

# NUMERICAL COMPUTATIONS FOR AN EFFECTIVE MODEL OF TWISTED BILAYER GRAPHENE

ÉRIC CANCÈS, LOUIS GARRIGUE AND DAVID GONTIER

## 1. STANDARD MONOLAYER

We choose for the microscopic lattice, the orientation **NOT THE RIGHT ONES** and for the Macroscopic lattice, we choose the orientation

$$b_1 = b \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \quad b_2 = b \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, \quad b_1^* = \frac{4\pi}{b\sqrt{3}} \begin{pmatrix} -\frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, \quad b_2^* = \frac{4\pi}{b\sqrt{3}} \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix} \quad (1)$$

so  $-Jb_j^* = \frac{a}{b}a_j^*$  and  $Jb_j = \frac{b}{a}a_j$  and

$$\mathcal{M}_b := \begin{pmatrix} b_1 & b_2 \end{pmatrix} = \frac{b}{2} \begin{pmatrix} -1 & 1 \\ \sqrt{3} & \sqrt{3} \end{pmatrix}$$

In reduced coordinates, with

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

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

and

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

**1.1. 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. From  $q$  to  $m_q$ .** Suppose you know  $q$  in cartesian coordinates and you want to compute  $m^q$ , its reduced coordinates, that is  $m^q a = q$ , then since  $m^q a = (a_1^* a_2^*) \begin{pmatrix} m_1^q \\ m_2^q \end{pmatrix} = 2\pi (\mathcal{M}^{-1})^* \begin{pmatrix} m_1^q \\ m_2^q \end{pmatrix}$ ,

$$\begin{pmatrix} m_1^q \\ m_2^q \end{pmatrix} = \frac{1}{2\pi} \mathcal{M}^* q \quad (2)$$

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

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

hence any function can be decomposed as

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

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

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

where  $\Gamma := \sqrt{L|\Omega|}$  and the reconstruction formula is

$$f(\mathbf{x}, z) = \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ m_z \in \mathbb{Z}}} \frac{e^{i(\mathbf{m}a^* \cdot \mathbf{x} + m_z \frac{2\pi}{L} z)}}{\Gamma} \hat{f}_{\mathbf{m},m_z} \quad (3)$$

We define the scalar product

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

and compute Plancherel's formula

$$\langle f, g \rangle = \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ m_z \in \mathbb{Z}}} \overline{\hat{f}_{\mathbf{m},m_z}} \hat{g}_{\mathbf{m},m_z}. \quad (4)$$

Hence, as a verification, we test that the normalization of the  $\hat{u}_j$ 's is the right one by checking that  $\|u_j\|_{L^2}^2 = 1$  via (4).

We implement the Fourier transforms

```
myfft(a,B) = fft(a)*sqrt(B)/length(a)
myifft(a) = ifft(a)*length(a)/sqrt(B)
```

where  $B = \Gamma^2 = L|\Omega|$  in  $3d$ ,  $B = L$  in  $1d$  in  $z$ , and  $B = |\Omega|$  in  $2d$  in  $(x, y)$ . 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.

**1.4. 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  $f$ .

**1.5. Action of mirror.** We define  $M := \text{diag}(-1, 1, -1)$ , we have

$$\mathbb{M}u(x) := u(Mx)$$

With the lattice  $a$  defined in (??), we obtain

## 2. COMPARISON WITH EXISTING RESULTS

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

**2.1. Reduction of Fourier coefficients in  $2d$  to  $1d$ .** This is used to compute  $V_{\text{int}}$ . We take a function  $f$  and define its average

$$g(z) := \frac{1}{|\Omega|} \int_{\Omega} f$$

and since

$$\hat{f}_{0,m_z} = \frac{1}{\sqrt{L}|\Omega|} \int_{\Omega} f(x, z) e^{-i \frac{2\pi}{L} m_z z} dx dz$$

then

$$\hat{g}_{m_z} = \frac{1}{|\Omega| \sqrt{L}} \int_{\Omega \times [0, L]} f(x, z) e^{-i \frac{2\pi}{L} m_z z} dx dz = \frac{\hat{f}_{0,m_z}}{\sqrt{|\Omega|}}$$

## 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

$$\begin{aligned} V_{\text{int}, \mathbf{s}}(z) &:= \frac{1}{|\Omega|} \int_{\Omega} \left( V_{\mathbf{s}}^{(2)}(\mathbf{x}, z) - V(\mathbf{x}, z + \frac{d}{2}) - V(\mathbf{x} - \mathbf{s}, z - \frac{d}{2}) \right) d\mathbf{x} \\ &= \frac{1}{|\Omega|} \int_{\Omega} \left( V_{\mathbf{s}}^{(2)}(\mathbf{x}, z) - V(\mathbf{x}, z + \frac{d}{2}) - V(\mathbf{x}, z - \frac{d}{2}) \right) d\mathbf{x} \\ &= \frac{1}{|\Omega|^{\frac{3}{2}}} \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ m_z \in \mathbb{Z}}} \left( \widehat{\left( V_{\mathbf{s}}^{(2)} \right)}_{\mathbf{m}, m_z} - \widehat{V}_{\mathbf{m}, m_z} e^{im_z \frac{2\pi}{L} \frac{d}{2}} - \widehat{V}_{\mathbf{m}, m_z} e^{-im_z \frac{2\pi}{L} \frac{d}{2}} \right) \\ &\quad \times \int_{\Omega} e^{i(\mathbf{m} a^* \cdot \mathbf{x} + m_z \frac{2\pi}{L} z)} d\mathbf{x} \\ &= \frac{1}{\sqrt{|\Omega|}} \sum_{m_z \in \mathbb{Z}} e^{im_z \frac{2\pi}{L} z} \left( \widehat{\left( V_{\mathbf{s}}^{(2)} \right)}_{0, m_z} - 2\widehat{V}_{0, m_z} \cos(m_z \frac{\pi d}{L}) \right) \end{aligned}$$

and we obtain the Fourier coefficients

$$\left(\widehat{V_{\text{int},\mathbf{s}}}\right)_{m_z} = \frac{1}{\sqrt{|\Omega|}} \left( \left(\widehat{V_{\mathbf{s}}^{(2)}}\right)_{0,m_z} - 2\widehat{V}_{0,m_z} \cos\left(m_z \frac{\pi d}{L}\right) \right)$$

We then compute

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

and finally obtain the Fourier coefficients

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

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

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

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

#### 4. EFFECTIVE POTENTIALS

We defined

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

and

$$\boxed{\langle\langle f, g \rangle\rangle^{\eta, \eta'} := e^{i\frac{1}{2}(\eta - \eta')\mathbf{K} \cdot J\mathbf{X}} \langle\langle f, g \rangle\rangle^{\eta, \eta'}}$$

and in particular since  $q_1 = JK$ , then  $\langle\langle f, g \rangle\rangle^{+-} = e^{-iq_1 x} \langle\langle f, g \rangle\rangle^{+-}$ . Now we make the approximation

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

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 (3),

$$\begin{aligned} ((f, g))^{\eta, \eta'} &= \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{i\frac{1}{2}(\eta - \eta')ma^* \cdot J\mathbf{X}} \sum_{m_z \in \mathbb{Z}} e^{i(\eta - \eta')\frac{2\pi}{L}m_z} \overline{\widehat{f}_{m, m_z}} \widehat{g}_{m, m_z} \\ &= \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{e^{-i\frac{1}{2}(\eta - \eta')ma^* \cdot J\mathbf{X}}}{\sqrt{|\Omega_M|}} C_{-\mathbf{m}} \end{aligned}$$

where

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

We have  $((f, g))^{++} = ((f, g))^{--} = \langle f, g \rangle = \sum_{m, m_z} \overline{\widehat{f}_{m, m_z}} \widehat{g}_{m, m_z}$ .

We also define, for  $\eta \in \{-1, 1\}$ ,

$$C_{\mathbf{m}}^{\eta} := \sqrt{|\Omega_M|} \sum_{m_z \in \mathbb{Z}} e^{\eta i 2 \frac{d\pi}{L} m_z} \overline{\widehat{f}_{-\eta m, m_z}} \widehat{g}_{-\eta m, m_z}$$

We have  $a_M^* = Ja^*$  hence  $ma^* \cdot JX = -ma_M^* \cdot X$  and

$$((f, g))^{+-} = \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{e^{ima_M^* \cdot \mathbf{X}}}{\sqrt{|\Omega_M|}} C_{\mathbf{m}}^+, \quad ((f, g))^{-+} = \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{e^{ima_M^* \cdot \mathbf{X}}}{\sqrt{|\Omega_M|}} C_{\mathbf{m}}^-$$

For the potentials, we finally need to implement

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

**4.1.  $\mathbb{W}$ 's  $V_{\text{int}}$  term.** We write  $V_{\text{int}}(z) = \frac{1}{\sqrt{L}} \sum_{m_z \in \mathbb{Z}} \widehat{V}_{\text{int}}^{m_z} e^{i\frac{2\pi}{L}m_z z}$  hence

$$\begin{aligned} \langle u_j, V_{\text{int}} u_{j'} \rangle &= \frac{1}{L^{\frac{3}{2}}} \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ m_z, m'_z, M_z \in \mathbb{Z}}} (\widehat{\bar{u}}_j)_{\mathbf{m}, m_z} (\widehat{u}_{j'})_{\mathbf{m}, m'_z} (\widehat{V_{\text{int}}})_{M_z} \int_z e^{iz\frac{2\pi}{L}(M_z + m'_z - m_z)} \\ &= \frac{1}{\sqrt{L}} \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ m_z, m'_z \in \mathbb{Z}}} (\widehat{\bar{u}}_j)_{\mathbf{m}, m_z} (\widehat{u}_{j'})_{\mathbf{m}, m'_z} (\widehat{V_{\text{int}}})_{m_z - m'_z} \end{aligned}$$

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

In the function  $\mathbb{V}(X) = \langle u_j, V u_i \rangle(X)$ , when  $V \rightarrow V + V_{\text{int}}$ , we have

$$\widetilde{\mathbb{V}}(X) = \langle u_j, (V + V_{\text{int}}) u_i \rangle(X) = \mathbb{V}(X) + \langle u_j, V_{\text{int}} u_i \rangle$$

but at the level of Fourier coefficients,

$$\widehat{\widetilde{\mathbb{V}}}_0 = \widehat{\mathbb{V}}_0 + \frac{\langle u_j, V_{\text{int}} u_i \rangle}{\sqrt{|\Omega|}}$$

so when we add it to the Fourier Hamiltonian, we should not forget to divide by  $\sqrt{|\Omega|}$

**4.2. Adding a constant.** We have

$$g(x) := f(x) + c \quad \implies \quad \widehat{g}_0 = \widehat{f}_0 + \sqrt{|\Omega_M|} c$$

4.3. **Subtracting the mean of  $\mathbb{W}^+$ .** To do this, we do it for a function  $f$ ,

$$\frac{1}{|\Omega|} \int f = \frac{\widehat{f}_0}{\sqrt{|\Omega|}}$$

hence

$$g(x) := f(x) - \frac{1}{|\Omega|} \int f \quad \implies \quad \widehat{g}_0 = 0$$

4.4.  $V_{\text{int}}^{3d}$ . We have  $V_{\text{int}}^{3d}(x, z) := V_{\text{int}}(z)$  hence  $\left(\widehat{V}_{\text{int}}^{3d}\right)_{m, m_z} = \sqrt{|\Omega_M|} \left(\widehat{V}_{\text{int}}\right)_{m_z}$

## 5. BM CONFIGURATION

From [1], the BM Hamiltonian is

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

where

$$T_1 = \begin{pmatrix} w_{AA} & w_{AB} \\ w_{AB} & w_{AA} \end{pmatrix}, \quad T_2 = \begin{pmatrix} w_{AA} & w_{AB}e^{-i\phi} \\ w_{AB}e^{i\phi} & w_{AA} \end{pmatrix}, \quad T_3 = \begin{pmatrix} w_{AA} & w_{AB}e^{i\phi} \\ w_{AB}e^{-i\phi} & w_{AA} \end{pmatrix}$$

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

$$T(x) := \sum_{j=1}^3 T_j e^{-iq_j \cdot x} = \begin{pmatrix} w_{AA}G(x) & w_{AB}\overline{F(-x)} \\ w_{AB}F(x) & w_{AA}G(x) \end{pmatrix}$$

Now, since  $q_{2,3} - q_1 = a_{M,j}^*$ , we know that

$$\begin{aligned} G(x) &= e^{-iq_1 x} \left( 1 + e^{-ia_{M,1}^* x} + e^{-ia_{M,2}^* x} \right) \\ F(x) &= e^{-iq_1 x} \left( 1 + \omega e^{-ia_{M,1}^* x} + \omega^2 e^{-ia_{M,2}^* x} \right) \end{aligned}$$

We have  $\mathbb{V}^{1,1} \simeq w_{AA}G$  so  $\langle G, \mathbb{V} \rangle \simeq w_{AA} \int_{\Omega_M} |G|^2 = 3 |\Omega_M| w_{AA}$  and hence

$$\begin{aligned} w_{AA} &\simeq \frac{\langle G, \mathbb{V}^{1,1} \rangle}{3 |\Omega_M|} = \frac{1}{3\sqrt{|\Omega_M|}} \left( \widehat{\mathbb{V}}_{0,0}^{1,1} + \widehat{\mathbb{V}}_{-1,0}^{1,1} + \widehat{\mathbb{V}}_{0,-1}^{1,1} \right) \\ w_{AB} &\simeq \frac{\langle F, \mathbb{V}^{1,2} \rangle}{3 |\Omega_M|} = \frac{1}{3\sqrt{|\Omega_M|}} \left( \widehat{\mathbb{V}}_{0,0}^{1,2} + \omega \widehat{\mathbb{V}}_{-1,0}^{1,2} + \omega^2 \widehat{\mathbb{V}}_{0,-1}^{1,2} \right) \end{aligned}$$

## 6. OPERATORS IN BASIS

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

$$\boxed{\mathcal{H}\psi = \varepsilon_\theta \mathcal{S}E\psi}$$

remark that energies have to be rescaled by  $\varepsilon_\theta$  ! The operator  $\mathcal{S}$  is Hermitian and positive and

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

where

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

**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  $\langle e_n, V e_m \rangle = \widehat{V}_{n-m}$  and

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

**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

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

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

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

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

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

## 7. SYMMETRIES

**7.1. 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

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

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

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

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

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

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

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

## 8. NON LOCAL TERM

From the theoretical investigations, we have

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

and

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

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

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

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

$$\varphi_s(\mathbf{y}, z) = \sum_{m, m_z} \frac{e^{i(ma^* \mathbf{y} + m_z \frac{2\pi}{L} z)}}{\Gamma} \widehat{\varphi}_{s, \mathbf{m}, m_z}, \quad u_j(\mathbf{y}, z) = \sum_{\mathbf{m}, m_z} \frac{e^{i(\mathbf{m}\mathbf{y} + \frac{2\pi}{L} m_z z)}}{\Gamma} \widehat{(u_j)}_{\mathbf{m}, m_z}$$

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

$$\begin{aligned} F^{\eta,j,s}(\mathbf{X}) &= \sum_{\mathbf{m}, m_z} e^{i(\mathbf{m}\mathbf{a}^*(\mathbf{a}_s - 2\eta J\mathbf{X}) - \eta \frac{2\pi}{L} m_z d)} \widehat{\varphi}_{s,\mathbf{m},m_z}(\widehat{u_j})_{\mathbf{m},m_z} \\ &= \sum_{\mathbf{m}, m_z} e^{i(\mathbf{m}\mathbf{a}_M^*(\frac{1}{2}J\mathbf{a}_s + \eta\mathbf{X}) - \eta \frac{2\pi}{L} m_z d)} \widehat{\varphi}_{s,\mathbf{m},m_z}(\widehat{u_j})_{\mathbf{m},m_z} \\ &= \sum_{\mathbf{m}, m_z} e^{i(\mathbf{m}\mathbf{a}_M^*(\frac{1}{2}J\mathbf{a}_s + \mathbf{X}) - \eta \frac{2\pi}{L} m_z d)} \widehat{\varphi}_{s,\eta\mathbf{m},m_z}(\widehat{u_j})_{\eta\mathbf{m},m_z} \end{aligned}$$

has Fourier coefficients

$$(\widehat{F^{\eta,j,s}})_{\mathbf{m}} = e^{i\frac{1}{2}\mathbf{m}\mathbf{a}_M^* \cdot J\mathbf{a}_s} \sum_{m_z} e^{-i\eta \frac{2\pi}{L} m_z d} \widehat{\varphi}_{s,\eta\mathbf{m},m_z}(\widehat{u_j})_{\eta\mathbf{m},m_z}$$

On the functions given by DFTK, we remark that  $\varphi_s[m]$  given is periodic and that

$$\mathcal{R}_{\frac{2\pi}{3}} \varphi_{\text{Bl},s} = \tau^s \varphi_{\text{Bl},s}.$$

**8.1. Symmetries.** We have

$$\begin{aligned} \mathcal{R}_{\frac{2\pi}{3}} F^{\eta,j,s} &= \int_{\mathbb{R}^3} \overline{\varphi_{\text{Bl},s}(\mathbf{y}, z)} \Phi_j \left( R_{-\frac{2\pi}{3}} \left( R_{\frac{2\pi}{3}} \mathbf{y} + R_{\frac{2\pi}{3}} \mathbf{a}_s - 2\eta J\mathbf{X} \right), z - \eta d \right) d\mathbf{y} dz \\ &= \int_{\mathbb{R}^3} \overline{\mathcal{R}_{\frac{2\pi}{3}} \varphi_{\text{Bl},s}(\mathbf{y}, z)} \left( \mathcal{R}_{\frac{2\pi}{3}} \Phi_j \right) \left( \mathbf{y} + R_{\frac{2\pi}{3}} \mathbf{a}_s - 2\eta J\mathbf{X}, z - \eta d \right) d\mathbf{y} dz \\ &= \tau^{j-s} \int_{\mathbb{R}^3} \overline{\varphi_{\text{Bl},s}(\mathbf{y}, z)} \Phi_j \left( \mathbf{y} + R_{\frac{2\pi}{3}} \mathbf{a}_s - 2\eta J\mathbf{X}, z - \eta d \right) d\mathbf{y} dz \end{aligned}$$

and if  $\varphi_{\text{Bl},s}(y + R_{\frac{2\pi}{3}} a_s) = \varphi_{\text{Bl},s}(y + a_s)$ , then

$$\mathcal{R}_{\frac{2\pi}{3}} \left( \overline{F^{\eta,j,s}} F^{\eta,j',s} \right) = \tau^{j'-j} \overline{F^{\eta,j,s}} F^{\eta,j',s}$$

## 9. CHANGE OF BASIS FOR GETTING $\Phi_j \in L^2_{\tau, \bar{\tau}}$

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  $e^{i\beta} = \pm 1$  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  $\pi$  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  $u_2(x) = \overline{u_1(-x)}$ .

#### 10. CHANGE OF GAUGE ON THE PHASIS OF WAVEFUNCTIONS

When we change  $\Phi_1 \rightarrow \Phi_1 e^{i\theta}$ , then  $u_1 \rightarrow u_1 e^{i\theta}$ ,  $u_2 \rightarrow u_2 e^{-i\theta}$  because  $u_2(x) = \overline{u_1(-x)}$ , and hence

$$\overline{u_1} u_2 \rightarrow \overline{u_1} u_2 e^{-2i\theta}$$

We define

$$\mathcal{U} := \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}$$

have

$$\begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix} \begin{pmatrix} \mathbb{W}^+ & \mathbb{V} \\ \mathbb{V}^* & \mathbb{W}^- \end{pmatrix} \begin{pmatrix} U^* & 0 \\ 0 & U^* \end{pmatrix} = \begin{pmatrix} U\mathbb{W}^+U^* & U\mathbb{V}U^* \\ U\mathbb{V}^*U^* & U\mathbb{W}^-U^* \end{pmatrix}$$

and with  $U := \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}$ , we have

$$U \begin{pmatrix} B^+ & B \\ B^* & B^- \end{pmatrix} U^* = \begin{pmatrix} B^+ & B e^{2i\theta} \\ B^* e^{-2i\theta} & B^- \end{pmatrix}$$

hence if we define  $H_\theta$  to be  $H$  with  $u_1 \rightarrow u_1 e^{i\theta}$ , we have that

$$\mathcal{U} H_\theta \mathcal{U}^*$$

is constant in  $\theta$ .

## 11. PLAN

Given a macroscopic model, BM of ours, we need to proceed the following way to build the band diagrams numerically

- (1) We rescale the model and remove dimensions by applying the conjugation  $\frac{1}{v_0 k_\theta^3} S \cdot S^*$  as in (5)
- (2) We conjugate by  $U = \begin{pmatrix} e^{-iK_2 x} & 0 \\ 0 & e^{iK_1 x} \end{pmatrix}$  to remove the  $e^{-iq_1 x}$  factors

11.1. **From  $a^*$  to  $c^*$ .** The lattice  $c^*$  enables to plot the bands diagram. Since  $a_1^* = c_1^*$  and  $a_2^* = c_1^* + c_2^*$ , we have

$$\sum_m f_m \frac{e^{ima^*x}}{\sqrt{|\Omega_M|}} = \sum_m f_m \frac{e^{i\left(\frac{m_1+m_2}{m_2}\right)c^*x}}{\sqrt{|\Omega_M|}} = \sum_m f_m \frac{e^{i(A^{-1}m)c^*x}}{\sqrt{|\Omega_M|}} = \sum_m f_{Am} \frac{e^{imc^*x}}{\sqrt{|\Omega_M|}}$$

where  $A = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}$ .

## 12. TREATING THE BISTRITZER-MACDONAL MODEL

In this section, we apply the plan of Section 11 to treat the BM model.

12.1. **Rescaling.** We consider

$$T(x) = \sum_{j=1}^3 T_j e^{-iq_j x}, \quad q_{2,3} = \begin{pmatrix} \pm\sqrt{3}/2 \\ 1/2 \end{pmatrix}, \quad q_1 = -q_2 - q_3.$$

The BM Hamiltonian is

$$\begin{pmatrix} -iv_0\sigma\nabla & wT(k_\theta x) \\ wT^*(k_\theta x) & -iv_0\sigma\nabla \end{pmatrix}.$$

We consider the rescaling

$$Su(x) := u\left(\frac{x}{k_\theta}\right), \quad S^*u(y) = k_\theta^2 u(k_\theta y), \quad SS^* = k_\theta^2$$

where we defined  $S^*$  as  $\int_\Omega \bar{f} Sg = \int_{L\Omega/k_\theta} g \overline{S^*f}$ . We have  $\nabla S^* = k_\theta S^* \nabla$  so  $S \nabla S^* = k_\theta^3 \nabla$  and  $SfS^* = k_\theta^2 f\left(\frac{x}{k_\theta}\right)$  so when  $x = yk_\theta$  is the microscopic scale

$$\frac{1}{k_\theta^3 v_0} S \left( \begin{pmatrix} -iv_0\sigma\nabla & wT(k_\theta x) \\ wT^*(k_\theta x) & -iv_0\sigma\nabla \end{pmatrix} - E \right) S^* = \begin{pmatrix} -i\sigma\nabla & \alpha T(x) \\ \alpha T^*(x) & -i\sigma\nabla \end{pmatrix} - \varepsilon =: H_{BM} \quad (5)$$

where  $\alpha := \frac{w}{k_\theta v_0}$  and where  $\varepsilon = \frac{E}{v_0 k_\theta}$  is the unit of [4, Fig 1] defined in the caption, and

12.2. **Removing  $e^{-iq_1x}$ .** With

$$U := \begin{pmatrix} e^{-iK_2x} & 0 \\ 0 & e^{-iK_1x} \end{pmatrix}, \quad (6)$$

we have

$$\begin{aligned} U^* H_{BM} U &= \begin{pmatrix} \sigma \cdot (-i\nabla - K_2) & T(x)e^{i(K_2-K_1)x} \\ T(x)^* e^{i(K_1-K_2)x} & \sigma \cdot (-i\nabla - K_1) \end{pmatrix} \\ &= \begin{pmatrix} \sigma \cdot (-i\nabla - K_2) & \mathbf{T} \\ \mathbf{T}^* & \sigma \cdot (-i\nabla - K_1) \end{pmatrix} \end{aligned}$$

From (9), that we consider again, we want  $K_2 - K_1 = q_1$ , so

$$\begin{aligned} \mathbf{T}(\mathbf{x}) &:= T(x)e^{i(K_2-K_1)x} = T(x)e^{iq_1x} = T_1 + T_2e^{i(q_1-q_2)x} + T_3e^{i(q_1-q_3)x} \\ &= T_1 + T_2e^{-ic_1^*x} + T_3e^{-i(c_1^*+c_2^*)x} \end{aligned}$$

where

$$\begin{aligned} a_1^* &= q_2 - q_1 = k_\theta \sqrt{3} \left( \frac{1/2}{\sqrt{3}/2} \right), & a_2^* &= q_3 - q_1 = k_\theta \sqrt{3} \left( \frac{-1/2}{\sqrt{3}/2} \right) \\ & & q_1 &= -q_2 - q_3 \end{aligned}$$

and

$$q_3 = \frac{1}{3}(-a_1^* + 2a_2^*), \quad q_2 = \frac{1}{3}(2a_1^* - a_2^*), \quad q_1 = \frac{1}{3}(-a_1^* - a_2^*)$$

and

$$\begin{aligned} c_1^* &:= q_2 - q_1 = a_1^* = k_\theta \sqrt{3} \left( \frac{1/2}{\sqrt{3}/2} \right), \\ c_2^* &:= q_3 - q_2 = -a_1^* + a_2^* = k_\theta \sqrt{3} \begin{pmatrix} -1 \\ 0 \end{pmatrix}, & a_2^* &= c_1^* + c_2^* \end{aligned}$$

hence

$$q_1 = \frac{1}{3}(-2c_1^* - c_2^*), \quad q_2 = \frac{1}{3}(c_1^* - c_2^*), \quad q_3 = \frac{1}{3}(c_1^* + 2c_2^*)$$

We choose

$$K_1 = \frac{1}{3}(c_1^* + 2c_2^*) \quad K_2 = \frac{1}{3}(-c_1^* + c_2^*),$$

so that  $K_2 - K_1 = \frac{1}{3}(-2c_1^* - c_2^*) = q_1$

### 13. TREATING OUR MODEL

Our Hamiltonian is

$$\mathcal{H}_{d,\theta} = \varepsilon_\theta^{-1} \mathcal{V}_d + c_\theta T_d + \varepsilon_\theta T_d^{(1)}, \quad \mathcal{H}_{d,\theta} \psi = \frac{E}{\varepsilon_\theta} \psi \quad (7)$$

where the three operators  $\mathcal{V}_d$ ,  $T_d$ , and  $T_d^{(1)}$  are of the form

$$\begin{aligned} \mathcal{S}_d &= \begin{pmatrix} \mathbb{I}_2 & \Sigma_d(\mathbf{X}) \\ \Sigma_d^*(\mathbf{X}) & \mathbb{I}_2 \end{pmatrix} \quad \text{and} \quad \mathcal{V}_d = \begin{pmatrix} \mathbb{W}_d^+(\mathbf{X}) & \mathbb{V}_d(\mathbf{X}) \\ \mathbb{V}_d(\mathbf{X})^* & \mathbb{W}_d^-(\mathbf{X}) \end{pmatrix}, \\ T_d &= \begin{pmatrix} v_F \boldsymbol{\sigma} \cdot (-i\nabla) & J(-i\nabla \Sigma_d)(\mathbf{X}) \cdot (-i\nabla) \\ -J(-i\nabla \Sigma_d^*)(\mathbf{X}) \cdot (-i\nabla) & v_F \boldsymbol{\sigma} \cdot (-i\nabla) \end{pmatrix}, \end{aligned}$$

$$T_d^{(1)} = -\frac{1}{2} \operatorname{div} (\mathcal{S}_d(\mathbf{X}) \nabla \bullet) + \frac{1}{2} \begin{pmatrix} -v_F \sigma \cdot J(-i\nabla) & 0 \\ 0 & v_F \sigma \cdot J(-i\nabla) \end{pmatrix}. \quad (8)$$

and with  $A = -i\nabla \Sigma$ ,

$$-\frac{1}{2} \operatorname{div} (\mathcal{S}_d(\mathbf{X}) \nabla \bullet) = \frac{1}{2} \begin{pmatrix} -\Delta & -\Sigma \Delta \\ -\Sigma^* \Delta & -\Delta \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0 & A \cdot (-i\nabla) \\ A^* \cdot (-i\nabla) & 0 \end{pmatrix}$$

**13.1. Application to our effective model.** Still with  $U$  defined in (6), we have

$$U^* \begin{pmatrix} 0 & \mathbb{V} \\ \mathbb{V}^* & 0 \end{pmatrix} U = \begin{pmatrix} 0 & \tilde{\mathbb{V}} \\ \tilde{\mathbb{V}}^* & 0 \end{pmatrix}, \quad U^* \begin{pmatrix} \mathbb{W}^+ & 0 \\ 0 & \mathbb{W}^- \end{pmatrix} U = \begin{pmatrix} \mathbb{W}^+ & 0 \\ 0 & \mathbb{W}^- \end{pmatrix}$$

and

$$U^* \begin{pmatrix} 0 & \Sigma \\ \Sigma^* & 0 \end{pmatrix} U = \begin{pmatrix} 0 & \tilde{\Sigma} \\ \tilde{\Sigma}^* & 0 \end{pmatrix}$$

$$U^* \begin{pmatrix} \sigma(-i\nabla) & 0 \\ 0 & \sigma(-i\nabla) \end{pmatrix} U = \begin{pmatrix} \sigma(-i\nabla - K_2) & 0 \\ 0 & \sigma(-i\nabla - K_1) \end{pmatrix}$$

and as presented in Section 14, with  $A := -i\nabla \Sigma$ ,

$$U^* \begin{pmatrix} 0 & JA(-i\nabla) \\ (JA)^*(-i\nabla) & \end{pmatrix} U = \begin{pmatrix} 0 & J\tilde{A} \cdot (-i\nabla - K_1) \\ (J\tilde{A})^* \cdot (-i\nabla - K_2) & 0 \end{pmatrix}$$

Moreover,

$$\begin{aligned} U^* \frac{1}{2} \begin{pmatrix} -v_F \sigma \cdot J(-i\nabla) & 0 \\ 0 & v_F \sigma \cdot J(-i\nabla) \end{pmatrix} U \\ = \frac{1}{2} \begin{pmatrix} -v_F \sigma \cdot J(-i\nabla - K_2) & 0 \\ 0 & v_F \sigma \cdot J(-i\nabla - K_1) \end{pmatrix} \end{aligned}$$

and

$$U^* \begin{pmatrix} -\Delta & -\Sigma \Delta \\ -\Sigma^* \Delta & -\Delta \end{pmatrix} U = \begin{pmatrix} (-i\nabla - K_2)^2 & \tilde{\Sigma}(-i\nabla - K_1)^2 \\ (\tilde{\Sigma})^* (-i\nabla - K_2)^2 & (-i\nabla - K_1)^2 \end{pmatrix}$$

**13.1.1. Factor  $\sqrt{|\Omega_M|}$ .** With  $\mathbb{V} = \sum_m V_m e_m$ ,  $e_m := \frac{e^{imc^*x}}{\sqrt{|\Omega_M|}}$ , we have

$$\boxed{\langle e_n, \mathbb{V} e_p \rangle = \frac{V_m}{\sqrt{|\Omega_M|}}}$$

hence

$$\langle e_n, \sigma \cdot (-i\nabla) e_p \rangle = \delta_{n-p} \sigma \cdot mc^*$$

and

$$\begin{aligned} & \left\langle e_n, \left( \begin{pmatrix} \sigma \cdot (-i\nabla) & \mathbb{V} \\ \mathbb{V}^* & \sigma \cdot (-i\nabla) \end{pmatrix} - \begin{pmatrix} \mathbb{1} & \Sigma \\ \Sigma^* & \mathbb{1} \end{pmatrix} E \right) e_p \right\rangle \\ &= \begin{pmatrix} \delta_{n-p} \sigma \cdot pc^* & \frac{\mathbb{V}_{n-p}}{\sqrt{|\Omega_M|}} \\ \frac{\overline{\mathbb{V}_{p-n}}}{\sqrt{|\Omega_M|}} & \delta_{n-p} \sigma \cdot pc^* \end{pmatrix} - \begin{pmatrix} \delta_{n-p} \mathbb{1} & \frac{\Sigma_{n-p}}{\sqrt{|\Omega_M|}} \\ \frac{\Sigma_{p-n}^*}{\sqrt{|\Omega_M|}} & \delta_{n-p} \mathbb{1} \end{pmatrix} E \end{aligned}$$



## 14. MAGNETIC TERM

We have

$$A := -i\nabla\Sigma = e^{-iq_1x} (-i\nabla - q_1) ((u_j, u_{j'}))^{+-}$$

hence with  $\tilde{f} := e^{iq_1x}f$ ,

$$\tilde{A} = (-i\nabla - q_1) \tilde{\Sigma}$$

$$\begin{aligned} U^* \begin{pmatrix} 0 & JA(-i\nabla) \\ JA^*(-i\nabla) & 0 \end{pmatrix} U \\ = \begin{pmatrix} 0 & e^{i(K_2-K_1)x} JA \cdot (-i\nabla - K_1) \\ e^{i(K_1-K_2)x} JA^* \cdot (-i\nabla - K_2) & 0 \end{pmatrix} \\ = \begin{pmatrix} 0 & e^{iq_1x} JA \cdot (-i\nabla - K_1) \\ e^{-iq_1x} JA^* \cdot (-i\nabla - K_2) & 0 \end{pmatrix} \\ = \begin{pmatrix} 0 & J\tilde{A} \cdot (-i\nabla - K_1) \\ J\tilde{A}^* \cdot (-i\nabla - K_2) & 0 \end{pmatrix} \end{aligned}$$

Now

$$\operatorname{div} JA = 0, \quad -i \operatorname{div} J\tilde{A} = q_1 J\tilde{A}$$

and since  $\tilde{A}^* = e^{-iq_1x}A^*$ , then  $-i \operatorname{div} J(\tilde{A}^*) = -q_1 J(\tilde{A}^*)$

With  $A$  a  $4 \times 4$  matrix, computing  $\langle v, Au \rangle = \left\langle \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \right\rangle$ , we compute that  $A^*$  is indeed the hermitian conjugate for any  $x$ . We remark also that  $JAJ = -(A^{-1})^T$ . The action of  $J$  is on the composants of  $A$ , not on  $u$  !!! So we have

$$A = \begin{pmatrix} A^{(1)} \\ A^{(2)} \end{pmatrix} =: \begin{pmatrix} C \\ B \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \\ \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \end{pmatrix}$$

and  $A$  acts on  $u$  as  $Au = \begin{pmatrix} A^{(1)}u \\ A^{(2)}u \end{pmatrix}$  hence  $A^* = \begin{pmatrix} (A^{(1)})^* \\ (A^{(2)})^* \end{pmatrix}$  and

$$JA = \begin{pmatrix} -A^{(2)} \\ A^{(1)} \end{pmatrix}, \quad (JA)^* = \begin{pmatrix} -(A^{(2)})^* \\ (A^{(1)})^* \end{pmatrix} = JA^* \neq -A^*J!!$$

We recall that  $\partial_j$  acts on  $L^2(\mathbb{R}^d, \mathbb{C}^2)$  as

$$-i\partial_j u = \begin{pmatrix} -i\partial_j u_1 \\ -i\partial_j u_2 \end{pmatrix}, \quad -i\nabla u = \begin{pmatrix} -i\partial_1 u \\ -i\partial_2 u \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} -i\partial_1 u_1 \\ -i\partial_1 u_2 \end{pmatrix} \\ \begin{pmatrix} -i\partial_2 u_1 \\ -i\partial_2 u_2 \end{pmatrix} \end{pmatrix}$$

so  $(-i\partial_j)^* = -i\partial_j$  and  $(-i\nabla)^* = -i\nabla$ . For any  $4 \times 4$  valued function  $B$ , we have

$$\partial_j (Bu) = \partial_j \begin{pmatrix} B_{11}u_1 + B_{12}u_2 \\ B_{21}u_1 + B_{22}u_2 \end{pmatrix} = B\partial_j u + (\partial_j B)u$$

where

$$\partial_j B := \begin{pmatrix} \partial_j B_{11} & \partial_j B_{12} \\ \partial_j B_{21} & \partial_j B_{22} \end{pmatrix}$$

i.e  $\partial_j$  acts pointwise on vectors and matrices. Moreover, for  $A = \begin{pmatrix} A^{(1)} \\ A^{(2)} \end{pmatrix}$ , we have

$$\begin{aligned} \operatorname{div} Au &= \partial_1 (A^{(1)}u) + \partial_2 (A^{(2)}u) = \sum_j A^{(j)} \partial_j u + (\partial_j A^{(j)}) u \\ &= (\operatorname{div} A) u + A \cdot \nabla u \end{aligned}$$

where we also define  $\operatorname{div}$  acting pointwise on the  $4 \times 4$  matrices, i.e

$$\operatorname{div} A := (\operatorname{div} A_{ij})_{1 \leq i, j \leq 2} = \left( \partial_1 A_{ij}^{(1)} + \partial_2 A_{ij}^{(2)} \right)_{ij}$$

In this case,  $\operatorname{div} J \nabla f = 0$  for any  $4 \times 4$  matrix valued function  $f$ . Moreover,

$$\begin{aligned} \langle V, -i \nabla u \rangle &= \left\langle \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}, -i \nabla u \right\rangle = \left\langle \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}, \begin{pmatrix} -i \partial_1 u \\ -i \partial_2 u \end{pmatrix} \right\rangle = \sum_j \langle V_j, -i \partial_j u \rangle \\ &= \sum_j \langle -i \partial_j V_j, u \rangle = \langle -i \operatorname{div} V, u \rangle \end{aligned}$$

Hence for  $A = -i \nabla \Sigma$ ,

$$\begin{aligned} \langle v, JA \cdot (-i \nabla - K_1) u \rangle &= \langle (JA)^* v, (-i \nabla - K_1) u \rangle = \langle JA^* v, (-i \nabla - K_1) u \rangle \\ &= \langle (-i \operatorname{div} - K_1) JA^* v, u \rangle \\ &= \langle ((-i \operatorname{div})(JA^*)) v, u \rangle + \langle (JA^*) \cdot (-i \nabla - K_1) v, u \rangle \\ &= \langle (JA^*) \cdot (-i \nabla - K_1) v, u \rangle \end{aligned}$$

Repeating the same computations, we find that

$$\begin{aligned} &\left\langle v, \left( J \tilde{A} \right) \cdot (-i \nabla - K_1) u \right\rangle \\ &= \left\langle \left( J \tilde{A}^* \right) \cdot (-i \nabla - K_1) v, u \right\rangle + \left\langle -i \operatorname{div} \left( J \tilde{A}^* \right) v, u \right\rangle \\ &= \left\langle \left( J \tilde{A}^* \right) \cdot (-i \nabla - K_2) v, u \right\rangle \end{aligned}$$

so

$$\left( \left( J \tilde{A} \right) \cdot (-i \nabla - K_1) \right)^* = \left( J \tilde{A}^* \right) \cdot (-i \nabla - K_2) = \left( J \tilde{A} \right)^* \cdot (-i \nabla - K_2)$$

## 15. ANNEXES

15.1.  $a_M^*$  **is not adapted to**  $K_1, K_2$ . In this appendix, we show that the lattice  $a_M^*$  is not adapted to be such that  $K_1$  and  $K_2$  are Dirac points, hence the necessity of using  $c^*$ .

In TKV, we have

$$\begin{aligned} a_1^* = q_2 - q_1 &= k_\theta \sqrt{3} \begin{pmatrix} 1/2 \\ \sqrt{3}/2 \end{pmatrix}, & a_2^* = q_3 - q_1 &= k_\theta \sqrt{3} \begin{pmatrix} -1/2 \\ \sqrt{3}/2 \end{pmatrix} \\ & & q_1 &= -q_2 - q_3 \end{aligned}$$

To have  $q_j$  in terms of  $a_j^*$ , we compute  $a_1^* \pm a_2^*$  and  $a_1^* = 2q_2 + q_3$ ,  $a_2^* = q_2 + 2q_3$  and

$$q_3 = \frac{1}{3}(-a_1^* + 2a_2^*), \quad q_2 = \frac{1}{3}(2a_1^* - a_2^*), \quad q_1 = \frac{1}{3}(-a_1^* - a_2^*)$$

$$R_{\frac{2\pi}{3}} q_1 = q_2, \quad R_{\frac{2\pi}{3}} q_2 = q_3, \quad R_{\frac{2\pi}{3}} q_3 = q_1$$

(this was triples checked, including with the cartesian coordinates). Moreover,

$$R_{-\frac{2\pi}{6}} a_1^* = a_1^* - a_2^*, \quad R_{-\frac{2\pi}{6}} a_2^* = a_1^*$$

$$R_{\frac{2\pi}{6}} a_1^* = a_2^*, \quad R_{\frac{2\pi}{6}} a_2^* = a_2^* - a_1^*$$

If

$$S := \begin{pmatrix} a_1^* & a_2^* \end{pmatrix} = k_\theta \sqrt{3} \begin{pmatrix} 1/2 & -1/2 \\ \sqrt{3}/2 & \sqrt{3}/2 \end{pmatrix}, \quad S^{-1} = \frac{2}{3k_\theta} \begin{pmatrix} \sqrt{3}/2 & 1/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix}$$

and

$$\mathcal{M} = \begin{pmatrix} a_1 & a_2 \end{pmatrix} = 2\pi (S^*)^{-1} = \frac{4\pi}{3k_\theta} \begin{pmatrix} \sqrt{3}/2 & -\sqrt{3}/2 \\ 1/2 & 1/2 \end{pmatrix}$$

$$\text{with } U := \begin{pmatrix} e^{-iK_2 x} & 0 \\ 0 & e^{-iK_1 x} \end{pmatrix}, \text{ and}$$

$$T(x) = T_1 e^{-iq_1 x} + T_2 e^{-iq_2 x} + T_3 e^{-iq_3 x}$$

we compute

$$U^* \begin{pmatrix} -i\sigma \nabla & T \\ T^* & -i\sigma \nabla \end{pmatrix} U = \begin{pmatrix} \sigma(-i\nabla - K_2) & T e^{i(K_2 - K_1)x} \\ T^* e^{i(K_1 - K_2)x} & \sigma(-i\nabla - K_1) \end{pmatrix} \quad (9)$$

and with  $K_2 - K_1 = q_1$ ,

$$T e^{i(K_2 - K_1)x} = T_1 + T_2 e^{i(-q_2 + q_1)x} + T_3 e^{i(-q_3 + q_1)x} = T_1 + T_2 e^{-ia_1^* x} + T_3 e^{-ia_2^* x}$$

and if  $K_1 = \frac{1}{3}(\alpha a_1^* + \beta a_2^*)$ , then

$$K_2 := R_{-\frac{2\pi}{6}} K_1 = \frac{1}{3}((\alpha + \beta) a_1^* - \alpha a_2^*)$$

$$K_2 - K_1 = \frac{1}{3}(\beta a_1^* + (-\beta - \alpha) a_2^*) = q_1 = \frac{1}{3}(-a_1^* - a_2^*)$$

so  $(\alpha, \beta) = (2, -1)$ ,  $K_1 = \frac{1}{3}(2a_1^* - a_2^*)$ ,  $K_2 = \frac{1}{3}(a_1^* - 2a_2^*)$

$$K_2 := R_{\frac{2\pi}{6}} K_1 = \frac{1}{3}(-\beta a_1^* + (\alpha + \beta) a_2^*)$$

$$K_2 - K_1 = \frac{1}{3}((-\alpha - \beta) a_1^* + \alpha a_2^*) = q_1 = \frac{1}{3}(-a_1^* - a_2^*)$$

so  $(\alpha, \beta) = (-1, 2)$ ,  $K_1 = \frac{1}{3}(-a_1^* + 2a_2^*)$ ,  $K_2 = \frac{1}{3}(-2a_1^* + a_2^*)$

## 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] G. TARNOPOLSKY, A. J. KRUCHKOV, AND A. VISHWANATH, *Origin of magic angles in twisted bilayer graphene*, Phys. Rev. Lett, 122 (2019), p. 106405.