

# 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. Dirac point.** We have

$$K = \frac{-a_1^* + a_2^*}{3}, \quad a_1^* \cdot a_2^* = -\frac{|a_j^*|^2}{2}, \quad |K| = \frac{|a_j^*|}{\sqrt{3}}$$

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

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

hence any function can be decomposed as

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

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  $z$ , and  $\int_{\mathbb{R}} dz \simeq \int_{[0, L]} dz$  so the Fourier transform is

$$(\mathcal{F}f)_{m, m_z} := \frac{1}{L |\Omega|} \int_{\Omega \times [0, L]} e^{-i(ma^* \mathbf{x} + m_z \frac{2\pi}{L} z)} f(\mathbf{x}, z) d\mathbf{x} dz$$

and the reconstruction formula is

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

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).

We implement the Fourier transform

```
myfft(a) = fft(a)/length(a)
myifft(a) = ifft(a)*length(a)
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so that if  $a_i = f(x_i)$  are the actual values of the functions, then  $myfft(a)[m] \simeq (\mathcal{F}f)_{m-1}$  up to Riemann series errors.

**1.3. 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

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

where  $\mathcal{L}$  is the action of  $M$  on the Fourier coefficients of  $f$ .

## 2. COMPARISON WITH EXISTING RESULTS

From [2], we verified that with  $T = 0$ , we have Fig 3(a), with the right energies

3. COMPUTATION OF  $V_{\text{int}}$ 

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

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

and we obtain the Fourier coefficients

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

We then compute

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

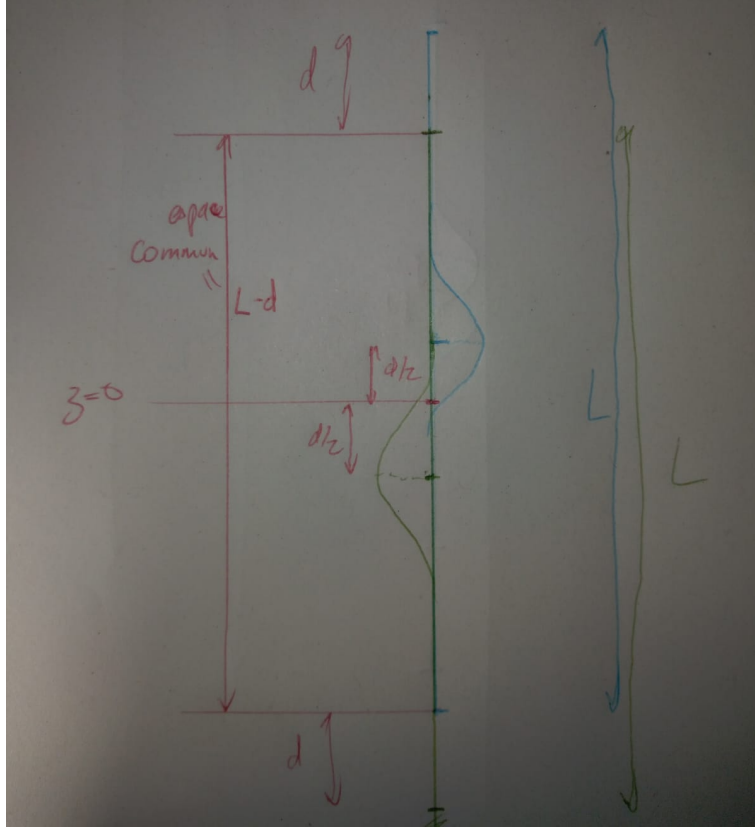
and finally obtain the Fourier coefficients

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

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  $V_{\text{int}}(-z) = V_{\text{int}}(z)$ .

FIGURE 1. Situation on the  $z$  coordinate

## 4. EFFECTIVE POTENTIALS

We defined

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

and

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

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 4. 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),

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

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,

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

Hence

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

and

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

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

Similarly

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

For the potentials, we finally need to implement

$$\begin{aligned} \mathbb{W}_{j, j'}^+ &= ((\bar{u}_j u_{j'}, V))^{+-}, \quad \mathbb{W}_{j, j'}^- = ((\bar{u}_j u_{j'}, V))^{-+}, \\ \mathbb{V}_{j, j'} &= \langle\langle (V + V_{\text{int}}) u_j, u_{j'} \rangle\rangle^{+-} \end{aligned}$$

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  $\mathbb{V}(-X)^* = \mathbb{V}(X)$

**4.1. 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

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

so

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

so we can implement

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

4.2. **W's  $V_{\text{int}}$  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  $M_{11} = M_{22}$ .

## 5. 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

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

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

$$\begin{aligned} q_1^c &= \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = a_1^* + a_2^*, \\ q_2^c &= \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} = -a_2^*, \quad q_3^c = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} = -a_1^*, \end{aligned}$$

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

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

Or

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

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

## 6. OPERATORS IN BASIS

**6.1. 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

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

and their Bloch transform becomes

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

and we want the middle of the spectrum of

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

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

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

**6.3. 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

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

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

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

**6.5. 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.

**6.6. 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

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

**6.7. 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

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

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  $f(x) = \sum_m \hat{f}_m e^{ima^*x}$

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

so

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

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  $V = \sum_m \hat{V}_m e^{ima^*x}$ , we have  $V^* = \sum_m \hat{V}_m^* e^{-ima^*x}$  and we compute

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

## 7. RENORMALIZATION OF THE EQUATION

We know that

$$(-i\nabla + k + A(x)(-i\nabla) + v(x))\psi = E\psi$$

with  $x = \lambda y$ , we define  $\phi(y) := \psi(\lambda y)$  and

$$((( -i\nabla + k) + A(\lambda y)(-i\nabla) + v(\lambda y))\psi)(\lambda y) = E\psi(\lambda y)$$

but  $(\nabla\psi)(\lambda y) = \frac{1}{\lambda}\nabla\phi(y)$ , so

$$\left(\frac{-i\nabla}{\lambda} + k + \frac{A(\lambda y)}{\lambda}(-i\nabla) + v(\lambda y)\right)\phi = E\phi$$

We enter  $V\left(\frac{3}{2}JX\right)$  for each potential  $V$ , hence we need to apply a coefficient  $\frac{2}{3}$  to each derivation operator.

## 8. SYMMETRIES

8.1. **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

$$SHS = -H$$

We compute

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

For any function  $B$  and any vector function  $\mathbf{A}$ , we have

$$\begin{aligned} \mathcal{S} \begin{pmatrix} 0 & B(\mathbf{X}) \\ B^*(\mathbf{X}) & 0 \end{pmatrix} \mathcal{S} &= - \begin{pmatrix} 0 & B^*(-\mathbf{X}) \\ B(-\mathbf{X}) & 0 \end{pmatrix} \\ \mathcal{S} \begin{pmatrix} 0 & B(\mathbf{X})\Delta \\ B^*(\mathbf{X})\Delta & 0 \end{pmatrix} \mathcal{S} &= - \begin{pmatrix} 0 & B^*(-\mathbf{X})\Delta \\ B(-\mathbf{X})\Delta & 0 \end{pmatrix} \\ \mathcal{S} \begin{pmatrix} 0 & i\mathbf{A}(\mathbf{X}) \cdot \nabla \\ i\mathbf{A}(\mathbf{X})^* \cdot \nabla & 0 \end{pmatrix} \mathcal{S} &= \begin{pmatrix} 0 & i\mathbf{A}(-\mathbf{X})^* \cdot \nabla \\ i\mathbf{A}(-\mathbf{X}) \cdot \nabla & 0 \end{pmatrix}, \end{aligned}$$

we also compute that

$$\mathcal{S} \begin{pmatrix} \sigma \cdot \nabla & 0 \\ 0 & \sigma \cdot \nabla \end{pmatrix} \mathcal{S} = - \begin{pmatrix} \sigma \cdot \nabla & 0 \\ 0 & \sigma \cdot \nabla \end{pmatrix},$$

hence if the operator  $\Gamma$  is a linear combination of the terms

$$\begin{aligned} &\begin{pmatrix} \sigma \cdot (-i\nabla) & 0 \\ 0 & \sigma \cdot (-i\nabla) \end{pmatrix}, \begin{pmatrix} \sigma \cdot J(-i\nabla) & 0 \\ 0 & \sigma \cdot J(-i\nabla) \end{pmatrix}, \\ &\begin{pmatrix} 0 & \mathbb{V} \\ \mathbb{V}^* & 0 \end{pmatrix}, \begin{pmatrix} 0 & \Sigma \\ \Sigma^* & 0 \end{pmatrix}, \begin{pmatrix} 0 & \Sigma\Delta \\ \Sigma^*\Delta & 0 \end{pmatrix} \end{aligned}$$

it satisfies the symmetry  $\mathcal{S}\Gamma\mathcal{S} = -\Gamma$ , and those are the particle-hole symmetric terms of our effective Hamiltonian. However, if  $\Gamma$  is a linear combination of the operators

$$\begin{pmatrix} 0 & \mathcal{A} \cdot (-i\nabla) \\ \mathcal{A}^* \cdot (-i\nabla) & 0 \end{pmatrix}, \begin{pmatrix} 0 & \mathcal{A} \cdot J(-i\nabla) \\ \mathcal{A}^* \cdot J(-i\nabla) & 0 \end{pmatrix}, \\ \begin{pmatrix} -\frac{1}{2}\Delta & 0 \\ 0 & -\frac{1}{2}\Delta \end{pmatrix}, \begin{pmatrix} \mathbb{W} & 0 \\ 0 & \mathbb{W}^* \end{pmatrix}, \begin{pmatrix} \mathbb{1}_{2 \times 2} & 0 \\ 0 & \mathbb{1}_{2 \times 2} \end{pmatrix}$$

of the effective Hamiltonian  $\mathcal{H}_{d,\theta}$ , it satisfies  $\mathcal{S}\Gamma\mathcal{S} = \Gamma$  and hence break the particle-hole symmetry.

But now we also compute that

$$\mathcal{S} \begin{pmatrix} k & 0 \\ 0 & k \end{pmatrix} \mathcal{S} = k, \\ \mathcal{S} \begin{pmatrix} \sigma(-i\nabla + k) & 0 \\ 0 & \sigma(-i\nabla + k) \end{pmatrix} \mathcal{S} = - \begin{pmatrix} \sigma(-i\nabla - k) & 0 \\ 0 & \sigma(-i\nabla - k) \end{pmatrix}$$

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

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

## 9. NON LOCAL TERM

From the theoretical investigations, we have

$$F_0^{\eta,j,s}(\mathbf{X}) := \int_{\mathbb{R}^3} \overline{\varphi_{\text{Bl}}(\mathbf{y}, z)} \Phi_j(\mathbf{y} + \mathbf{a}_s - 2\eta J\mathbf{X}, z - \eta d) \, d\mathbf{y} dz$$

and

$$\mathbb{W}_{\text{nl},-1}^{\eta}(\mathbf{X})_{jj'} := \frac{v_0}{|\Omega|} \sum_{s \in \{1,2\}} \overline{F_0^{\eta,j,s}(\mathbf{X})} F_0^{\eta,j',s}(\mathbf{X}).$$

Since  $\varphi_{\text{Bl}}$  is localized, we periodize it and we make the approximation

$$F_0^{\eta,j,s}(\mathbf{X}) \simeq \int_{\Omega \times [0,L]} \overline{\varphi_{\text{Bl}}(\mathbf{y}, z)} \Phi_j(\mathbf{y} + \mathbf{a}_s - 2\eta J\mathbf{X}, z - \eta d) \, d\mathbf{y} dz$$

and we define  $\varphi$  such that  $\varphi_{\text{Bl}} = e^{i\mathbf{K}\mathbf{y}}\varphi$ , because it is  $\widehat{\varphi}$  which is stored by DFTK, so

$$\begin{aligned} \varphi_{\text{Bl}}(\mathbf{y}, z) &= \sum_{\mathbf{G}, G_z} e^{i((\mathbf{G}+\mathbf{K})\mathbf{y}+G_z z)} \widehat{\varphi}_{\mathbf{G}, G_z}, \\ \Phi_j(\mathbf{y}, z) &= \sum_{\mathbf{G}, G_z} e^{i((\mathbf{G}+\mathbf{K})\mathbf{y}+G_z z)} \widehat{(u_j)}_{\mathbf{G}, G_z} \end{aligned}$$

where  $\mathbf{K}$  is the Dirac point, thus

$$\begin{aligned} F_0^{\eta,j,s}(\mathbf{X}) &= L |\Omega| \sum_{\mathbf{G}, G_z} e^{i(\mathbf{G}(\mathbf{a}_s - 2\eta J\mathbf{X}) - \eta G_z d)} \widehat{\varphi}_{\mathbf{G}, G_z} \widehat{(u_j)}_{\mathbf{G}, G_z} \\ F^{\eta,j,s}(\mathbf{X}) &:= F_0^{\eta,j,s}(-\tfrac{3}{2}J\mathbf{X}) \\ &= L |\Omega| \sum_{\mathbf{G}, G_z} e^{i(\mathbf{G}(\mathbf{a}_s - 3\eta J\mathbf{X}) - \eta G_z d)} \widehat{\varphi}_{\mathbf{G}, G_z} \widehat{(u_j)}_{\mathbf{G}, G_z} \\ &= L |\Omega| \sum_{\mathbf{G}, G_z} e^{i(\mathbf{G}(-\eta \frac{\mathbf{a}_s}{3} + \mathbf{X}) - \eta G_z d)} \widehat{\varphi}_{-\frac{\eta}{3}\mathbf{G}, G_z} \widehat{(u_j)}_{-\frac{\eta}{3}\mathbf{G}, G_z} \end{aligned}$$

has Fourier coefficients

$$\begin{aligned} \widehat{(F^{\eta,j,s})}_{\mathbf{G}} &= L |\Omega| \sum_{G_z} e^{-i\eta(\mathbf{G} \frac{\mathbf{a}_s}{3} + G_z d)} \widehat{\varphi}_{-\frac{\eta}{3}\mathbf{G}, G_z} \widehat{(u_j)}_{-\frac{\eta}{3}\mathbf{G}, G_z} \\ \widehat{(F^{\eta,j,s})}_{m_z} &= L |\Omega| \sum_{m_z} e^{-i\eta(m \mathbf{a}^* \frac{\mathbf{a}_s}{3} + \frac{2\pi}{L} m_z d)} \widehat{\varphi}_{-\frac{\eta}{3}m, m_z} \widehat{(u_j)}_{-\frac{\eta}{3}m, m_z} \\ &= L |\Omega| \sum_{m_z} e^{-i\eta\left(2\pi m \frac{\mathbf{a}_s^{\text{red}}}{3} + \frac{2\pi}{L} m_z d\right)} \widehat{\varphi}_{-\frac{\eta}{3}m, m_z} \widehat{(u_j)}_{-\frac{\eta}{3}m, m_z} \end{aligned}$$

10. 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 [3].

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  $\left( \mathcal{R}_{\frac{2\pi}{3}} - \tau \right) \phi_1 = 0$  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  $\cos^2 + \sin^2 = 1$ ,

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

and also choosing  $\alpha = 0$  if  $\cos \theta \geq 0$  and  $\pi$  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  $u_2(x) = \overline{u_1(-x)}$ .

## 11. THE 1/3 SCALING OF COORDINATES

Taken from [4, 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  $3q_j \in \mathbb{L}^*$ .

## REFERENCES

- [1] S. BECKER, M. EMBREE, J. WITTSTEN, AND M. ZWORSKI, *Spectral characterization of magic angles in twisted bilayer graphene*, Phys. Rev. B, 103 (2021), p. 165113.
- [2] S. FANG, S. CARR, Z. ZHU, D. MASSATT, AND E. KAXIRAS, *Angle-dependent  $\{it Ab initio\}$  low-energy hamiltonians for a relaxed twisted bilayer graphene heterostructure*, arXiv preprint arXiv:1908.00058, (2019).
- [3] C. FEFFERMAN AND M. WEINSTEIN, *Honeycomb lattice potentials and Dirac points*, J. Am. Math. Soc, 25 (2012), pp. 1169–1220.
- [4] A. B. WATSON AND M. LUSKIN, *Existence of the first magic angle for the chiral model of bilayer graphene*, J. Math. Phys, 62 (2021), p. 091502.