbf{X}})$$

where $\overline{\mathbf{X}} := (X_1, -X_2) =: M\mathbf{X}$, it satisfies $\mathcal{M} = \mathcal{M}^{-1} = \mathcal{M}^*$.

Next,

$$\mathcal{M} \begin{pmatrix} 0 & B(\mathbf{X}) \\ B(\mathbf{X})^* & 0 \end{pmatrix} \mathcal{M} = \begin{pmatrix} 0 & \sigma_1 B^*(\overline{\mathbf{X}})\sigma_1 \\ \sigma_1 B(\overline{\mathbf{X}})\sigma_1 & 0 \end{pmatrix}$$

In cartesian coordinates, we have

$$T(M\mathbf{X}) = \sum_{j=1}^{3} T_j e^{ix\cdot M^* q_j^c} = \sum_{j=1}^{3} T_j e^{ix\cdot M q_j^c}$$

because $M^* = M$. But

$$\sigma_1 T^*(M\mathbf{X})\sigma_1 = \begin{pmatrix} w_0 \left(\sum_{j=1}^3 e^{ix\cdot Mq_j}\right) & w_1 \left(e^{ix\cdot Mq_1} + e^{i\phi} e^{ixMq_2} + e^{i2\phi} e^{ix\cdot Mq_3}\right) \\ \cdot & \cdot \end{pmatrix}$$

$$= \begin{pmatrix} w_0 \left(\sum_{j=1}^3 e^{ix\cdot q_j}\right) & w_1 \left(e^{ix\cdot q_1} + e^{-i\phi} e^{ixq_2} + e^{-i2\phi} e^{ix\cdot q_3}\right) \\ \cdot & \cdot \end{pmatrix} = T(\mathbf{X})$$

where we used that $Mq_1^c = q_1^c$, $Mq_2^c = q_3^c$ and $Mq_3^c = q_2^c$.

We search the action on reduced Fourier coefficients. We have

$$f(Mx) = \sum_m e^{ix\cdot M(ma^*)} = \sum_m e^{ix\cdot (M^r m)a^*}$$

where $M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$,

$$M^r = S^{-1}MS = \mathcal{M}^* M \left(\mathcal{M}^*\right)^{-1} = \sigma_1$$

7. Change of basis for getting $\Phi_j \in L^2_{\tau,\overline{\tau}}$

Numerically, DFTK gives

$$\phi, \psi \in \operatorname{Ker}\left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right) + \operatorname{Ker}\left(\mathcal{R}_{\frac{2\pi}{3}} - \overline{\tau}\right)$$

but we want to separate the spaces and obtain $\phi_1 \in \operatorname{Ker}\left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right)$ so that $\phi_2(x,z) := \overline{\phi_1}(-x,z) \in \operatorname{Ker}\left(\mathcal{R}_{\frac{2\pi}{3}} - \overline{\tau}\right)$, which existence is ensured by [2].

First we define

$$c := \left\| \left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right) \phi_a \right\|_{L^2}^2, \qquad s := \left\langle \left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right) \phi_a, \left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right) \phi_b \right\rangle.$$

Then we parametrize

$$\phi_1 = e^{i\alpha} \left(\frac{s}{|s|} \cos\theta \phi_a + e^{i\beta} \sin\theta \phi_b \right)$$

and we want $\left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right)\phi_1 = 0$ which is equivalent to

$$\frac{s}{|s|}\cos\theta\left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right)\phi_a + e^{i\beta}\sin\theta\left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right)\phi_b = 0$$

and we take the scalar product with $\left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right)\phi_a$ so that

$$\frac{c}{|s|}\cos\theta + e^{i\beta}\sin\theta = 0$$

Now we necessarily have $e^{i\beta} = \pm$ so $\cos\theta = \mp\frac{|s|}{c}\sin\theta$ and finally using $\cos^2 + \sin^2 = 1$,

$$|\cos\theta| = \frac{1}{\sqrt{1 + \left(\frac{c}{|s|}\right)^2}}, \qquad |\sin\theta| = \frac{1}{\sqrt{1 + \left(\frac{|s|}{c}\right)^2}},$$

and also choosing $\alpha = 0$ if $\cos\theta \geqslant 0$ and π otherwise, which does not change anything, we have

$$\phi_1 = \frac{s}{|s|}\frac{1}{\sqrt{1 + \left(\frac{c}{|s|}\right)^2}}\phi_a \pm \frac{1}{\sqrt{1 + \left(\frac{|s|}{c}\right)^2}}\phi_b$$

and $\phi_2(x) = \overline{\phi_1(-x)}$. By multiplying by e^{-iKx}, we also obtain

$$\boxed{u_1 = \frac{s}{|s|}\frac{1}{\sqrt{1 + \left(\frac{c}{|s|}\right)^2}}u_a \pm \frac{1}{\sqrt{1 + \left(\frac{|s|}{c}\right)^2}}u_b}$$

and $u_2(x) = \overline{u_1(-x)}$.

8. The 1/3 scaling of coordinates

Taken from [3, Appendix G.3, G.4] for instance, the moiré lattice vectors are

$$a_1 = \frac{2\pi}{3k_\theta}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix}, \qquad a_2 = \frac{2\pi}{3k_\theta}\begin{pmatrix}-\sqrt{3}\\ 1\end{pmatrix}$$

and $T(x) = \sum_{j=1}^{3} T_j e^{-iq_j x}$ has

$$q_1 = k_\theta\begin{pmatrix}0\\ -1\end{pmatrix}, \qquad q_{2,3} = \frac{k_\theta}{2}\begin{pmatrix}\pm\sqrt{3}\\ 1\end{pmatrix}$$

and we remark that $a_1 \cdot q_1 = -\frac{2\pi}{3}$ so actually $q_j \notin \mathbb{L}^*$ but $3q_j \in \mathbb{L}^*$.

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