NUMERICAL COMPUTATIONS FOR AN EFFECTIVE MODEL OF TWISTED BILAYER GRAPHENE

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Abstract. We give here details on the implementation of the code corresponding to the article [2], which proposes a derivation of effective moiré models from continuous Schrödinger operators.

1. Standard monolayer

We choose

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

We define the matrix going from reduced to cartesian coordinates

$$\mathcal{M} : \mathbb{T}^2 \simeq [0,1]^2 \to \Omega,$$
$$\mathcal{M} := \frac{a}{2} \begin{pmatrix} 1 & 1 \\ -\sqrt{3} & \sqrt{3} \end{pmatrix} = \begin{pmatrix} a_1 & a_2 \end{pmatrix}, \qquad \mathcal{M}^{-1} = \frac{1}{a} \begin{pmatrix} 1 & -1/\sqrt{3} \\ 1 & 1/\sqrt{3} \end{pmatrix}$$

and

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

where $k_D := \frac{4\pi}{3a}$.

1.1. Dirac point.

We have

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

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

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

so

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

1.3. **Fourier conventions.** We will manipulate functions which are Ω-periodic in $\mathbf{x}$, but not in z. We make the approximation that L is large enough so that the z-periodized systems are equal. So now we consider that f and g are L-periodic in z, and $\int_{\mathbb{R}} \mathrm{d}z \simeq cst \int_{[0,L]} \mathrm{d}z$ 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

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

We define the scalar product

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

and compute Plancherel's formula

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

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

We implement the Fourier transforms

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

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 define $R_\theta := \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$. 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

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

1.5. **Action of mirror.** We define $G := \mathrm{diag}\ (1,-1)$ and the action $\mathcal{G}f(x) := f(Gx)$, we compute

$$G^{\mathrm{red}} = \mathcal{M}^* G (\mathcal{M}^*)^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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

Numerically, DFTK gives

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

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

First we define

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

Then we parametrize

$$\phi_1 = e^{i\alpha} \left(\frac{s}{|s|} \cos\theta \phi_a + e^{i\beta} \sin\theta \phi_b \right)$$

and we want $\left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right) \phi_1 = 0$ which is equivalent to

$$\frac{s}{|s|} \cos\theta \left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right) \phi_a + e^{i\beta} \sin\theta \left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right) \phi_b = 0$$

and we take the scalar product with $\left(\mathcal{R}_{\frac{2\pi}{3}} - \tau\right) \phi_a$ so that

$$\frac{c}{|s|} \cos\theta + e^{i\beta} \sin\theta = 0$$

Now we necessarily have $e^{i\beta} = \pm$ so $\cos\theta = \mp \frac{|s|}{c} \sin\theta$ and finally using $\cos^2 + \sin^2 = 1$,

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

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

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

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

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

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

3. Computation of V_{int}

3.1. **Reduction of Fourier coefficients in $2d$ to $1d$.** In $1d$, the Fourier transform is

$$(\mathcal{F}h)_{m_z} := \frac{1}{\sqrt{L}} \int_{[0,L]} e^{-im_z \frac{2\pi}{L} z} h(z) \mathrm{d}z$$

and the reconstruction formula is

$$h(z) = \frac{1}{\sqrt{L}} \sum_{m_z \in \mathbb{Z}} e^{im_z \frac{2\pi}{L} z} \widehat{h}_{m_z}$$

We take a function f in $3d$ and define its average

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

and since

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

then

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

3.2. **Computation.** For $\mathbf{s} \in \Omega := [0,1]\mathbf{a}_1 + [0,1]\mathbf{a}_2$, we denote by $V_{\mathbf{s}}^{(2)}$ the true Kohn-Sham mean-field potential for the configuration where the two sheets are aligned (no angle), but with the upper one shifted by a vector $\mathbf{s}$. We set

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

and we obtain the Fourier coefficients

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

We then compute

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

and finally obtain the Fourier coefficients

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

and we expect $V_{\text{int},\mathbf{s}}$ not to depend too much on $\mathbf{s}$, that is we expect that the following quantity is small

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

4. Effective potentials

We are now in $2d$ and $|\Omega_{\text{M}}| = |\Omega|$. 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 $\langle\!\langle f,g\rangle\!\rangle^{+-} = e^{-iq_1 x}(\!(f,g)\!)^{+-}$.

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

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

Using the Fourier decomposition (2) in $2d$, and using $a_{\text{M}}^* = Ja^*$ and $ma^* \cdot JX = -ma_{\text{M}}^* \cdot X$, $\iota_{\eta'}^\eta := \frac{1}{2}(\eta - \eta')$, when $\eta \neq \eta'$,

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

To sum up,

$$\boxed{(\!(f,g)\!)^{\eta,\eta'} = \delta_{\eta=\eta'}\langle f,g\rangle + \delta_{\eta\neq\eta'} \sum_{m\in\mathbb{Z}^2} \frac{e^{ima_{\text{M}}^*\cdot J\mathbf{X}}}{\sqrt{|\Omega_{\text{M}}|}} C_m^{\iota_{\eta'}^\eta}}$$

For the potentials, we finally need to implement

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

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

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

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

In the function $\mathbb{V}(X) = \langle u_j, V u_i \rangle (X)$, when $V \to V + V_{\text{int}}$, we have

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

but at the level of Fourier coefficients,

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

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

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

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

$$\frac{1}{|\Omega|} \int_{\Omega_{\mathrm{M}}} f = \frac{\widehat{f}_0}{\sqrt{|\Omega|}}$$

hence

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

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

5. 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

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

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

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

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

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

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

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

has Fourier coefficients

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

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

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

Finally, we analyze a symmetry. 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

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

6. Effective BM coefficients from potential

From [1], the BM Hamiltonian is

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

where

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

and where

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

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

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

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

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

7. Change of gauge on the phasis of wavefunctions

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

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

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 $U := \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}$, we have

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

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

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

is constant in α, where $\mathcal{U} := \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}$.

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

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

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

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

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

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

we also compute that

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

hence if the operator Γ is a linear combination of the terms

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

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

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

of the effective Hamiltonian $\mathcal{H}_{d,\theta}$, it satisfies $\mathcal{S}\Gamma\mathcal{S} = \Gamma$ and hence break the particle-hole symmetry.

But now we also compute that

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

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

The mirror operator for the BM Hamiltonian is

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

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

Next,

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

and for BM's potential, $\sigma_1 T^*(M\mathbf{X})\sigma_1 = T(\mathbf{X})$

9. 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 $\frac{1}{v_{\mathrm{F}} k_\theta^3} S \cdot S^*$ as in (4)

(2) We conjugate by $U = \begin{pmatrix} e^{iK_1 x} & 0 \\ 0 & e^{iK_2 x} \end{pmatrix}$ to remove the $e^{-iq_1 x}$ factors

10. Treating the Bistritzer-MacDonal model

In this section, we apply the plan of Section 9 to treat the BM model.

10.1. **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

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

We consider the rescaling

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

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

$$\frac{1}{k_\theta^3 v_{\mathrm{F}}} S\left(\begin{pmatrix} -iv_{\mathrm{F}}\sigma\nabla & wT(k_\theta x) \\ wT^*(k_\theta x) & -iv_{\mathrm{F}}\sigma\nabla \end{pmatrix} - E\right) S^* = \begin{pmatrix} -i\sigma\nabla & \alpha T\left(x\right) \\ \alpha T^*(x) & -i\sigma\nabla \end{pmatrix} - \varepsilon =: H_{BM} \tag{4}$$

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

10.2. **Removing $e^{-iq_1 x}$.** With

$$U := \begin{pmatrix} e^{iK_1 x}\mathbb{1}_2 & 0 \\ 0 & e^{iK_2 x}\mathbb{1}_2 \end{pmatrix}, \tag{5}$$

we have

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

where $\mathbf{T}$ is moiré-periodic.

11. Treating our model

11.1. **Goal.** Our Hamiltonian is

$$\mathcal{H} = \varepsilon_\theta^{-1}\mathcal{V} + c_\theta T + \varepsilon_\theta T^{(1)}, \qquad \mathcal{H}\psi = \frac{E}{\varepsilon_\theta}\mathcal{S}\psi \tag{6}$$

where the three operators $\mathcal{V}$, T, and $T^{(1)}$ are

$$\mathcal{S} = \begin{pmatrix} \mathbb{I}_2 & \Sigma \\ \Sigma^* & \mathbb{I}_2 \end{pmatrix} \qquad \text{and} \qquad \mathcal{V} = \begin{pmatrix} \mathbb{W}^+ & \mathbb{V} \\ \mathbb{V}^* & \mathbb{W}^- \end{pmatrix},$$

$$T = \begin{pmatrix} v_F\boldsymbol{\sigma}\cdot(-\mathrm{i}\nabla) & J(-\mathrm{i}\nabla\Sigma)\cdot(-\mathrm{i}\nabla) \\ J(-\mathrm{i}\nabla\Sigma^*)\cdot(-\mathrm{i}\nabla) & v_F\boldsymbol{\sigma}\cdot(-\mathrm{i}\nabla) \end{pmatrix},$$

$$T^{(1)} = -\frac{1}{2}\mathrm{div}\mathcal{S}\nabla\bullet + \frac{1}{2}\begin{pmatrix} -v_F\boldsymbol{\sigma}\cdot J(-\mathrm{i}\nabla) & 0 \\ 0 & v_F\boldsymbol{\sigma}\cdot J(-\mathrm{i}\nabla) \end{pmatrix}. \tag{7}$$

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

Numerically, we will discretize $\mathcal{H}$ and $\mathcal{S}$ and compute the eigenvalues of $\mathcal{S}^{-\frac{1}{2}}\mathcal{H}\mathcal{S}^{-\frac{1}{2}}$.

11.2. **Gauge change.** We recall that

$$U := \begin{pmatrix} e^{iK_1 x}\mathbb{1}_2 & 0 \\ 0 & e^{iK_2 x}\mathbb{1}_2 \end{pmatrix},$$

and that we work on $U\mathcal{H}U^*$

11.2.1. *Electric potentials and mass matrix.* We have

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

and

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

11.2.2. *First order differential operators.* We compute

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

and as presented in Section 13, with $A := -i\nabla\Sigma$,

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

Moreover,

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

11.2.3. *Second order differential operator.* We have

$$-i\operatorname{div} e^{iK_1 x}\circ = -i\operatorname{div} + K_1, \qquad -i\nabla e^{-iK_2 x}\circ = -i\nabla - K_2$$

so

$$\begin{aligned}e^{iK_1x}(-i\operatorname{div})\Sigma(-i\nabla)e^{-iK_2x} &= (-i\operatorname{div} - K_1)\, e^{i(K_1-K_2)x}\Sigma\,(-i\nabla - K_2)\\ &= (-i\operatorname{div} - K_1)\,\widetilde{\Sigma}\,(-i\nabla - K_2)\end{aligned}$$

and as operator compositions,

$$\begin{aligned}U(-i\operatorname{div})\mathcal{S}(-i\nabla)U^* &= U\begin{pmatrix}-\Delta & (-i\operatorname{div})\Sigma(-i\nabla)\\ (-i\operatorname{div})\Sigma^*(-i\nabla) & -\Delta\end{pmatrix}U^*\\ = &\begin{pmatrix}(-i\nabla - K_1)^2 & (-i\operatorname{div} - K_1)\,\widetilde{\Sigma}\,(-i\nabla - K_2)\\ (-i\operatorname{div} - K_2)\,\widetilde{\Sigma}^*\,(-i\nabla - K_1) & (-i\nabla - K_2)^2\end{pmatrix}\end{aligned}$$

12. Discretization

Now we take the basis

$$e_m^a := e^a \otimes \frac{e^{ima^*_{\mathrm{M}}x}}{\sqrt{|\Omega_{\mathrm{M}}|}}$$

where

$$e^1 := \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \dots$$

12.1. **Electric potentials.** With $\mathbb{V} = \sum_m V_m e_m$, $e_m := \frac{e^{ima^*_{\mathrm{M}}x}}{\sqrt{|\Omega_{\mathrm{M}}|}}$, we have

$$\langle e_n, \mathbb{V} e_p \rangle = \frac{V_{n-p}}{\sqrt{|\Omega_{\mathrm{M}}|}}$$

so for multiplication operatos A, B, C, D,

$$\left\langle e_n, \begin{pmatrix} A & B \\ C & D \end{pmatrix} e_p \right\rangle = \frac{1}{\sqrt{|\Omega_{\mathrm{M}}|}} \begin{pmatrix} A_{n-p} & B_{n-p} \\ C_{n-p} & D_{n-p} \end{pmatrix}$$

12.2. **First order differential operators.** We have

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

and with $\mathbb{A} = \sum_m A_m e_m$,

$$\langle e_n, \mathbb{A} \cdot (-i\nabla) e_p \rangle = \frac{A_{n-p}}{\sqrt{|\Omega_{\mathrm{M}}|}} \cdot p a^*_{\mathrm{M}}$$

hence

$$\left\langle e_n, U \begin{pmatrix} \sigma\,(-i\nabla) & 0 \\ 0 & \sigma\,(-i\nabla) \end{pmatrix} U^* e_p \right\rangle = \delta_{n-p} \begin{pmatrix} \sigma\,(n a^*_{\mathrm{M}} - K_1) & 0 \\ 0 & \sigma\,(n a^*_{\mathrm{M}} - K_2) \end{pmatrix}$$

and

$$\begin{aligned} &\left\langle e_n, U \begin{pmatrix} 0 & JA(-i\nabla) \\ (JA)^*\,(-i\nabla) & \end{pmatrix} U^* e_p \right\rangle \\ &\quad = \frac{1}{\sqrt{|\Omega_{\mathrm{M}}|}} \begin{pmatrix} 0 & \left(J\widetilde{A}\right)_{n-p} \cdot (p a^*_{\mathrm{M}} - K_2) \\ \left(J\widetilde{A}\right)^*_{n-p} \cdot (p a^*_{\mathrm{M}} - K_1) & 0 \end{pmatrix} \end{aligned}$$

Moreover,

$$\begin{aligned} &\left\langle e_n, U \begin{pmatrix} -v_F \sigma \cdot J(-i\nabla) & 0 \\ 0 & v_F \sigma \cdot J(-i\nabla) \end{pmatrix} U^* e_p \right\rangle \\ &\quad = \delta_{n-p} \begin{pmatrix} -v_F \sigma \cdot J(p a^*_{\mathrm{M}} - K_1) & 0 \\ 0 & v_F \sigma \cdot J(p a^*_{\mathrm{M}} - K_2) \end{pmatrix} \end{aligned}$$

12.3. **Second order differential operator.** We have

$$\langle e_p, -i\,\mathrm{div}\,(\Sigma\,(-i\nabla)\, e_m) \rangle = \langle (-i\nabla)\, e_p, \Sigma\,(-i\nabla)\, e_m \rangle = p a^*_{\mathrm{M}} \cdot m a^*_{\mathrm{M}} \frac{\Sigma_{p-m}}{\sqrt{|\Omega_{\mathrm{M}}|}}$$

so

$$\frac{1}{2}\left\langle e_n, U(-i\operatorname{div})\mathcal{S}(-i\nabla)U^* e_p\right\rangle = \frac{1}{2}U\begin{pmatrix} -\Delta & (-i\operatorname{div})\Sigma(-i\nabla) \\ (-i\operatorname{div})\Sigma^*(-i\nabla) & -\Delta \end{pmatrix}U^*$$

$$= \frac{1}{2}\begin{pmatrix} (pa^*_{\mathrm{M}} - K_1)^2 & (pa^*_{\mathrm{M}} - K_1)\cdot(na^*_{\mathrm{M}} - K_2)\,\frac{\widetilde{\Sigma}_{n-p}}{\sqrt{|\Omega_{\mathrm{M}}|}} \\ (pa^*_{\mathrm{M}} - K_2)\cdot(na^*_{\mathrm{M}} - K_1)\,\frac{\widetilde{\Sigma}^*_{n-p}}{\sqrt{|\Omega_{\mathrm{M}}|}} & (pa^*_{\mathrm{M}} - K_2)^2 \end{pmatrix}$$

13. Appendix : more on the magnetic term

We have

$$A := -i\nabla\Sigma = e^{-iq_1x}\left(-i\nabla - q_1\right)\left(\left(u_j, u_{j'}\right)\right)^{+-}$$

hence with $\widetilde{f} := e^{iq_1x}f$,

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

$$U\begin{pmatrix} 0 & JA(-i\nabla) \\ JA^*(-i\nabla) & \end{pmatrix}U^*$$

$$= \begin{pmatrix} 0 & e^{i(K_1-K_2)x}JA\cdot(-i\nabla - K_2) \\ e^{i(K_2-K_1)x}JA^*\cdot(-i\nabla - K_1) & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & e^{iq_1x}JA\cdot(-i\nabla - K_2) \\ e^{-iq_1x}JA^*\cdot(-i\nabla - K_1) & 0 \end{pmatrix}$$

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

Now

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

and since $\widetilde{A}^* = e^{-iq_1x}A^*$, then $-i\operatorname{div} J\left(\widetilde{A}^*\right) = -q_1 J\left(\widetilde{A}^*\right)$. We have

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

With A a $4{\times}4$ 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^{*m}, the pointwise dual of A at each x, is indeed the hermitian conjugate for any x. More precisely,

$$\langle u, v\rangle = \int_X \langle u, v\rangle_{mat}$$

so

$$\langle u, Vv\rangle = \int_X \langle u(x), V(x)v(x)\rangle_{mat} = \int_X \langle V(x)^{*m}u(x), v(x)\rangle_{mat} = \langle V^{*m}u, v\rangle$$

and

$$\boxed{V^* = V^{*m}}$$

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

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

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 $A = -i\nabla\Sigma$,

$$\begin{aligned}\langle v, JA\cdot(-i\nabla - K_2)\,u\rangle &= \langle (JA)^*\,v, (-i\nabla - K_2)\,u\rangle = \langle JA^* v, (-i\nabla - K_2)\,u\rangle \\ &= \langle (-i\operatorname{div} - K_2)\,JA^* v, u\rangle \\ &= \langle ((-i\operatorname{div})\,(JA^*))\,v, u\rangle + \langle (JA^*)\cdot(-i\nabla - K_2)\,v, u\rangle \\ &= \langle (JA^*)\cdot(-i\nabla - K_2)\,v, u\rangle\end{aligned}$$

Repeating the same computations, we find that

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

so

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

We can compute (double checked) that for a 1-component potential V, $\langle u, Vv\rangle = \left\langle \overline{V}u, v\right\rangle$ hence $V^{*_f} = \overline{V}$ and $\left(V^{*_f}\right)_m = \overline{V}_{-m}$

Next,

$$\begin{aligned}\langle u, A\cdot(-i\nabla)v\rangle &= \int \overline{\overline{A}u}\cdot(-i\nabla)v = \int v\overline{(-i\nabla)\overline{A}u} \\ &= \left\langle \left(-i\operatorname{div}\overline{A}\right)u, v\right\rangle + \left\langle \overline{A}\cdot(-i\nabla)u, v\right\rangle\end{aligned}$$

hence

$$(A\cdot(-i\nabla))^{*_f} = -i\operatorname{div}\overline{A} + \overline{A}\cdot(-i\nabla)$$

and $-i\operatorname{div} A = q_1\cdot A$ implies $-i\operatorname{div}\overline{A} = -q_1\cdot\overline{A}$. Now for a 4×4 matrix function V, we have

$$\begin{aligned}\langle e_i\otimes e_I, V^{*_f *_m} e_j\otimes e_J\rangle &= (V^{*_f *_m})^{IJ}_{i-j} = \langle Ve_i\otimes e_I, e_j\otimes e_J\rangle \\ &= \overline{\langle e_j\otimes e_J, Ve_i\otimes e_I\rangle} = \overline{V^{JI}_{j-i}}\end{aligned}$$

hence

$$(V^{*_f *_m})^{IJ}_m = \overline{V^{JI}_{-m}}, \qquad V^{*_f *_m} = V^*$$

13.1. **Stuff.** Let us consider an operator H and its discretization

$$H^{ab}_{ij} := \left\langle e^a_i, He^b_j\right\rangle \qquad (H^*)^{ab}_{ij} = \overline{H^{ba}_{ji}}$$

and we want to build the Hermitian operator

$$\begin{pmatrix} 0 & H \\ H^* & 0\end{pmatrix}$$

$$(H^*)^t = \overline{H}, \qquad \left((H^*)^t\right)^{ab}_{ij} = \overline{H^{ab}_{ij}}$$

For $H = V$, we have

$$H^{ab}_{ij} := V^{ab}_{i-j} \qquad (H^*)^{ab}_{ij} = \overline{V^{ba}_{j-i}}, \qquad \overline{H}^{ab}_{ij} = \overline{V^{ab}_{i-j}}$$

and in the code we implement $\overline{H^{ab}_{ij}}$.

Let us assume that $-i\operatorname{div} A = q_1 \cdot A$, so in Fourier space this is written

$$ma^*_{\mathrm{M}} \cdot A_m = q_1 \cdot A_m \tag{8}$$

but be careful, this relation is true only for $m \in \{-N/2, \dots, N/2\}$!!!! Now $e^a_m := e^a \otimes \frac{e^{ima^*_{\mathrm{M}}x}}{\sqrt{|\Omega_{\mathrm{M}}|}}$,

$$H^{ab}_{ij} := \left\langle e^a_i, A \cdot (-i\nabla - K_1)\, e^b_j \right\rangle = A^{ab}_{i-j} \cdot (ja^*_{\mathrm{M}} - K_1)$$

where

$$\begin{aligned}(H^*)^{ab}_{ij} = \overline{H^{ba}_{ji}} &= \overline{\left\langle e^b_j, A\,(-i\nabla - K_1)\, e^a_i \right\rangle} = \left\langle e^a_i, A^* \cdot (-i\nabla - K_2)\, e^b_j \right\rangle \\ &= \overline{A^{ba}_{j-i}}(ja^*_{\mathrm{M}} - K_2) \underset{8}{=} \overline{A^{ba}_{j-i}} \cdot (ia^*_{\mathrm{M}} - K_1) = \overline{H^{ba}_{ji}}\end{aligned}$$

and

$$\overline{H}^{ab}_{ij} = \overline{A^{ab}_{i-j}} \cdot (ja^*_{\mathrm{M}} - K_1) = \overline{A^{ab}_{i-j}} \cdot (ia^*_{\mathrm{M}} - K_2)$$

and the last inequality is true only when $i - j \in \{-N/2, \dots, N/2\}$!!!

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