NUMERICAL COMPUTATIONS FOR AN EFFECTIVE MODEL OF TWISTED BILAYER GRAPHENE

ÉRIC CANCÈS, DAVID GONTIER AND LOUIS GARRIGUE

1. Standard monolayer

We recall that

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

In reduced coordinates, with

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

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

and

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

1.1. Fourier conventions.

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

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

hence any function can be decomposed as

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

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

1.2. Rotation action.

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

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

and

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

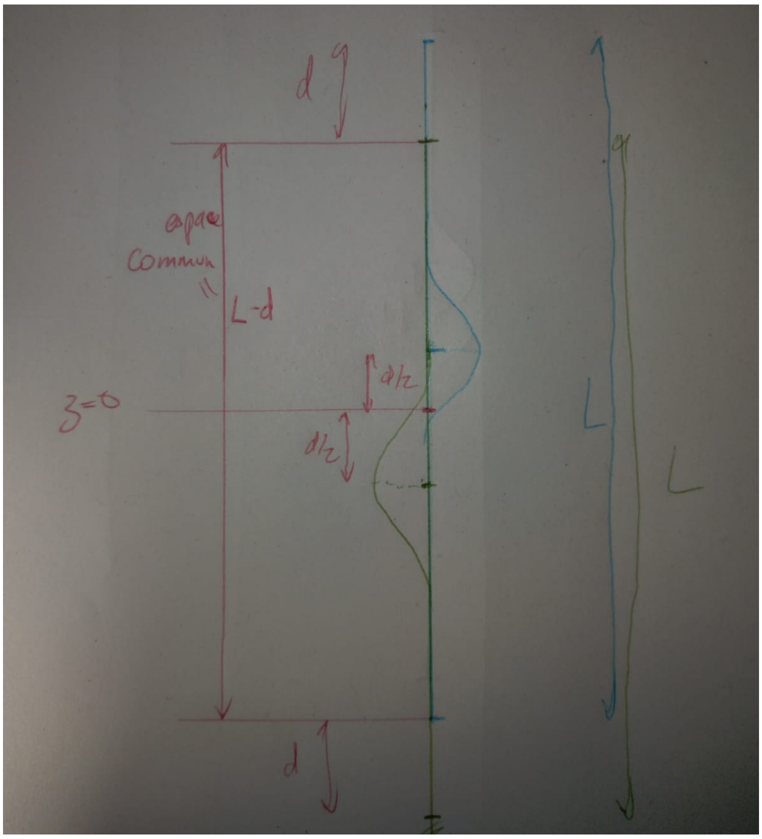

FIGURE 1. Situation on the z coordinate

2. Effective potentials

We defined

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

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

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

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

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

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

The situation is drawn on Figure 2. 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,

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

where

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

Then,

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

Hence

$$\begin{aligned}
(\!(f,g)\!)^{+-}\left(-\tfrac{3}{2}J\mathbf{X}\right) &= \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{i3ma^*\cdot\mathbf{X}} C_{\mathbf{m}} = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{ima^*\cdot\mathbf{X}} C_{\frac{\mathbf{m}}{3}}, \\
\langle\!\langle f,g\rangle\!\rangle^{+-}\left(-\tfrac{3}{2}J\mathbf{X}\right) &= \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{i3(m+m_k)a^*\cdot\mathbf{X}} C_{\mathbf{m}} = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{ima^*\cdot\mathbf{X}} C_{\frac{\mathbf{m}-3\mathbf{m}_K}{3}}
\end{aligned}$$

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

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

As for he magnetic term, we have

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

so

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

and

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

so we can implement

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

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

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

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

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

hence

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

and with

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

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

and hence

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

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

3. 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

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

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

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

4. Rotation of $\frac{\pi}{2}$

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

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

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

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

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

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

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

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

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 $\mathcal{R}_{\frac{2\pi}{3}} (\tau_X T) = \tau_X T$.

5. Without rotation

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

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

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

Or

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

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

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

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

6. Operators in basis

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

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

and M is also Hermitian.

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

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

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

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

7. Symmetries

7.1. **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

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

8. 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

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

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 4×4 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

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

9. 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 $S_1 = (S^*S)^{-\frac{1}{2}}$