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

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

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

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

In reduced coordinates, with

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

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

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

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

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

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

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

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

We define the scalar product

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

and compute Plancherel's formula

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

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

We implement the Fourier transforms

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myfft(a,B) = fft(a)*sqrt(B)/length(a)
myifft(a) = ifft(a)*length(a)/sqrt(B)
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where $B = \Gamma^2 = L|\Omega|$ in $3d$, $B = L$ in $1d$ in z, and $B = |\Omega|$ in $2d$ in (x,y). If $a_i = f(x_i)$ are the actual values of the functions, then $myfft(a)[m] \simeq (\mathcal{F}f)_{m-1}$ up to Riemann series errors.

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

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

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

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

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

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

2. Comparision with existing results

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

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

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

and since

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

then

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

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

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

and we obtain the Fourier coefficients

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

We then compute

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

and finally obtain the Fourier coefficients

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

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

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

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

4. Effective potentials

We defined

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

and

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

and in particular since $q_1 = JK$, then $\langle\!\langle f,g\rangle\!\rangle^{+-} = e^{-iq_1x}(\!(f,g)\!)^{+-}$. Now we make the approximation

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

The functions are defined on $[-L/2, L/2]$ but we need to integrate on the common segment, which is $[-\frac{L-d}{2}, \frac{L-d}{2}]$, so on $[-L/2, L/2]$ to recover the initial domain.

Firstly, using the Fourier decomposition (3),

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

where

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

We have $\langle\!\langle f, g\rangle\!\rangle^{++} = \langle\!\langle f, g\rangle\!\rangle^{--} = \langle f, g\rangle = \sum_{m,m_z} \overline{\widehat{f}_{m,m_z}}\widehat{g}_{m,m_z}$.
We also define, for $\eta \in \{-1, 1\}$,

$$C^{\eta}_{\mathbf{m}} := \sqrt{|\Omega_{\mathrm{M}}|} \sum_{m_z\in\mathbb{Z}} e^{\eta i2\frac{d\pi}{L}m_z} \overline{\widehat{f}_{-\eta m,m_z}}\widehat{g}_{-\eta m,m_z}$$

We have $a^*_{\mathrm{M}} = Ja^*$ hence $ma^* \cdot JX = -ma^*_{\mathrm{M}} \cdot X$ and

$$\langle\!\langle f, g\rangle\!\rangle^{+-} = \sum_{\mathbf{m}\in\mathbb{Z}^2} \frac{e^{ima^*_{\mathrm{M}}\cdot\mathbf{X}}}{\sqrt{|\Omega_{\mathrm{M}}|}} C^{+}_{\mathbf{m}}, \qquad \langle\!\langle f, g\rangle\!\rangle^{-+} = \sum_{\mathbf{m}\in\mathbb{Z}^2} \frac{e^{ima^*_{\mathrm{M}}\cdot\mathbf{X}}}{\sqrt{|\Omega_{\mathrm{M}}|}} C^{-}_{\mathbf{m}}$$

For the potentials, we finally need to implement

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

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

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

and the matrix $M_{j,j'} := \left\langle u_j, V_{\mathrm{int}} u_{j'}\right\rangle$ is such that $M^* = M$ and $M_{11} = M_{22}$.
In the function $\mathbb{V}(X) = \langle u_j, V u_i\rangle (X)$, when $V \to V + V_{\mathrm{int}}$, we have

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

but at the level of Fourier coefficients,

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

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

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

$$g(x) := f(x) + c \qquad \Longrightarrow \qquad \widehat{g}_0 = \widehat{f}_0 + \sqrt{|\Omega_{\mathrm{M}}|}c$$

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

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

hence

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

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

5. BM configuration

From [1], the BM Hamiltonian is

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

where

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

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

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

Now, since $q_{2,3} - q_1 = a^*_{\mathrm{M},j}$, we know that

$$G(x) = e^{-iq_1 x}\left(1 + e^{-ia^*_{\mathrm{M},1}x} + e^{-ia^*_{\mathrm{M},2}x}\right)$$
$$F(x) = e^{-iq_1 x}\left(1 + \omega e^{-ia^*_{\mathrm{M},1}x} + \omega^2 e^{-ia^*_{\mathrm{M},2}x}\right)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

For a general $V = \sum_m \widehat{V}_m e^{ima^* \cdot x}$, we have $V^* = \sum_m \widehat{V}_m^* e^{-ima^* \cdot x}$ and we compute

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

7. Symmetries

7.1. Particle-hole. We define

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

We have

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

We have $T(-x)^* = T(x)$ hence we should have that

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

We compute

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

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

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

7.2. **Mirror.** First, for any function B, we have $\sigma_1 B^*\sigma_1 = \begin{pmatrix} \overline{B_{22}} & \overline{B_{12}} \\ \overline{B_{21}} & \overline{B_{11}} \end{pmatrix}$.

The mirror operator for the BM Hamiltonian is

$$\mathcal{M}u(\mathbf{X}) := \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix} u(\overline{\mathbf{X}})$$

where $\overline{\mathbf{X}} := (X_1, -X_2) =: M\mathbf{X}$, it satisfies $\mathcal{M} = \mathcal{M}^{-1} = \mathcal{M}^*$.

Next,

$$\mathcal{M}\begin{pmatrix} 0 & B(\mathbf{X}) \\ B(\mathbf{X})^* & 0 \end{pmatrix}\mathcal{M} = \begin{pmatrix} 0 & \sigma_1 B^*(\overline{\mathbf{X}})\sigma_1 \\ \sigma_1 B(\overline{\mathbf{X}})\sigma_1 & 0 \end{pmatrix}$$

In cartesian coordinates, we have

$$T(M\mathbf{X}) = \sum_{j=1}^{3} T_j e^{ix\cdot M^* q_j^c} = \sum_{j=1}^{3} T_j e^{ix\cdot M q_j^c}$$

because $M^* = M$. But

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

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

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

8. Non Local term

From the theoretical investigations, we have

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

and

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

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

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

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

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

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

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

has Fourier coefficients

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

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

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

8.1. **Symmetries.** We have

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

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

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

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

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

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

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

10. 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.

11. Plan

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

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

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

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

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

12. Treating the Bistritzer-MacDonal model

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

12.1. **Rescaling.** We consider

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

The BM Hamiltonian is

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

We consider the rescaling

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

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

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

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

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

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

we have

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

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

$$\begin{aligned} \mathbf{T}(\mathbf{x}) &:= T(x)e^{i(K_2-K_1)x} = T(x)e^{iq_1x} = T_1 + T_2 e^{i(q_1-q_2)x} + T_3 e^{i(q_1-q_3)x} \\ &= T_1 + T_2 e^{-ic_1^*x} + T_3 e^{-i\left(c_1^*+c_2^*\right)x} \end{aligned}$$

where

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

$$q_1 = -q_2 - q_3$$

and

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

and

$$c_1^* := q_2 - q_1 = a_1^* = k_\theta\sqrt{3}\begin{pmatrix} 1/2 \\ \sqrt{3}/2 \end{pmatrix},$$

$$c_2^* := q_3 - q_2 = -a_1^* + a_2^* = k_\theta\sqrt{3}\begin{pmatrix} -1 \\ 0 \end{pmatrix}, \qquad a_2^* = c_1^* + c_2^*$$

hence

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

We choose

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

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

13. Treating our model

Our Hamiltonian is

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

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

$$\mathcal{S}_d = \begin{pmatrix} \mathbb{I}_2 & \Sigma_d(\mathbf{X}) \\ \Sigma_d^*(\mathbf{X}) & \mathbb{I}_2 \end{pmatrix} \qquad \text{and} \qquad \mathcal{V}_d = \begin{pmatrix} \mathbb{W}_d^+(\mathbf{X}) & \mathbb{V}_d(\mathbf{X}) \\ \mathbb{V}_d(\mathbf{X})^* & \mathbb{W}_d^-(\mathbf{X}) \end{pmatrix},$$

$$T_d = \begin{pmatrix} v_F\boldsymbol{\sigma}\cdot(-\mathrm{i}\nabla) & J(-\mathrm{i}\nabla\Sigma_d)(\mathbf{X})\cdot(-\mathrm{i}\nabla) \\ -J(-\mathrm{i}\nabla\Sigma_d^*)(\mathbf{X})\cdot(-\mathrm{i}\nabla) & v_F\boldsymbol{\sigma}\cdot(-\mathrm{i}\nabla) \end{pmatrix},$$

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

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

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

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

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

and

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

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

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

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

Moreover,

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

and

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

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

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

hence

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

and

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

14. Magnetic term

We have

$$A := -i\nabla\Sigma = e^{-iq_1 x}\left(-i\nabla - q_1\right)\left(\left(u_j, u_{j'}\right)\right)^{+-}$$

hence with $\widetilde{f} := e^{iq_1 x} f$,

$$\widetilde{A} = \left(-i\nabla - q_1\right)\widetilde{\Sigma}$$

$$\begin{aligned} &U^* \begin{pmatrix} 0 & JA(-i\nabla) \\ JA^*(-i\nabla) & \end{pmatrix} U \\ &= \begin{pmatrix} 0 & e^{i(K_2-K_1)x} JA\cdot(-i\nabla - K_1) \\ e^{i(K_1-K_2)x} JA^*\cdot(-i\nabla - K_2) & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & e^{iq_1 x} JA\cdot(-i\nabla - K_1) \\ e^{-iq_1 x} JA^*\cdot(-i\nabla - K_2) & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & J\widetilde{A}\cdot(-i\nabla - K_1) \\ J\widetilde{A}^*\cdot(-i\nabla - K_2) & 0 \end{pmatrix} \end{aligned}$$

Now

$$\operatorname{div} JA = 0, \qquad -i\operatorname{div} J\widetilde{A} = q_1 J\widetilde{A}$$

and since $\widetilde{A}^* = e^{-iq_1 x}A^*$, then $-i\operatorname{div} J\left(\widetilde{A}^*\right) = -q_1 J\left(\widetilde{A}^*\right)$. We have

$$\operatorname{div} A = \sum_m \left(A_m^1 \left(ma^*\right)_1 + A_m^2 \left(ma^*\right)_2\right)\frac{e^{ima^* x}}{\sqrt{|\Omega_{\mathrm{M}}|}}$$

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

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

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

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

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

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

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

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

where

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

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

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

where we also define div acting pointwise on the 4×4 matrices, i.e

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

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

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

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

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

Repeating the same computations, we find that

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

so

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

15. Annexes

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

In TKV, we have

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

$$q_1 = -q_2 - q_3$$

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

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

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

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

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

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

If

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

and

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

with $U := \begin{pmatrix}e^{-iK_2x} & 0\\ 0 & e^{-iK_1x}\end{pmatrix}$, and

$$T(x) = T_1 e^{-iq_1x} + T_2 e^{-iq_2x} + T_3 e^{-iq_3x}$$

we compute

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

and with $K_2 - K_1 = q_1$,

$$Te^{i(K_2-K_1)x} = T_1 + T_2e^{i(-q_2+q_1)x} + T_3e^{i(-q_3+q_1)x} = T_1 + T_2e^{-ia_1^*x} + T_3e^{-ia_2^*x}$$

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

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

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

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

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

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

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

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