

# NUMERICAL COMPUTATIONS FOR AN EFFECTIVE MODEL OF TWISTED BILAYER GRAPHENE

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## 1. STANDARD MONOLAYER

We recall that

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

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  $\Omega$ -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

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

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

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

## 2. 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

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

and we obtain the Fourier coefficients

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

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

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

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

$$\int_{\Omega \times \mathbb{R}} \simeq \int_{\Omega \times [-\frac{L}{2}, \frac{L}{2}]} = \int_{\Omega \times [0, L]}$$

The situation is drawn on Figure 3. Numerically 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),

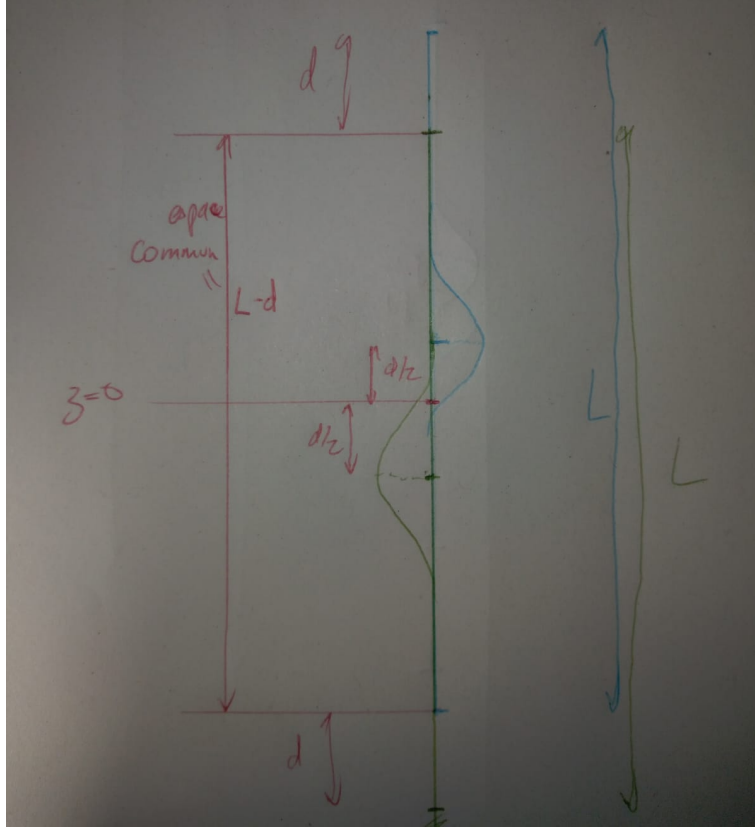
$$\begin{aligned}((f, g))^{\eta, \eta'} &= L \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{i(\eta - \eta')\mathbf{m} a^* \cdot J\mathbf{X}} \sum_{m_z \in \mathbb{Z}} e^{i(\eta - \eta') \frac{2\pi}{L} m_z \frac{d}{2}} \overline{\widehat{f}_{m, m_z}} \widehat{g}_{m, m_z} \\ &= \sum_{\mathbf{m} \in \mathbb{Z}^2}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

where

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

Then,

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

FIGURE 1. Situation on the  $z$  coordinate

Hence

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

and

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

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

For the potentials, we finally need to implement

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

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

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

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. **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

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

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

$$j^\ell \nabla \Phi_\ell(x) = \nabla \mathcal{R}_{\frac{2\pi}{3}} \Phi_\ell(x) = R_{\frac{2\pi}{3}} \mathcal{R}_{\frac{2\pi}{3}} \nabla \Phi_\ell$$

hence

$$\mathcal{R}_{\frac{2\pi}{3}} (\nabla \Phi_\ell) = j^\ell R_{-\frac{2\pi}{3}} (\nabla \Phi_\ell)$$

and with

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

$$\mathcal{R}_{\frac{2\pi}{3}} ((\Phi_\ell, \nabla \Phi_{\ell'}))^{\eta, \eta'} = j^{\ell' - \ell} R_{-\frac{2\pi}{3}} ((\Phi_\ell, \nabla \Phi_{\ell'}))^{\eta, \eta'}$$

and hence

$$\mathcal{R}_{\frac{2\pi}{3}} \mathcal{A} = R_{-\frac{2\pi}{3}} : U \mathcal{A} U^*$$

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. BM CONFIGURATION

From [?], the BM Hamiltonian is

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

where

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

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

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

### 5. ROTATION OF $\frac{\pi}{2}$

From [?], we have vectors (in the reference, without the factor  $\frac{4\pi}{a\sqrt{3}}$ )

$$\widetilde{q}_1^c = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \quad \widetilde{q}_{2,3}^c = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} \pm \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix} = \frac{2\pi}{a} \begin{pmatrix} \pm 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}$$

For them to be adapted to our lattice, we turn them and define  $q_j^c := R_{-\frac{\pi}{2}} \widetilde{q}_j^c$ , so that

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

so after a rotation of  $-\frac{\pi}{2}$ , we have

$$T^c(x) = T_1 e^{-iq_1^c \cdot x} + T_2 e^{-ia_2^* \cdot x} + T_3 e^{-ia_1^* \cdot x}$$

On reduced coordinates, we have

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

where  $q_j := -\mathcal{M}^* q_j^c / 2\pi$ , so

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

Writing a drawing and placing the  $q_i$ 's, we have

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

so

$$\mathcal{R}_{\frac{2\pi}{3}} T(x) = T_1 e^{-iq_2 x} + T_2 e^{-iq_3 x} + T_3 e^{-iq_1 x}$$

We don't have  $\mathcal{R}_{\frac{2\pi}{3}} T = T$  but this is true for the diagonal elements and for the off-diagonal, there exists  $X$  such that  $\mathcal{R}_{\frac{2\pi}{3}}(\tau_X T) = \tau_X T$ .

### 6. WITHOUT ROTATION

Without rotation, we have  $q_j := -\widetilde{\mathcal{M}}^* \widetilde{q}_j^c / 2\pi$  so

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

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

Or

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

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

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

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

## 7. OPERATORS IN BASIS

For a general  $W = \sum_k W^{ika^* \cdot x}$ , we have

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

and  $M$  is also Hermitian.

For a general  $V = \sum_k V^{ika^* \cdot x}$ , we have

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

For a general  $A = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}$ ,  $A_j = \sum_k (A_j)_k e^{ika^* \cdot x}$ , we compute

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

## 8. SYMMETRIES

8.1. **Particle-hole.** we have

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

we also have, for any operator  $A$ ,

$$\mathcal{S} \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \mathcal{S} = P \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} P$$

where  $Pu(x) := u(-x)$ . Hence

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

but since  $P\sigma \cdot kP = \sigma \cdot k$ ,

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

so it is not  $\mathcal{S}$  symmetric ! We have  $T(-x)^* = T(x)$  hence defining

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

we should have that

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

We compute

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

## 9. NUMERICS

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

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

and for  $V_{ij} := E_{ij}v_{ij}$  where  $v_{ij}$  is a potential in  $\mathbb{R}^2$  and  $E_{ij} := |e_i\rangle \langle e_j|$  being the  $4 \times 4$  matrix having a one at line  $i$  and column  $j$ ,

$$V_{\gamma,\eta}e_{\alpha,m} = \delta_{\eta,\alpha}e_{\gamma} \otimes v_{\gamma,\eta}e_m$$



and we recall that  $ve_m = \sum_k v_k e_{k+m}$  hence

$$\langle e_n, ve_m \rangle = v_{n-m}$$

and

$$\langle e_{\beta,n}, V_{\gamma,\eta} e_{\alpha,m} \rangle = \delta_{\eta,\alpha} \delta_{\beta,\gamma} \langle e_n, v_{\gamma,\eta} e_m \rangle = \delta_{\eta,\alpha} \delta_{\beta,\gamma} (v_{\gamma,\eta})_{n-m}$$

#### 10. EIGENVALUE EQUATION

We have  $H\psi = ES\psi$  is equivalent to  $S^*H\psi = ES^*S\psi$  and

$$(S^*S)^{-\frac{1}{2}} S^*H (S^*S)^{-\frac{1}{2}} \psi = E\psi$$

and in the code we define  $S_2 := (S^*S)^{-\frac{1}{2}} S^*$  and  $S_1 = (S^*S)^{-\frac{1}{2}}$