Enlarged unit cell, decomposition of κ, and Bloch Hamiltonian

1 Enlarged unit cell, decomposition of κ, and Bloch Hamiltonian

1.1 Lattice and supercell

We work on the honeycomb in brick-wall coordinates with original integer coordinates $(i, j) \in \mathbb{Z}^2$. We enlarge to a 2×2 supercell with

$$\mathbf{a} = 2\hat{i}, \qquad \mathbf{b} = 2\hat{j},$$

and four internal offsets

$$r_0 = (0,0), \qquad r_1 = (1,0), \qquad r_2 = (0,1), \qquad r_3 = (1,1).$$

A supercell position is $\mathbf{R} = m\,\mathbf{a} + n\,\mathbf{b}$. Sites are labeled $(\mathbf{R}, r, s)$ with $r \in \{0,1,2,3\}$ and sublattice $s \in \{A, B\}$. We use the Bloch basis

$$\Psi_{\mathbf{K}} = (A_0, A_1, A_2, A_3;\ B_0, B_1, B_2, B_3)^{\mathsf{T}},$$

and define

$$\mathbf{K}\cdot\mathbf{a} = 2K_i, \qquad \mathbf{K}\cdot\mathbf{b} = 2K_j, \qquad \mathbf{K}\cdot(\mathbf{a}-\mathbf{b}) = 2(K_i - K_j).$$

1.2 Nearest-neighbor (Kitaev) map in real space

Using the convention

$$J_x:\ B_{i,j} \to A_{i,j}, \quad J_y:\ B_{i,j} \to A_{i+1,j}, \quad J_z:\ B_{i,j} \to A_{i,j+1},$$

the Majorana hopping Hamiltonian (itinerant $c^z \equiv c$; flux-free gauge) is

$$H_J = i\sum_{\mathbf{R}}\Big[J_x\sum_{r=0}^{3} c_{B,\mathbf{R},r}c_{A,\mathbf{R},r} + J_y\big(c_{B,\mathbf{R},r_0}c_{A,\mathbf{R},r_1} + c_{B,\mathbf{R},r_2}c_{A,\mathbf{R},r_3} + c_{B,\mathbf{R},r_1}c_{A,\mathbf{R}+\mathbf{a},r_0} + c_{B,\mathbf{R},r_3}c_{A,\mathbf{R}+\mathbf{a},r_2}\big)$$
$$+ J_z\big(c_{B,\mathbf{R},r_0}c_{A,\mathbf{R},r_2} + c_{B,\mathbf{R},r_1}c_{A,\mathbf{R},r_3} + c_{B,\mathbf{R},r_2}c_{A,\mathbf{R}+\mathbf{b},r_0} + c_{B,\mathbf{R},r_3}c_{A,\mathbf{R}+\mathbf{b},r_1}\big)\Big].$$

1.3 Twelve vertex-disjoint κ subsets in real space

We decompose the chiral term into 12 commuting blocks indexed by sublattice class $S \in \{A, B\}$ (A–A or B–B), next-nearest-neighbor direction $d \in \{+i,\, -j,\, j-i\}$, and parity $p \in \{\text{even}, \text{odd}\}$. Each block is a *matching* (no shared sites), so $\exp(-i\theta H_\kappa^{S,d,p})$ is exact per block. With a fixed orientation $J \to K = J + d$, the A–A blocks carry signs $(+,-,+)$ for $d = (+i, -j, j-i)$, while B–B blocks carry the opposite $(-,+,-)$.

For the 2×2 supercell:

$$
\begin{aligned}
H_\kappa^{A,+i,\text{even}} &= i \sum_{\mathbf{R}} \kappa_{A,+i,\text{e}} \big(c_{A,\mathbf{R},r_0} c_{A,\mathbf{R},r_1} + c_{A,\mathbf{R},r_2} c_{A,\mathbf{R},r_3} \big), \\
H_\kappa^{A,+i,\text{odd}} &= -i \sum_{\mathbf{R}} \kappa_{A,+i,\text{o}} \big(c_{A,\mathbf{R},r_0} c_{A,\mathbf{R}-\mathbf{a},r_1} + c_{A,\mathbf{R},r_2} c_{A,\mathbf{R}-\mathbf{a},r_3} \big), \\
H_\kappa^{A,-j,\text{even}} &= -i \sum_{\mathbf{R}} \kappa_{A,-j,\text{e}} \big(c_{A,\mathbf{R},r_0} c_{A,\mathbf{R},r_2} + c_{A,\mathbf{R},r_1} c_{A,\mathbf{R},r_3} \big), \\
H_\kappa^{A,-j,\text{odd}} &= +i \sum_{\mathbf{R}} \kappa_{A,-j,\text{o}} \big(c_{A,\mathbf{R},r_0} c_{A,\mathbf{R}-\mathbf{b},r_2} + c_{A,\mathbf{R},r_1} c_{A,\mathbf{R}-\mathbf{b},r_3} \big), \\
H_\kappa^{A,j-i,\text{even}} &= i \sum_{\mathbf{R}} \kappa_{A,j-i,\text{e}} \big(c_{A,\mathbf{R},r_1} c_{A,\mathbf{R},r_2} + c_{A,\mathbf{R},r_3} c_{A,\mathbf{R}+\mathbf{b},r_0} \big), \\
H_\kappa^{A,j-i,\text{odd}} &= -i \sum_{\mathbf{R}} \kappa_{A,j-i,\text{o}} \big(c_{A,\mathbf{R},r_1} c_{A,\mathbf{R}+\mathbf{a}-\mathbf{b},r_2} + c_{A,\mathbf{R},r_3} c_{A,\mathbf{R}+\mathbf{a},r_0} \big),
\end{aligned}
$$

and analogously for B–B with the opposite signs:

$$
\begin{aligned}
H_\kappa^{B,+i,\text{even}} &= -i \sum_{\mathbf{R}} \kappa_{B,+i,\text{e}} \big(c_{B,\mathbf{R},r_0} c_{B,\mathbf{R},r_1} + c_{B,\mathbf{R},r_2} c_{B,\mathbf{R},r_3} \big), \\
H_\kappa^{B,+i,\text{odd}} &= +i \sum_{\mathbf{R}} \kappa_{B,+i,\text{o}} \big(c_{B,\mathbf{R},r_0} c_{B,\mathbf{R}-\mathbf{a},r_1} + c_{B,\mathbf{R},r_2} c_{B,\mathbf{R}-\mathbf{a},r_3} \big), \\
H_\kappa^{B,-j,\text{even}} &= +i \sum_{\mathbf{R}} \kappa_{B,-j,\text{e}} \big(c_{B,\mathbf{R},r_0} c_{B,\mathbf{R},r_2} + c_{B,\mathbf{R},r_1} c_{B,\mathbf{R},r_3} \big), \\
H_\kappa^{B,-j,\text{odd}} &= -i \sum_{\mathbf{R}} \kappa_{B,-j,\text{o}} \big(c_{B,\mathbf{R},r_0} c_{B,\mathbf{R}-\mathbf{b},r_2} + c_{B,\mathbf{R},r_1} c_{B,\mathbf{R}-\mathbf{b},r_3} \big), \\
H_\kappa^{B,j-i,\text{even}} &= -i \sum_{\mathbf{R}} \kappa_{B,j-i,\text{e}} \big(c_{B,\mathbf{R},r_1} c_{B,\mathbf{R},r_2} + c_{B,\mathbf{R},r_3} c_{B,\mathbf{R}+\mathbf{b},r_0} \big), \\
H_\kappa^{B,j-i,\text{odd}} &= +i \sum_{\mathbf{R}} \kappa_{B,j-i,\text{o}} \big(c_{B,\mathbf{R},r_1} c_{B,\mathbf{R}+\mathbf{a}-\mathbf{b},r_2} + c_{B,\mathbf{R},r_3} c_{B,\mathbf{R}+\mathbf{a},r_0} \big).
\end{aligned}
$$

Summing all 12 blocks yields $H_\kappa = \sum_{S,d,p} H_\kappa^{S,d,p}$.

1.4 Bloch Hamiltonian $H(\mathbf{K})$ as an explicit 8×8 matrix

In the Bloch basis, the total Hamiltonian is

$$H(\mathbf{K}) = \begin{pmatrix} H_{AA} & H_{AB} \\ H_{AB}^{\dagger} & H_{BB} \end{pmatrix}, \qquad H_{ij}(\mathbf{K}) = H_{ji}(\mathbf{K})^*.$$

A–A block (kappa, ABA). Nonzero entries:

$$\begin{aligned}
&H_{AA}[0,1] = i\big(\kappa_{A,+i,\mathrm{e}} - \kappa_{A,+i,\mathrm{o}}\, e^{-2iK_i}\big)\,, \quad H_{AA}[2,3] = i\big(\kappa_{A,+i,\mathrm{e}} - \kappa_{A,+i,\mathrm{o}}\, e^{-2iK_i}\big)\,,\\
&H_{AA}[0,2] = i\big(-\kappa_{A,-j,\mathrm{e}} + \kappa_{A,-j,\mathrm{o}}\, e^{-2iK_j}\big)\,, \quad H_{AA}[1,3] = i\big(-\kappa_{A,-j,\mathrm{e}} + \kappa_{A,-j,\mathrm{o}}\, e^{-2iK_j}\big)\,,\\
&H_{AA}[1,2] = i\Big(\kappa_{A,j-i,\mathrm{e}} - \kappa_{A,j-i,\mathrm{o}}\, e^{+2i(K_i-K_j)}\Big)\,,\\
&H_{AA}[3,0] = i\big(\kappa_{A,j-i,\mathrm{e}}\, e^{+2iK_j} - \kappa_{A,j-i,\mathrm{o}}\, e^{+2iK_i}\big)\,,
\end{aligned}$$

with $H_{AA}[j,i] = H_{AA}[i,j]^*$ and all diagonal elements zero.

B–B block (kappa, BAB). Nonzero entries:

$$\begin{aligned}
&H_{BB}[0,1] = i\big(-\kappa_{B,+i,\mathrm{e}} + \kappa_{B,+i,\mathrm{o}}\, e^{-2iK_i}\big)\,, \quad H_{BB}[2,3] = i\big(-\kappa_{B,+i,\mathrm{e}} + \kappa_{B,+i,\mathrm{o}}\, e^{-2iK_i}\big)\,,\\
&H_{BB}[0,2] = i\big(\kappa_{B,-j,\mathrm{e}} - \kappa_{B,-j,\mathrm{o}}\, e^{-2iK_j}\big)\,, \quad H_{BB}[1,3] = i\big(\kappa_{B,-j,\mathrm{e}} - \kappa_{B,-j,\mathrm{o}}\, e^{-2iK_j}\big)\,,\\
&H_{BB}[1,2] = i\Big(-\kappa_{B,j-i,\mathrm{e}} + \kappa_{B,j-i,\mathrm{o}}\, e^{+2i(K_i-K_j)}\Big)\,,\\
&H_{BB}[3,0] = i\big(-\kappa_{B,j-i,\mathrm{e}}\, e^{+2iK_j} + \kappa_{B,j-i,\mathrm{o}}\, e^{+2iK_i}\big)\,,
\end{aligned}$$

with $H_{BB}[j,i] = H_{BB}[i,j]^*$ and zero diagonals.

A–B block (nearest-neighbor J). Nonzero entries $H_{AB}[\mathrm{A},\mathrm{B}]$:

$$\begin{aligned}
&J_x: \quad H_{AB}[0,0] = iJ_x,\;\; H_{AB}[1,1] = iJ_x,\;\; H_{AB}[2,2] = iJ_x,\;\; H_{AB}[3,3] = iJ_x,\\
&J_y: \quad H_{AB}[1,0] = iJ_y,\;\; H_{AB}[0,1] = iJ_y\, e^{+2iK_i},\;\; H_{AB}[3,2] = iJ_y,\;\; H_{AB}[2,3] = iJ_y\, e^{+2iK_i},\\
&J_z: \quad H_{AB}[2,0] = iJ_z,\;\; H_{AB}[0,2] = iJ_z\, e^{+2iK_j},\;\; H_{AB}[3,1] = iJ_z,\;\; H_{AB}[1,3] = iJ_z\, e^{+2iK_j}.
\end{aligned}$$

The lower-left block is $H_{BA} = H_{AB}^{\dagger}$.

1.5 Remarks

- Each of the 12 κ-blocks is a vertex-disjoint matching $\Rightarrow$ exact exponentiation per subset (no intra-block Trotter error).

- Summing even + odd for fixed (S, d) produces the expected sine structure factor along d; summing the three directions reproduces the usual real $\Delta(\mathbf{k})$ sitting with opposite signs on the A/B diagonals.

- Hermiticity is enforced everywhere by $H_{ij}(\mathbf{K}) = H_{ji}(\mathbf{K})^*$.