NUMERICAL COMPUTATIONS FOR AN EFFECTIVE MODEL OF TWISTED BILAYER GRAPHENE

ÉRIC CANCÈS, LOUIS GARRIGUE AND DAVID GONTIER

1. Standard monolayer

We recall that

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

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

In reduced coordinates, with

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

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

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. **Dirac point.** We have

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

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 $m^q a = (a_1^* a_2^*) \begin{pmatrix} m_1^q \\ m_2^q \end{pmatrix} = 2\pi \left(\mathcal{M}^{-1}\right)^* \begin{pmatrix} m_1^q \\ m_2^q \end{pmatrix}$,

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

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

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

hence any function can be decomposed as

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

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

Now we consider that f and g are L-periodic in z, and $\int_{\mathbb{R}} \mathrm{d}z \simeq \int_{[0,L]} \mathrm{d}z$ so the Fourier transform is

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

and the reconstruction formula is

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

We define the scalar product

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

and compute Plancherel's formula

$$\langle f,g\rangle = L\,|\Omega| \sum_{\substack{\mathbf{m}\in\mathbb{Z}^2\\ m_z\in\mathbb{Z}}} \overline{\widehat{f}_{\mathbf{m},m_z}}\widehat{g}_{\mathbf{m},m_z}. \tag{3}$$

Hence, as a verification, we test that the normalization of the $\widehat{u_j}$'s is the right one by checking that $\|u_j\|^2_{L^2} = 1$ via (3).

We implement the Fourier transform

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

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.

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

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

and

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

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

$$R^{\mathrm{red}}_{\frac{\pi}{2}} = S^{-1}R_{\frac{\pi}{2}}S = \frac{1}{\sqrt{3}}\begin{pmatrix}-1 & 2\\ -2 & 1\end{pmatrix}, \qquad R^{\mathrm{red}}_{-\frac{\pi}{2}} = \frac{1}{\sqrt{3}}\begin{pmatrix}1 & -2\\ 2 & -1\end{pmatrix} =: \frac{1}{\sqrt{3}}M$$

and

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

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

2. Comparision with existing results

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

3. Computation of $V_{\rm int}$

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

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

and we obtain the Fourier coefficients

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

We then compute

$$V_{\rm int}(z) := \frac{1}{|\Omega|}\int_\Omega V_{\mathrm{int},\mathbf{s}}(z)\mathrm{d}\mathbf{s} = \frac{1}{N^2}\sum_{s_x,s_y\in[\![1,N]\!]} V^{\rm array}_{\mathrm{int},(\mathrm{s_x},\mathrm{s_y})}(z)$$

and finally obtain the Fourier coefficients

$$\boxed{\left(\widehat{V_{\rm int}}\right)_{m_z} = \frac{1}{N^2}\sum_{s_x,s_y\in[\![1,N]\!]} \left(\widehat{V_{\mathrm{int},\mathbf{s}}}\right)_{m_z}}$$

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

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

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

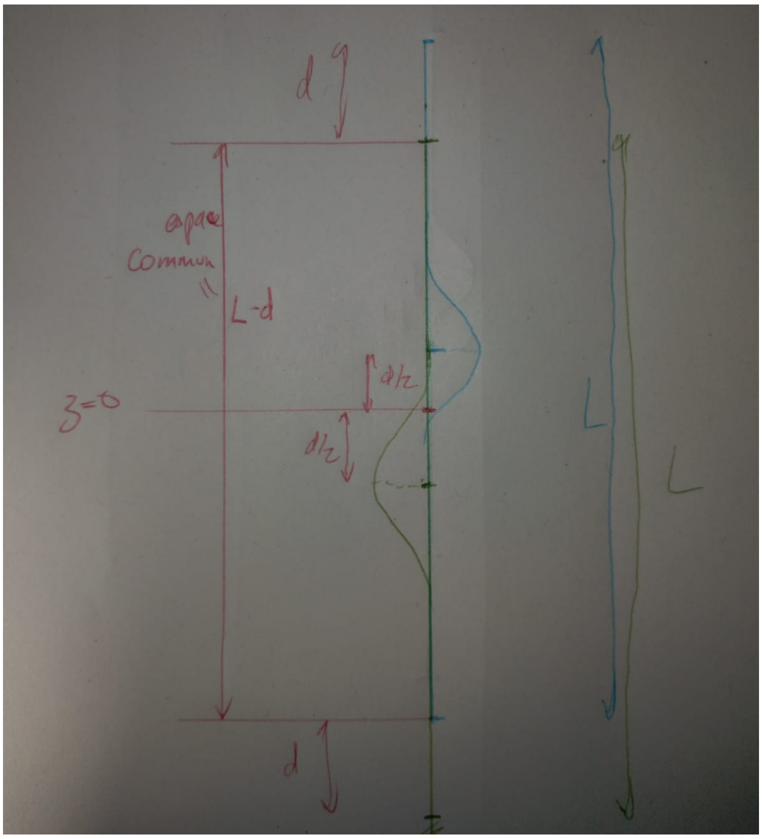

FIGURE 1. Situation on the z coordinate

4. Effective potentials

We defined

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

and

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

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 (2),

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

where

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

and we also define

$$C^{\pm}_{\mathbf{m}} := L\sum_{m_z\in\mathbb{Z}} e^{\pm i2\frac{d\pi}{L}m_z}\overline{\widehat{f}_{m,m_z}}\widehat{g}_{m,m_z}$$

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

$$\boxed{(\!(f,g)\!)^{+-}\left(-\tfrac{3}{2}J\mathbf{X}\right) = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{i3ma^*\cdot\mathbf{X}} C^+_{\mathbf{m}} = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{ima^*\cdot\mathbf{X}} C^+_{\frac{\mathbf{m}}{3}},}$$

and

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

where $C_{\frac{\mathbf{m}}{n}} := 0$ if n does not divide m_1 and m_2. Numerically, there is no loss of information since all C_m's are taken into account if the "ecut" is large enough.

Similarly

$$(\!(f,g)\!)^{-+}\left(-\tfrac{3}{2}J\mathbf{X}\right) = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{-i3ma^*\cdot\mathbf{X}} C^-_{\mathbf{m}} = \sum_{\mathbf{m}\in\mathbb{Z}^2} e^{ima^*\cdot\mathbf{X}} C^-_{-\frac{\mathbf{m}}{3}},$$

For the potentials, we finally need to implement

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

If $f(z) = \varepsilon f(-z)$, then $\widehat{f}_{-m_z} = \varepsilon\widehat{f}_{m_z}$, from this we see that $\overline{C^{u_{j'},u_j}_{\mathbf{m}}} = C^{u_j,u_{j'}}_{\mathbf{m}}$ and hence $\mathbb{V}(-X)^* = \mathbb{V}(X)$

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

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

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

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

so

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

so we can implement

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

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

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

and the matrix $M_{j,j'} := \left\langle u_j, V_{\mathrm{int}} u_{j'}\right\rangle$ 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

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

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

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

and

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

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

where we took rotated q_j^c's by J with respect to [1], and with a rescaling of $\frac{4\pi}{a\sqrt{3}}$.

We define the reduced dual vectors $q_j := -\mathcal{M}^* q_j^c/2\pi$ so

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

and we compute

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

Or

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

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

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 ε_θ ! 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

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

and their Bloch transform becomes

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

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

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

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

$$\begin{aligned}\langle e_n, A\cdot(-i\nabla + k)e_m\rangle &= \sum_\ell \left(\widehat{A_1}\right)_\ell (ma^*+k)_1 \left\langle e_n, e^{i\ell a^*\cdot x} e_m\right\rangle \\ &\quad + \left(\widehat{A_2}\right)_\ell (ma^*+k)_2 \left\langle e_n, e^{i\ell a^*\cdot x} e_m\right\rangle \\ &= \left(\widehat{A_1}\right)_{n-m} (ma^*+k)_1 + \left(\widehat{A_2}\right)_{n-m} (ma^*+k)_2 = \widehat{A}_{n-m}\cdot(ma^*+k)\end{aligned}$$

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

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

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

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

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

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

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

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

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

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

Then

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

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

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

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

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

so

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

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

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

so

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

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

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

7. Renormalization of the equation

We know that

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

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

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

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

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

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

$$\mathcal{S}u(x) := i\begin{pmatrix} 0 & -\mathbb{1}_{2\times2} \\ \mathbb{1}_{2\times2} & 0 \end{pmatrix} u(-x)$$

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

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

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

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

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 Γ is a linear combination of the terms

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

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

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

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

$$\sigma_1 T^*(M\mathbf{X})\sigma_1 = \begin{pmatrix}w_0\left(\sum_{j=1}^3 e^{ix\cdot Mq_j}\right) & w_1\left(e^{ix\cdot Mq_1} + e^{i\phi}e^{ixMq_2} + e^{i2\phi}e^{ix\cdot Mq_3}\right)\\ \cdot & \cdot\end{pmatrix}$$
$$= \begin{pmatrix}w_0\left(\sum_{j=1}^3 e^{ix\cdot q_j}\right) & w_1\left(e^{ix\cdot q_1} + e^{-i\phi}e^{ixq_2} + e^{-i2\phi}e^{ix\cdot q_3}\right)\\ \cdot & \cdot\end{pmatrix} = T(\mathbf{X})$$

where we used that $Mq_1^c = q_1^c$, $Mq_2^c = q_3^c$ and $Mq_3^c = q_2^c$.

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

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

9. Non Local term

From the theoretical investigations, we have

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

and

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

Since φ_{Bl} is localized, we periodize it and we make the approximation

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

and we define φ 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

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

has Fourier coefficients

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

10. Change of basis for getting $\Phi_j \in L^2_{\tau,\overline{\tau}}$

Numerically, DFTK gives

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

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

First we define

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

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 $\cos^2 + \sin^2 = 1$,

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

and also choosing $\alpha = 0$ if $\cos\theta \geqslant 0$ and π otherwise, which does not change anything, we have

$$\phi_1 = \frac{s}{|s|}\frac{1}{\sqrt{1 + \left(\frac{c}{|s|}\right)^2}}\phi_a \pm \frac{1}{\sqrt{1 + \left(\frac{|s|}{c}\right)^2}}\phi_b$$

and $\phi_2(x) = \overline{\phi_1(-x)}$. By multiplying by e^{-iKx}, we also obtain

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

and $u_2(x) = \overline{u_1(-x)}$.

11. The 1/3 scaling of coordinates

Taken from [5, Appendix G.3, G.4] for instance, the moiré lattice vectors are

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

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

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

and we remark that $a_1 \cdot q_1 = -\frac{2\pi}{3}$ so actually $q_j \notin \mathbb{L}^*$ but $3q_j \in \mathbb{L}^*$.

12. Change of gauge on the phasis of wavefunctions

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

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

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

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

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

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

is constant in θ.

12.1. BM.

From [4], we have

$$T(x) = \sum_j T_j e^{-iq_j x}, q_1 = \begin{pmatrix}0\\ -1\end{pmatrix}, q_{2,3} = \begin{pmatrix}\pm\frac{\sqrt{3}}{2}\\ \frac{1}{2}\end{pmatrix}, q_1 = -q_2 - q_3$$

so from (1) we deduce that

$$T(x) = \sum_j T_j e^{im_{q_j} a^* x}$$

where $k_D = 4\pi/(3a)$

$$m_{q_1} = \frac{1}{3k_D}\begin{pmatrix}1\\ -1\end{pmatrix}, \qquad m_{q_2} =$$

We compute, for $j \in \{1,2,3\}$,

$$\begin{aligned} v_\theta^m(x) &= v_m e^{ima^*\left(\cos\frac{\theta}{2}x + \sin\frac{\theta}{2}Jx\right)} + v_m e^{ima^*\left(\cos\frac{\theta}{2}x - \sin\frac{\theta}{2}Jx\right)} \\ &= 2iv_m e^{ima^*\cos\frac{\theta}{2}x} \sin ma^* \sin\frac{\theta}{2}Jx \\ &= 2iv_m e^{ima^*\cos\frac{\theta}{2}x} \sin m\frac{a^*}{2k_D}k_\theta Jx \end{aligned}$$

and

$$\frac{a_1^*}{2k_D} = \frac{\sqrt{3}}{2}\begin{pmatrix}\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix} = -\frac{\sqrt{3}}{2}Jq_2, \qquad \frac{a_2^*}{2k_D} = \frac{\sqrt{3}}{2}\begin{pmatrix}\frac{1}{2}\\ -\frac{\sqrt{3}}{2}\end{pmatrix} = -\frac{\sqrt{3}}{2}Jq_3$$

We deduce that

$$v_\theta^m(x) = -2iv_m e^{ima^*\cos\frac{\theta}{2}x} \sin k_\theta \frac{\sqrt{3}}{2} m b^* \cdot x$$

where $b_1^* := q_2$, $b_2^* := q_3$. We define $m_2 = (1,0)$, $m_3 = (0,1)$, $m_1 = (-1,-1)$, so the three modes are

$$m_j b^* = q_j$$

and

$$v_\theta^{m_j}(x) = \cdot \sin k_\theta \frac{\sqrt{3}}{2} q_j \cdot x$$

12.2. **Rescaling.** We consider the rescaling

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

where we defined S^* as $\int_\Omega \overline{f}\, Sg = \int_{L\Omega/k_\theta} g\, \overline{S^* f}$.

We define the BM potential at moiré scale

$$T(y) := \sum_j T_j e^{im_{q_j} a_M^* y}$$

We have $\nabla S^* = k_\theta^2 S \nabla$ so $S\nabla S^* = k_\theta^2 \nabla$ and $SfS^* = k_\theta f\left(\frac{x}{k_\theta}\right)$ so when $x = yk_\theta$ is the microscopic scale

$$\frac{1}{k_\theta^2 v_0} S\left(\begin{pmatrix} -iv_0\sigma\nabla & w_1 T(k_\theta x) \\ w_1 T^*(k_\theta x) & -iv_0\sigma\nabla \end{pmatrix} - E\right) S^* = \begin{pmatrix} -i\sigma\nabla & \alpha T(x) \\ \alpha T^*(x) & -i\sigma\nabla \end{pmatrix} - \varepsilon$$

where $\alpha := \frac{w_1}{k_\theta^2 v_0}$ where $\varepsilon = \frac{E}{v_0 k_\theta}$ is the unit of [4, Fig 1] defined in the caption. In [4] below (3) they define $k_D = 4\pi/(3a)$ which corresponds to our situation.

We will do another rescaling because in our numerical simulations we do not implement m_{q_j} but a transformation of it.

$$Gu(x) := u\left(Lx\right), \qquad G^*u(y) = \frac{1}{|\det L|} u\left(L^{-1}y\right), \qquad GG^* = \frac{1}{|\det L|}$$

where we defined G^* as $\int_\Omega \overline{f}\, Gg = \int_{L\Omega} g\, \overline{G^* f}$, and the multiplication operator T transforms as

$$GTG^* = \frac{1}{|\det L|} T\left(Lx\right), \qquad G\nabla G^* = \frac{1}{|\det L|}\left(L^{-1}\right)^* \nabla$$

and

$$T\left(Lx\right)=\sum T_{j}e^{im_{q_{j}}a^{*}\cdot Lx}=\sum T_{j}e^{i\left(\widetilde{L}m_{q_{j}}\right)a^{*}x}=\sum T_{j}e^{im_{Q_{j}}a^{*}x}$$
$$=:\widetilde{T}(x)$$

where $\widetilde{L}=\mathcal{M}^{*}L^{*}\left(\mathcal{M}^{*}\right)^{-1}$. From the numerical needs, we want

$$\widetilde{L}=\begin{pmatrix}-1 & 2\\ -2 & 1\end{pmatrix}$$

and hence

$$L=\mathcal{M}\left(\widetilde{L}\right)^{*}\mathcal{M}^{-1}=-\sqrt{3}J,\qquad\left(L^{-1}\right)^{*}=-\frac{1}{\sqrt{3}}J$$

$$\left|\det L\right|G\begin{pmatrix}-i\sigma\nabla-\varepsilon & \alpha T\left(x\right)\\ \alpha T^{*}(x) & -i\sigma\nabla-\varepsilon\end{pmatrix}G^{*}=\begin{pmatrix}i\frac{1}{\sqrt{3}}\sigma J\nabla-\varepsilon & \alpha\widetilde{T}\left(x\right)\\ \alpha\widetilde{T}^{*}(x) & i\frac{1}{\sqrt{3}}\sigma J\nabla-\varepsilon\end{pmatrix}$$

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.

[5] 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.