NUMERICAL COMPUTATIONS FOR AN EFFECTIVE MODEL OF TWISTED BILAYER GRAPHENE

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1. Standard monolayer

We choose for the microscopic lattice, the orientation

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

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

and for the Macroscopic lattice, we choose the orientation

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

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

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

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

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

$$\begin{pmatrix} m_1^q \\ m_2^q \end{pmatrix} = \frac{1}{2\pi} \mathcal{M}^* q \tag{3}$$

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

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

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

$$\boxed{f(\mathbf{x},z) = \sum_{\substack{\mathbf{m}\in\mathbb{Z}^2\\ m_z\in\mathbb{Z}}} e^{i\left(\mathbf{ma}^*\cdot\mathbf{x}+m_z\frac{2\pi}{L}z\right)}\widehat{f}_{\mathbf{m},m_z}} \tag{4}$$

We define the scalar product

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

and compute Plancherel's formula

$$\langle f,g\rangle = L|\Omega|\sum_{\substack{\mathbf{m}\in\mathbb{Z}^2\\ m_z\in\mathbb{Z}}}\overline{\widehat{f}_{\mathbf{m},m_z}}\widehat{g}_{\mathbf{m},m_z}. \tag{5}$$

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 (5).

We implement the Fourier transform

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

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

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

and

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

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

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

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

With the lattice a defined in (1), we obtain

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_{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

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

and we obtain the Fourier coefficients

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

We then compute

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

and finally obtain the Fourier coefficients

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

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

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

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

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

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

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 (4),

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

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

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

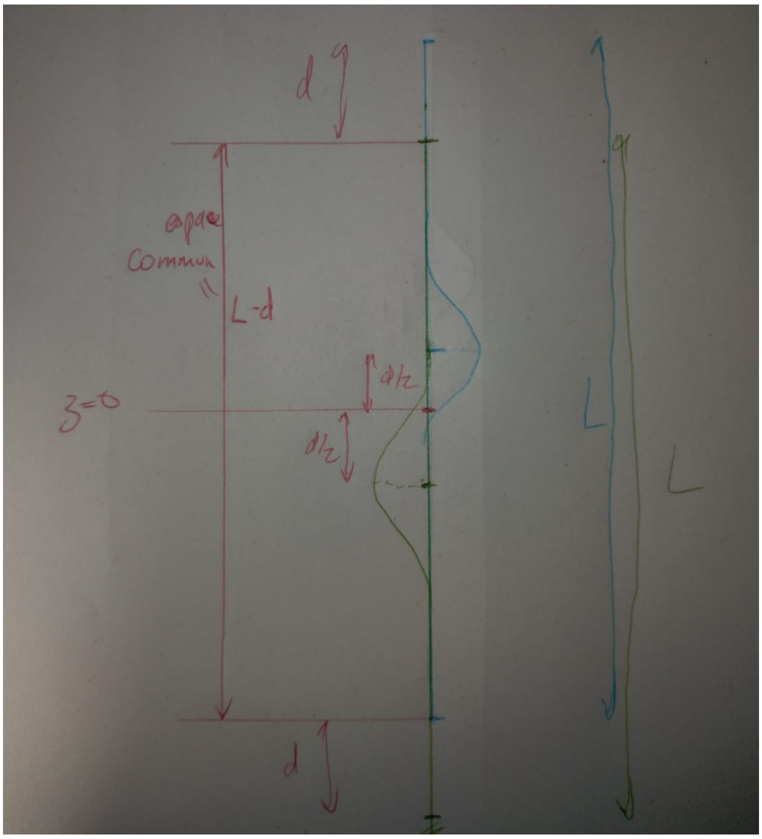

FIGURE 1. Situation on the z coordinate

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 $\overline{C_{\mathbf{m}}^{u_{j'},u_j}} = C_{\mathbf{m}}^{u_j,u_{j'}}$ and hence $\mathbb{V}(-X)^* = \mathbb{V}(X)$

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

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

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 $V_{\text{int}}(z) = \sum_{m_z\in\mathbb{Z}} \widehat{V}_{\text{int}}^{m_z} e^{i\frac{2\pi}{L} m_z z}$ hence

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

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

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

$$T := v_{\mathrm{F}} \begin{pmatrix} \boldsymbol{\sigma} \cdot (-i\nabla) & \boldsymbol{\mathcal{A}} \cdot (-i\nabla) \\ \boldsymbol{\mathcal{A}}^* \cdot (-i\nabla) & \boldsymbol{\sigma} \cdot (-i\nabla) \end{pmatrix},$$

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

$$\mathcal{V} := \begin{pmatrix} \mathbb{W} & \mathbb{V} \\ \mathbb{V}^* & \mathbb{W} \end{pmatrix},$$

and their Bloch transform becomes

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

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

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

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

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

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

For $V = \sum_\ell \widehat{V}_\ell e^{i\ell a^* x}$, we have $\langle e_n, V e_m \rangle = \widehat{V}_{n-m}$ and

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

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

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

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

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

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

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

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

$$\left\langle e_{\alpha,n}, \frac{1}{2}\left(-i\nabla+k\right)^2 e_{\beta,m}\right\rangle = \frac{1}{2}\left(ma^*+k\right)^2 \delta_{\alpha,\beta}\delta_{m-n}$$

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

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

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

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

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

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

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

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

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

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

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 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

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

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

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

and

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

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

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

$$= \int_{\Omega\times[0,L]} \overline{\varphi_s(\mathbf{y},z)}u_j\left(\mathbf{y} + \mathbf{a}_s - 2\eta J\mathbf{X}, z - \eta d\right)\mathrm{d}\mathbf{y}\mathrm{d}z$$

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

$$\varphi_s(\mathbf{y},z) = \sum_{\mathbf{G},G_z} e^{i(\mathbf{G}\mathbf{y}+G_z z)}\widehat{\varphi}_{s,\mathbf{G},G_z}, \qquad u_j(\mathbf{y},z) = \sum_{\mathbf{G},G_z} e^{i(\mathbf{G}\mathbf{y}+G_z z)}\widehat{(u_j)}_{\mathbf{G},G_z}$$

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

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

has Fourier coefficients

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

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

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

9.1. **Symmetries.**

We have

$$
\begin{aligned}
\mathcal{R}_{\frac{2\pi}{3}}F_0^{\eta,j,s} &= \int_{\mathbb{R}^3} \overline{\varphi_{\mathrm{Bl},s}(\mathbf{y},z)}\Phi_j\left(R_{-\frac{2\pi}{3}}\left(R_{\frac{2\pi}{3}}\mathbf{y}+R_{\frac{2\pi}{3}}\mathbf{a}_s-2\eta J\mathbf{X}\right), z-\eta d\right)\mathrm{d}\mathbf{y}\mathrm{d}z \\
&= \int_{\mathbb{R}^3} \overline{\mathcal{R}_{\frac{2\pi}{3}}\varphi_{\mathrm{Bl},s}(\mathbf{y},z)}\left(\mathcal{R}_{\frac{2\pi}{3}}\Phi_j\right)\left(\mathbf{y}+R_{\frac{2\pi}{3}}\mathbf{a}_s-2\eta J\mathbf{X}, z-\eta d\right)\mathrm{d}\mathbf{y}\mathrm{d}z \\
&= \tau^{j-s}\int_{\mathbb{R}^3} \overline{\varphi_{\mathrm{Bl},s}(\mathbf{y},z)}\Phi_j\left(\mathbf{y}+R_{\frac{2\pi}{3}}\mathbf{a}_s-2\eta J\mathbf{X}, z-\eta d\right)\mathrm{d}\mathbf{y}\mathrm{d}z
\end{aligned}
$$

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

$$
\mathcal{R}_{\frac{2\pi}{3}}\left(\overline{F_0^{\eta,j,s}}F_0^{\eta,j',s}\right) = \tau^{j'-j}\,\overline{F_0^{\eta,j,s}}F_0^{\eta,j',s}
$$

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

Numerically, DFTK gives

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

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

First we define

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

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.

13. Comparision between BM and our model

13.1. **Rescaling.** The BM Hamiltonian is

$$\begin{pmatrix} -iv_0 \sigma \nabla & w_1 T^{\mathrm{TKV}}(k_\theta x) \\ w_1 T^{*,\mathrm{TKV}}(k_\theta x) & -iv_0 \sigma \nabla \end{pmatrix}.$$

We consider the rescaling

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

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

$$\frac{1}{k_\theta^3 v_0} S \left(\begin{pmatrix} -iv_0 \sigma \nabla & w_1 T^{\mathrm{TKV}}(k_\theta x) \\ w_1 T^{*,\mathrm{TKV}}(k_\theta x) & -iv_0 \sigma \nabla \end{pmatrix} - E \right) S^* \\ = \begin{pmatrix} -i\sigma\nabla & \alpha T^{\mathrm{TKV}}(x) \\ \alpha T^{*,\mathrm{TKV}}(x) & -i\sigma\nabla \end{pmatrix} - \varepsilon$$

where $\alpha := \frac{w_1}{k_\theta v_0}$ and where $\varepsilon = \frac{E}{v_0 k_\theta}$ is the unit of [4, Fig 1] defined in the caption.

13.2. **Rotation and reduced coordinates of q.** In [4], the orientation of the lattice (one of the equations below (6)), is with reciprocal vectors

$$b_{1,2}^{*,\mathrm{TKV}} = \sqrt{3}\begin{pmatrix}\pm 1/2\\ \sqrt{3}/2\end{pmatrix}$$

and to compare with our lattice defined in (2), we have

$$-Jb_1^{*,\mathrm{TKV}} = b_1^*, \qquad -Jb_2^{*,\mathrm{TKV}} = -b_2^*, \qquad b = \frac{4\pi}{3}$$

corresponding to the direct lattice

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

The q_j's are

$$q_{2,3}^{\mathrm{TKV}} = \begin{pmatrix}\pm\frac{\sqrt{3}}{2}\\ \frac{1}{2}\end{pmatrix}, \qquad q_1^{\mathrm{TKV}} = -q_2^{\mathrm{TKV}} - q_3^{\mathrm{TKV}}$$

and we do a rotation, $q_j := -Jq_j^{\mathrm{TKV}}$,

$$q_1 = \begin{pmatrix}-1\\ 0\end{pmatrix}, \qquad q_{2,3} = \begin{pmatrix}\frac{1}{2}\\ \mp\frac{\sqrt{3}}{2}\end{pmatrix}, \qquad q_1 = -q_2 - q_3$$

We have

$$T(x) := T^{\mathrm{TKV}}(Jx) = \sum_j T_j e^{-iq_j x} \underset{(3)}{=} \sum_j T_j e^{i\widetilde{m}_{q_j} b^* x}$$

where $\widetilde{m}_{q_j} = -\frac{1}{2\pi}\mathcal{M}_b^* q_j$, that is

$$\widetilde{m}_{q_1} = \frac{1}{3}\begin{pmatrix}-1\\ 1\end{pmatrix}, \qquad \widetilde{m}_{q_2} = \frac{1}{3}\begin{pmatrix}2\\ 1\end{pmatrix}, \qquad \widetilde{m}_{q_3} = \frac{1}{3}\begin{pmatrix}-1\\ -2\end{pmatrix}$$

and we redefine

$$m_{q_1} = \begin{pmatrix}-1\\ 1\end{pmatrix}, \qquad m_{q_2} = \begin{pmatrix}2\\ 1\end{pmatrix}, \qquad m_{q_3} = \begin{pmatrix}-1\\ -2\end{pmatrix} \tag{6}$$

so

$$T(x) = \sum_j T_j e^{im_{q_j}\frac{b^*}{3}x} \tag{7}$$

We conjugate again and get

$$\mathcal{R}_{-\frac{\pi}{2}}\left(\begin{pmatrix}-i\sigma\nabla & \alpha T^{\mathrm{TKV}}(x)\\ \alpha T^{*,\mathrm{TKV}}(x) & -i\sigma\nabla\end{pmatrix} - \varepsilon\right)\mathcal{R}_{\frac{\pi}{2}} = \begin{pmatrix}-i\sigma\cdot J\nabla & \alpha T(x)\\ \alpha T^*(x) & -i\sigma\cdot J\nabla\end{pmatrix} - \varepsilon$$

the action of J corresponding to the rotation of the dual lattice vectors, so if we write ∇ in our new lattice b, we have

$$\begin{pmatrix}-i\sigma\nabla & \alpha T(x)\\ \alpha T^*(x) & -i\sigma\nabla\end{pmatrix} - \varepsilon$$

13.3. **Rescaling again.** To write the Fourier coefficients of T, we need to rescale, so ne define $Su(x) := u(3x)$ and as previously, doing "$k_\theta = 1/3$", we have $SS^* = 1/9$, $S\nabla S^* = \left(1/3^3\right)\nabla$

$$3^2 S\left(\begin{pmatrix} -i\sigma\nabla & \alpha T(x) \\ \alpha T^*(x) & -i\sigma\nabla \end{pmatrix} - \varepsilon\right)S^* = \begin{pmatrix} -\frac{1}{3}i\sigma\nabla & \alpha T(3x) \\ \alpha T^*(3x) & -\frac{1}{3}i\sigma\nabla \end{pmatrix} - \varepsilon$$

and now we can implement the Fourier coefficients of $T(3\cdot)$, given by (6), because

$$T(3x) = \sum_j T_j e^{im_{q_j} b^* x}$$

13.4. **Relation to our model.** 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

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

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

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

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