

NUMERICAL COMPUTATIONS FOR AN EFFECTIVE MODEL OF TWISTED BILAYER GRAPHENE

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1. STANDARD MONOLAYER

We recall that

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

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

In reduced coordinates, with

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

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

and

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

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

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

hence any function can be decomposed as

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

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

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,

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

We define the scalar product

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

and compute Plancherel's formula

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

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

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

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

and

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

Similarly, $R_{\frac{\pi}{2}}(ma^*) = \left(R_{\frac{\pi}{2}}^{\text{red}} m\right) a^*$ where

$$R_{\frac{\pi}{2}}^{\text{red}} = S^{-1} R_{\frac{\pi}{2}} S = \frac{1}{\sqrt{3}} \begin{pmatrix} -1 & 2 \\ -2 & 1 \end{pmatrix}, \quad R_{-\frac{\pi}{2}}^{\text{red}} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & -2 \\ 2 & -1 \end{pmatrix} =: \frac{1}{\sqrt{3}} M$$

and

$$\mathcal{R}_{\frac{\pi}{2}} f(x) = \sum_m f_m e^{i \left(R_{\frac{\pi}{2}}^{\text{red}} m\right) a^* \cdot x} = \sum_m f_{Mm} e^{i \frac{1}{\sqrt{3}} m a^* \cdot x}$$

2. COMPUTATION OF V_{int}

For $\mathbf{s} \in \Omega := [0, 1] \mathbf{a}_1 + [0, 1] \mathbf{a}_2$, we denote by $V_{\mathbf{s}}^{(2)}$ 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

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

and we obtain the Fourier coefficients

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

We then compute

$$V_{\text{int}}(z) := \frac{1}{|\Omega|} \int_{\Omega} V_{\text{int},\mathbf{s}}(z) d\mathbf{s} = \frac{1}{N^2} \sum_{s_x, s_y \in \llbracket 1, N \rrbracket} V_{\text{int},(s_x, s_y)}^{\text{array}}(z)$$

and finally obtain the Fourier coefficients

$$\left(\widehat{V_{\text{int}}} \right)_{m_z} = \frac{1}{N^2} \sum_{s_x, s_y \in \llbracket 1, N \rrbracket} \left(\widehat{V_{\text{int},\mathbf{s}}} \right)_{m_z}$$

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

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

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

3. EFFECTIVE POTENTIALS

We defined

$$((f, g))^{\eta, \eta'}(\mathbf{X}) := \frac{1}{|\Omega|} \int_{\Omega \times \mathbb{R}} \bar{f}(x - \eta J\mathbf{X}, z - \eta \frac{d}{2}) g(x - \eta' J\mathbf{X}, z - \eta' \frac{d}{2}) d\mathbf{x} dz$$

and

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

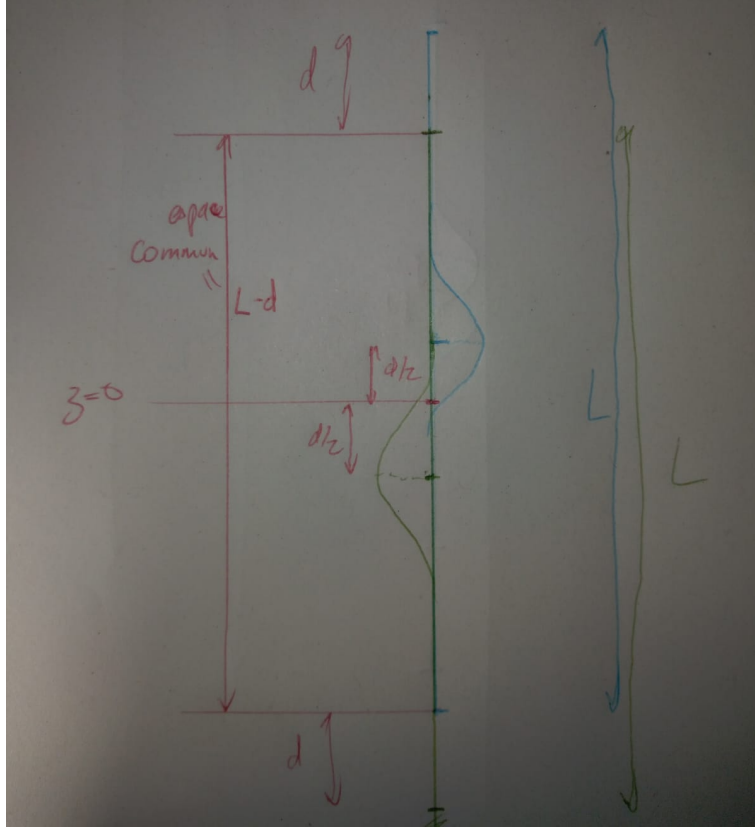
so $\langle\langle f, g \rangle\rangle^{\eta, \eta'} = e^{i(\eta - \eta')\mathbf{K} \cdot J\mathbf{X}} ((f, g))^{\eta, \eta'}$. Now we make the approximation

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

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),

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

FIGURE 1. Situation on the z coordinate

where

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

and we also define

$$C_{\mathbf{m}}^{\pm} := L \sum_{m_z \in \mathbb{Z}} e^{\pm i 2 \frac{d\pi}{L} m_z} \widehat{f_{m, m_z}} \widehat{g_{m, m_z}}$$

Then,

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

Hence

$$((f, g))^{+-} \left(-\frac{3}{2} J \mathbf{X}\right) = \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{i 3 m a^* \cdot \mathbf{X}} C_{\mathbf{m}}^+ = \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{i m a^* \cdot \mathbf{X}} C_{\frac{\mathbf{m}}{3}}^+,$$

and

$$((f, g))^{+-} \left(-\frac{3}{2} J \mathbf{X}\right) = \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{i 3(m + m_K) a^* \cdot \mathbf{X}} C_{\mathbf{m}}^+ = \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{i m a^* \cdot \mathbf{X}} C_{\frac{\mathbf{m} - 3m_K}{3}}^+$$

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

Similarly

$$((f, g))^{-+} \left(-\frac{3}{2}J\mathbf{X}\right) = \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{-i3\mathbf{m}\mathbf{a}^* \cdot \mathbf{X}} C_{\mathbf{m}}^- = \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{i\mathbf{m}\mathbf{a}^* \cdot \mathbf{X}} C_{-\frac{\mathbf{m}}{3}}^-$$

For the potentials, we finally need to implement

$$\mathbb{W}_{j,j'}^+ = ((\bar{u}_j u_{j'}, V))^{+-}, \quad \mathbb{W}_{j,j'}^- = ((\bar{u}_j u_{j'}, V))^{-+},$$

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

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

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

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

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

so

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

so we can implement

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

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

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

and the matrix $M_{j,j'} := \langle u_j, V_{\text{int}} u_{j'} \rangle$ 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 $x \in \mathbb{R}^2$,

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

and

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

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

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

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

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

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

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

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

and their Bloch transform becomes

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.7. Dirac operator. We have

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

where

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

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

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

Then

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

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

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

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

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

so

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

We have

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

We have

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

so

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

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

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

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

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

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

$$\begin{aligned} \sigma_1 T^*(M\mathbf{X}) \sigma_1 &= \begin{pmatrix} w_0 \left(\sum_{j=1}^3 e^{ix \cdot M q_j} \right) & w_1 \left(e^{ix \cdot M q_1} + e^{i\phi} e^{ix \cdot M q_2} + e^{i2\phi} e^{ix \cdot M q_3} \right) \\ \cdot & \cdot \end{pmatrix} \\ &= \begin{pmatrix} w_0 \left(\sum_{j=1}^3 e^{ix \cdot q_j} \right) & w_1 \left(e^{ix \cdot q_1} + e^{-i\phi} e^{ix \cdot q_2} + e^{-i2\phi} e^{ix \cdot q_3} \right) \\ \cdot & \cdot \end{pmatrix} = T(\mathbf{X}) \end{aligned}$$

where we used that $M q_1^c = q_1^c$, $M q_2^c = q_3^c$ and $M q_3^c = q_2^c$.

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

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

7. CHANGE OF BASIS FOR GETTING $\Phi_j \in L_{\tau, \bar{\tau}}^2$

Numerically, DFTK gives

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

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

First we define

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

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

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

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

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

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

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

and also choosing $\alpha = 0$ if $\cos \theta \geq 0$ 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

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

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

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

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

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

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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