

NUMERICAL COMPUTATIONS FOR AN EFFECTIVE MODEL OF TWISTED BILAYER GRAPHENE

ÉRIC CANCÈS, LOUIS GARRIGUE AND DAVID GONTIER

1. STANDARD MONOLAYER

We choose for the microscopic lattice, the orientation

$$\begin{aligned} a_1 &= a \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix}, & a_2 &= a \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix} \\ a_1^* &= \frac{2\pi}{a} \begin{pmatrix} \frac{1}{\sqrt{3}} \\ 1 \end{pmatrix} = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}, & a_2^* &= \frac{2\pi}{a} \begin{pmatrix} \frac{1}{\sqrt{3}} \\ -1 \end{pmatrix} = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} \end{aligned} \quad (1)$$

and for the Macroscopic lattice, we choose the orientation

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

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

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

In reduced coordinates, with

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

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

and

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

1.1. Dirac point. We have

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

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

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

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

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

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

hence any function can be decomposed as

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

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

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

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

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

$$f(\mathbf{x}, z) = \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ m_z \in \mathbb{Z}}} \frac{e^{i(\mathbf{m}a^* \cdot \mathbf{x} + m_z \frac{2\pi}{L} z)}}{\Gamma} \hat{f}_{\mathbf{m},m_z} \quad (4)$$

We define the scalar product

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

and compute Plancherel's formula

$$\langle f, g \rangle = \sum_{\substack{\mathbf{m} \in \mathbb{Z}^2 \\ m_z \in \mathbb{Z}}} \overline{\hat{f}_{\mathbf{m},m_z}} \hat{g}_{\mathbf{m},m_z}. \quad (5)$$

Hence, as a verification, we test that the normalization of the \hat{u}_j 's is the right one by checking that $\|u_j\|_{L^2}^2 = 1$ via (5).

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 $R_{\frac{2\pi}{3}}(ma^*) = \left(R_{\frac{2\pi}{3}}^{\text{red}} m\right) a^*$ where

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

and

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

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

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

and

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

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

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

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

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

2. COMPARISON 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

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

then

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

3. COMPUTATION OF V_{int}

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

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

and we obtain the Fourier coefficients

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

We then compute

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

and finally obtain the Fourier coefficients

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

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

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

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

4. EFFECTIVE POTENTIALS

We defined

$$\langle\langle f, g \rangle\rangle^{\eta, \eta'}(\mathbf{X}) := \int_{\Omega \times \mathbb{R}} \bar{f}(x - \eta J\mathbf{X}, z - \eta \frac{d}{2}) g(x - \eta' J\mathbf{X}, z - \eta' \frac{d}{2}) dx dz$$

and

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

and in particular since $q_1 = -2JK$, then

$$\langle\langle f, g \rangle\rangle^{+-} = e^{-iq_1 x} \langle\langle f, g \rangle\rangle^{+-}, \quad \langle\langle f, g \rangle\rangle^{-+} = e^{iq_1 x} \langle\langle f, g \rangle\rangle^{-+}$$

Now we make the approximation

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

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

Firstly, using the Fourier decomposition (4),

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

where

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

We have $((f, g))^{++} = ((f, g))^{--} = \langle f, g \rangle = \sum_{\mathbf{m}, m_z} \widehat{f}_{\mathbf{m}, m_z} \widehat{g}_{\mathbf{m}, m_z}$.

We also define, for $\eta \in \{-1, 1\}$,

$$C_{\mathbf{m}}^{\eta} := \sqrt{|\Omega_M|} \sum_{m_z \in \mathbb{Z}} e^{i\eta 2 \frac{d\pi}{L} m_z} \widehat{f}_{-\eta \mathbf{m}, m_z} \widehat{g}_{-\eta \mathbf{m}, m_z}$$

We have $a_M^* = 2Ja^*$ hence $2ma^* \cdot JX = -ma_M^* \cdot X$ and

$$((f, g))^{+-} = \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{e^{i\mathbf{m} a_M^* \cdot \mathbf{X}}}{\sqrt{|\Omega_M|}} C_{\mathbf{m}}^+, \quad ((f, g))^{-+} = \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{e^{i\mathbf{m} a_M^* \cdot \mathbf{X}}}{\sqrt{|\Omega_M|}} C_{\mathbf{m}}^-$$

Now, since $q_{2,3} - q_1 = a_{M,j}^*$, we know that

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

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

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

Then,

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

Moreover,

$$\begin{aligned} \mathcal{A} &= \frac{1}{2} J (-i \nabla) \Sigma = \frac{1}{2} J (-i \nabla) \left(e^{-iq_1 x} ((u_j, u_{j'}))^{+-} \right) \\ &= e^{-iq_1 x} \frac{1}{2} \sum_{\mathbf{m} \in \mathbb{Z}^2} J (ma_M^*) \frac{e^{i\mathbf{m} a_M^* \cdot \mathbf{X}}}{\sqrt{|\Omega_M|}} C_{\mathbf{m}}^{+, \Sigma} - \frac{1}{2} \Sigma J q_1, \\ &\stackrel{q_1 = -2JK}{=} e^{-iq_1 x} \sum_{\mathbf{m} \in \mathbb{Z}^2} \frac{e^{i\mathbf{m} a_M^* \cdot \mathbf{X}}}{\sqrt{|\Omega_M|}} C_{\mathbf{m}}^{+, \mathcal{A}} - \Sigma K, \\ C_m^{+, \mathcal{A}} &:= \frac{1}{2} J (ma_M^*) C_{\mathbf{m}}^{+, \Sigma} \end{aligned}$$

To plot, we will need to shift the exponent $e^{-iq_1 x} = e^{\frac{i}{3} (a_{M,1}^* + a_{M,2}^*) x}$

TO RECTIFY

Hence

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

and

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

where $C_{\frac{\mathbf{m}}{3}} := 0$ if n does not divide m_1 and m_2 . Numerically, there is no loss of information since all $C_{\mathbf{m}}$'s are taken into account if the “ecut” is large enough.

Similarly

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

For the potentials, we finally need to implement

$$\mathbb{W}_{j,j'}^+ = ((\bar{u}_j u_{j'}, V))^{+-}, \quad \mathbb{W}_{j,j'}^- = ((\bar{u}_j u_{j'}, V))^{-+},$$

$$\mathbb{V}_{j,j'} = \langle\langle (V + V_{\text{int}}) u_j, u_{j'} \rangle\rangle^{+-}$$

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

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

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

so

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

and

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

so

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

so we can implement

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

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

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

and the matrix $M_{j,j'} := \langle u_j, V_{\text{int}} u_{j'} \rangle$ 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 $V \rightarrow V + V_{\text{int}}$, 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 $\sqrt{|\Omega|}$

4.3. **Adding a constant.** We have

$$g(x) := f(x) + c \quad \implies \quad \widehat{g}_0 = \widehat{f}_0 + \sqrt{|\Omega_M|} c$$

4.4. **Subtracting 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

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

4.5. V_{int}^{3d} . We have $V_{\text{int}}^{3d}(x, z) := V_{\text{int}}(z)$ hence $\left(\widehat{V_{\text{int}}^{3d}} \right)_{m, m_z} = \sqrt{|\Omega_M|} \left(\widehat{V_{\text{int}}} \right)_{m_z}$

5. FORM

If we have

$$T(x) = \begin{pmatrix} e^{-iq_1 x} g(x) & e^{-iq_1 x} f(x) \\ e^{-iq_1 x} \bar{f}(-x) & e^{-iq_1 x} g(x) \end{pmatrix} = e^{-iq_1 x} \begin{pmatrix} g(x) & f(x) \\ \bar{f}(-x) & g(x) \end{pmatrix},$$

then

$$T^*(x) = e^{iq_1 x} \begin{pmatrix} \bar{g}(x) & f(-x) \\ \bar{f}(x) & \bar{g}(x) \end{pmatrix}$$

and \mathbb{W} does not have an exponent $e^{-iq_1 x}$.

5.1. **From $T(x)$ to $T(3x)$.** With $T(x) = e^{-iq_1 x} \sum T_m e^{i m a_M^* x}$, we have

$$\mathcal{T}(x) := T(3x) = e^{i(a_{1,M}^* + a_{2,M}^*)x} \sum T_m e^{i m a_M^* 3x} = \sum_m T_m \frac{\begin{pmatrix} 1 \\ 1 \end{pmatrix}}{3} e^{i m a_M^* x}$$

6. BM CONFIGURATION

From [1], the BM Hamiltonian is

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

where

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

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

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

and

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

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

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

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

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

and we compute

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

Or

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

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

7. OPERATORS IN BASIS

7.1. Goal. Our goal is to study the eigenvalue equation

$$\mathcal{H}\psi = \varepsilon_\theta \mathcal{S} E \psi$$

remark that energies have to be rescaled by ε_θ ! The operator \mathcal{S} is Hermitian and positive and

$$\mathcal{H} := \frac{1}{\varepsilon_\theta} \mathcal{V} + c_\theta T + \varepsilon_\theta T^{(1)}$$

where

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

and their Bloch transform becomes

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

and we want the middle of the spectrum of

$$\mathcal{H}_k := \mathcal{S}^{-\frac{1}{2}} \left(\frac{1}{\varepsilon_\theta} \mathcal{V} + c_\theta T_k + \varepsilon_\theta T_k^{(1)} \right) \mathcal{S}^{-\frac{1}{2}}$$

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

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

7.3. 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

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

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

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

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

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

7.5. Off-diagonal potential. For a general $V = \sum_m V_m e^{ima^* \cdot x}$, we have $V^* = \sum_m V_m^* e^{-ima^* \cdot x}$ and

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

and M is also Hermitian.

7.6. 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

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

7.7. 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

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

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

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

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

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

so

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

We have

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

We have

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

so

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

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

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

8. RENORMALIZATION OF THE EQUATION

We know that

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

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

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

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

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

We enter $V\left(\frac{3}{2}JX\right)$ for each potential V , hence we need to apply a coefficient $\frac{2}{3}$ to each derivation operator.

9. SYMMETRIES

9.1. **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 \mathbf{A} , we have

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

we also compute that

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

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

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

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

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

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

But now we also compute that

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

9.2. 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

$$\begin{aligned} \sigma_1 T^*(M\mathbf{X}) \sigma_1 &= \begin{pmatrix} w_0 \left(\sum_{j=1}^3 e^{ix \cdot M q_j} \right) & w_1 \left(e^{ix \cdot M q_1} + e^{i\phi} e^{ix \cdot M q_2} + e^{i2\phi} e^{ix \cdot M q_3} \right) \\ \cdot & \cdot \end{pmatrix} \\ &= \begin{pmatrix} w_0 \left(\sum_{j=1}^3 e^{ix \cdot q_j} \right) & w_1 \left(e^{ix \cdot q_1} + e^{-i\phi} e^{ix \cdot q_2} + e^{-i2\phi} e^{ix \cdot q_3} \right) \\ \cdot & \cdot \end{pmatrix} = T(\mathbf{X}) \end{aligned}$$

where we used that $M q_1^c = q_1^c$, $M q_2^c = q_3^c$ and $M q_3^c = q_2^c$.

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

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

10. NON LOCAL TERM

From the theoretical investigations, we have

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

and

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

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

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

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

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

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

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

has Fourier coefficients

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

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

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

10.1. Symmetries. We have

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

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

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

11. CHANGE OF BASIS FOR GETTING $\Phi_j \in L^2_{\tau, \bar{\tau}}$

Numerically, DFTK gives

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

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

First we define

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

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

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

and also choosing $\alpha = 0$ if $\cos \theta \geq 0$ 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

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

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

12. THE 1/3 SCALING OF COORDINATES

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

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

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

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

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

13. CHANGE OF GAUGE ON THE PHASIS OF WAVEFUNCTIONS

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

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

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

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

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

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

is constant in θ .

14. COMPARISON BETWEEN BM AND OUR MODEL

14.1. **Rescaling.** The BM Hamiltonian is

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

We consider the rescaling

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

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

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

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

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

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

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

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

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

corresponding to the direct lattice

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

The q_j 's are

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

so

$$\sqrt{3}Jq_{2,3}^{\text{TKV}} = \pm b_{2,1}^{*,\text{TKV}}$$

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

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

We have

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

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

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

and we redefine

$$m_{q_1} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \quad m_{q_2} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}, \quad m_{q_3} = \begin{pmatrix} -1 \\ -2 \end{pmatrix} \quad (6)$$

so

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

We conjugate again and get

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

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

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

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

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

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

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

14.4. Relation to our model. We compute, for $j \in \{1, 2, 3\}$,

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

and

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

We deduce that

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

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

$$m_j b^* = q_j$$

and

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

15. CODE

$$\begin{aligned} b_1^* &= \frac{4\pi\varepsilon}{a\sqrt{3}} \begin{pmatrix} -1/2 \\ -\sqrt{3}/2 \end{pmatrix} = k_\theta \sqrt{3} \begin{pmatrix} -1/2 \\ -\sqrt{3}/2 \end{pmatrix}, \quad b_2^* = k_\theta \sqrt{3} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ R_{\frac{2\pi}{3}} b_1^* &= b_2^*, \quad R_{\frac{2\pi}{3}} b_2^* = -b_1^* - b_2^* \\ K_1 &= \frac{1}{3} (b_1^* + 2b_2^*) = \frac{1}{3} (a_1^* - 2a_2^*) = k_\theta \begin{pmatrix} \sqrt{3}/2 \\ -1/2 \end{pmatrix} \\ K_2 &= \frac{1}{3} (-b_1^* + b_2^*) = \frac{1}{3} (2a_1^* - a_2^*) = k_\theta \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \end{pmatrix} = R_{\frac{2\pi}{6}} K_1 \end{aligned}$$

then

$$H = \begin{pmatrix} \sigma^\xi \cdot (-i\nabla + k - K_1) & T_\xi(x) \\ T_\xi(x)^* & \sigma^\xi \cdot (-i\nabla + k - K_2) \end{pmatrix}$$

where $\sigma^\xi := (\xi\sigma_1, \sigma_2)$ and $T_\xi(x) = T_1^\xi + T_2^\xi e^{-ib_1^*x} + T_3^\xi e^{-i(b_1^*+b_2^*)x}$ where

$$T_1^\xi = \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}, \quad T_2^\xi = \begin{pmatrix} \alpha & \beta e^{-i\xi\phi} \\ \beta e^{i\xi\phi} & \alpha \end{pmatrix} \quad T_3^\xi = \overline{T_2^\xi}$$

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

$$U^* H U = \begin{pmatrix} \sigma^\xi \cdot (-i\nabla + k) & T_\xi(x) e^{i(K_1-K_2)x} \\ T_\xi(x)^* e^{i(K_2-K_1)x} & \sigma^\xi \cdot (-i\nabla + k) \end{pmatrix}$$

and $K_1 - K_2 = \frac{1}{3}(2b_1^* + b_2^*)$ so

$$T_\xi(x) e^{i(K_1-K_2)x} = T_1 e^{i\frac{1}{3}(2b_1^*+b_2^*)x} + T_2 e^{i\frac{1}{3}(-b_1^*+b_2^*)x} + T_3 e^{i\frac{1}{3}(-b_1^*-2b_2^*)x}$$

If we define

$$Q_1 := \frac{1}{3}(2b_1^* + b_2^*) = k_\theta \begin{pmatrix} 0 \\ -1 \end{pmatrix} = q_1$$

$$Q_2 := \frac{1}{3}(-b_1^* + b_2^*), \quad Q_3 := \frac{1}{3}(-b_1^* - 2b_2^*)$$

we have

$$R_{\frac{2\pi}{3}} Q_1 = Q_2, \quad R_{\frac{2\pi}{3}} Q_2 = Q_3, \quad R_{\frac{2\pi}{3}} Q_3 = Q_1$$

and hence $Q_j = q_j$, of TKV, and $TT_\xi(x) e^{i(K_1-K_2)x} = T_\xi(x) e^{iq_1x} = T(x)$.

Also, we have $b_1^* + b_2^* = k_\theta \sqrt{3} \begin{pmatrix} 1/2 \\ -\sqrt{3}/2 \end{pmatrix} = -a_2^*$ and $b_1^* = -a_1^*$, so

$$b_1^* = -a_1^*, \quad b_2^* = a_1^* - a_2^*$$

15.1. **TKV.** In TKV, we have

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

$$q_1 = -q_2 - q_3$$

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

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

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

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

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

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

If

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

and

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

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

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

we compute

$$U^* \begin{pmatrix} -i\sigma\nabla & T \\ T^* & -i\sigma\nabla \end{pmatrix} U = \begin{pmatrix} \sigma(-i\nabla - K_1) & T e^{i(K_1-K_2)x} \\ T^* e^{i(K_2-K_1)x} & \sigma(-i\nabla - K_2) \end{pmatrix} \quad (8)$$

and with $K_1 - K_2 = q_1$,

$$T e^{i(K_1-K_2)x} = T_1 + T_2 e^{i(-q_2+q_1)x} + T_3 e^{i(-q_3+q_1)x} = T_1 + T_2 e^{-ia_1^*x} + T_3 e^{-ia_2^*x}$$

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

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

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

has no solution !!! We can try

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

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

so $(\alpha, \beta) = (1, 2)$ but then K_1 is not a Dirac point for this configuration !

15.2. Deductive from TKV. From (8), that we consider again, we want $K_1 - K_2 = q_1$, so

$$T(x) e^{i(K_1-K_2)x} = T(x) e^{iq_1x} = T_1 + T_2 e^{i(q_1-q_2)x} + T_3 e^{i(q_1-q_3)x}$$

$$= T_1 + T_2 e^{-ic_1^*x} + T_3 e^{-i(c_1^*+c_2^*)x}$$

where

$$c_1^* := q_2 - q_1 = a_1^*, \quad c_2^* := q_3 - q_2 = -a_1^* + a_2^*, \quad a_2^* = c_1^* + c_2^*$$

hence

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

and

$$R_{\frac{2\pi}{6}} c_1^* = c_1^* + c_2^*, \quad R_{\frac{2\pi}{6}} c_2^* = -c_1^*$$

so if $K_2 = \frac{1}{3}(\alpha c_1^* + \beta c_2^*)$, and if we impose $K_1 = R_{\frac{2\pi}{6}} K_2$, we have $K_1 = \frac{1}{3}((\alpha - \beta) c_1^* + \alpha c_2^*)$ and

$$\frac{1}{3}(-2c_1^* - c_2^*) = q_1 = K_1 - K_2 = \frac{1}{3}(-\beta c_1^* + (\alpha - \beta) c_2^*) \implies (\alpha, \beta) = (1, 2)$$

so

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

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