

Solid State Simulation Techniques.

Graphene Tight-Binding Homework.

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December 2025

The aim of this homework is to construct a p_Z tight-binding (TB) model for bulk graphene. We will use the simplest model, considering just one Slater-Koster type orbital for each of the two atoms in the graphene primitive cell.

1 Real-space Hamiltonian Construction

In this section, we construct the nearest-neighbor (1NN) Tight-Binding Hamiltonian for graphene. We begin by defining the lattice structure and basis, then explicitly identify the geometric relations between neighbors, and finally establish the rules for the matrix elements.

1.1 System Definition and Notation

We define the primitive lattice vectors for graphene as:

$$\mathbf{a}_1 = \frac{a}{2}(\hat{x} - \sqrt{3}\hat{y}), \quad (1)$$

$$\mathbf{a}_2 = \frac{a}{2}(\hat{x} + \sqrt{3}\hat{y}), \quad (2)$$

where a is the lattice constant. The unit cell contains two basis atoms, which we will refer to as A and B, with atom A fixed at the origin. Their positions within the unit cell are:

$$\mathbf{d}_A = 0, \quad (3)$$

$$\mathbf{d}_B = \frac{1}{3}(2\mathbf{a}_1 + \mathbf{a}_2) = \frac{a}{2}\left(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}\right). \quad (4)$$

The magnitude of \mathbf{d}_B corresponds to the carbon-carbon bond length, $a_{cc} = a/\sqrt{3}$.

To describe the electronic states, we use the basis $|\alpha, \mathbf{R}\rangle$, where $\alpha \in \{A, B\}$ denotes the sublattice and \mathbf{R} denotes the Bravais lattice vector of the unit cell. For example, $|A, 0\rangle$ represents atom A in the reference cell ($\mathbf{R} = 0$), while $|B, -\mathbf{a}_1\rangle$ refers to atom B in the unit cell shifted by $-\mathbf{a}_1$.

1.2 Nearest Neighbor Geometry

In the 1NN approximation, we consider only interactions between atoms separated by the bond length a_{cc} . Each atom A effectively "sees" three nearest B neighbors. To construct the Hamiltonian, we must identify the specific unit cell \mathbf{R} each neighbor belongs to and the explicit vector $\boldsymbol{\delta}$ connecting them.

As shown in Figure 1, fixing our reference at A_0 , we identify the three neighbors and calculate their relative position vectors $\boldsymbol{\delta}_i$ explicitly:

1. **Neighbor B_0 (Intra-cell):** The first neighbor is the B atom within the same unit cell ($\mathbf{R} = 0$). The bond vector is simply the position of B:

$$\boldsymbol{\delta}_1 = \mathbf{d}_B = \left(\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right). \quad (5)$$

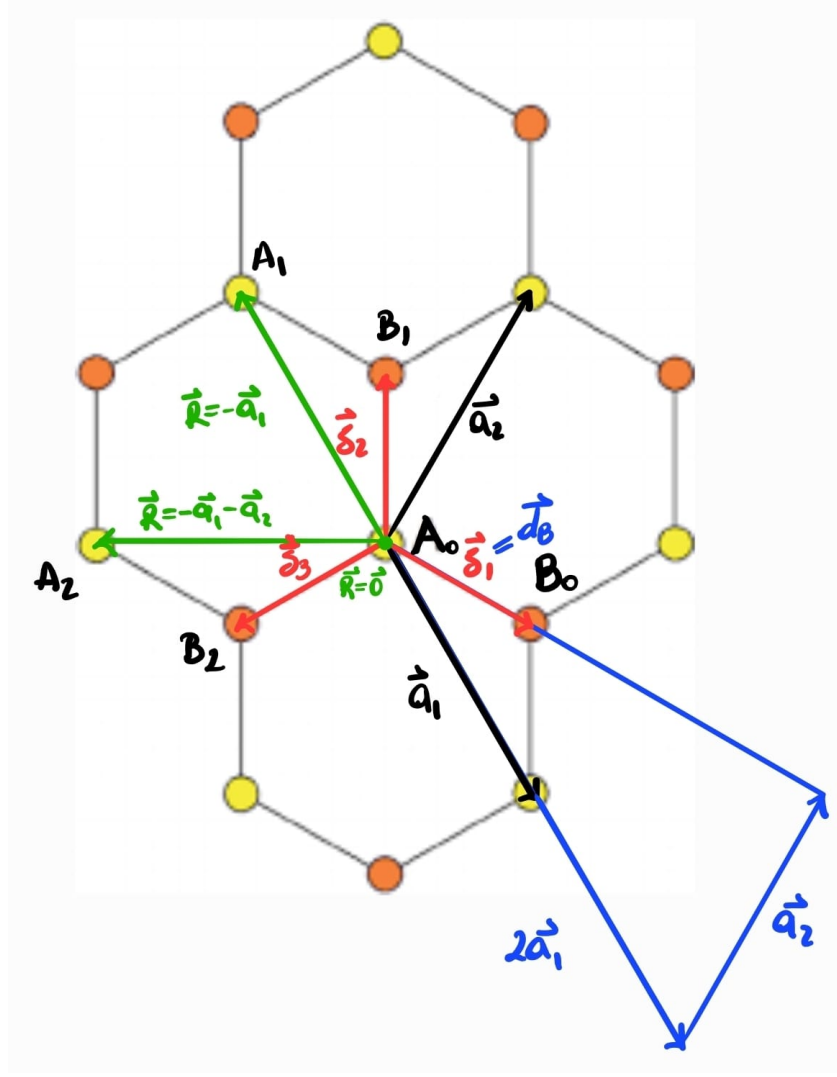


Figure 1: Lattice structure of graphene centered on atom A_0 . The three nearest neighbors (B_0, B_1, B_2) are connected by the bond vectors $\delta_{1,2,3}$ (red arrows). The green arrows indicate the lattice translation vectors \mathbf{R} required to reach the unit cell of each neighbor.

2. **Neighbor B_1 (Inter-cell 1):** The second neighbor lies in the unit cell shifted by $\mathbf{R} = -\mathbf{a}_1$. The bond vector is obtained by shifting the B position by this lattice vector:

$$\delta_2 = \mathbf{d}_B - \mathbf{a}_1 = \left(0, \frac{a}{\sqrt{3}}\right). \quad (6)$$

3. **Neighbor B_2 (Inter-cell 2):** The third neighbor lies in the unit cell shifted by $\mathbf{R} = -\mathbf{a}_1 - \mathbf{a}_2$. The explicit vector calculation yields:

$$\delta_3 = \mathbf{d}_B - \mathbf{a}_1 - \mathbf{a}_2 = \left(-\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right). \quad (7)$$

1.3 Hamiltonian Construction Rules

With the neighbors identified, we determine the Hamiltonian matrix elements based on the distance d between the orbitals. We decompose the Hamiltonian into 2×2 blocks $H_{0,\mathbf{R}}$ representing the coupling between the origin cell and a neighbor cell \mathbf{R} :

- If $d = 0$ (On-site): The energy (of diagonal elements) is E_z^0 .
- If $d = a_{cc}$ (Nearest Neighbor): The energy is the hopping parameter t . Based on our geometric analysis, this applies only to the interactions defined by δ_1 , δ_2 , and δ_3 .

- If $d > a_{cc}$: The interaction is effectively zero in the 1NN approximation.

This implies that the only non-zero off-diagonal blocks in our model will be $H_{0,0}$, $H_{0,-\mathbf{a}_1}$, and $H_{0,-\mathbf{a}_1-\mathbf{a}_2}$ (and their complex conjugates).

1.4 Calculation of Matrix Elements

Now we compute the interaction matrix elements between the orbitals in the reference unit cell ($\mathbf{R} = 0$) and those in a target unit cell \mathbf{R} . we do this by fixing the "Bra" (destination state) as atom A in the origin cell, denoted as $\langle A, 0 |$. We then systematically evaluate the distance to various "Ket" (source) atoms located in both the origin and neighboring cells. By applying the interaction rules defined previously, we identify which atomic pairs correspond to non-zero couplings (hopping parameters) or on-site energies.

We denote the Hamiltonian blocks as $H_{0,\mathbf{R}}$, and for each block, we evaluate four specific matrix elements:

1. $\langle A, 0 | H | A, \mathbf{R} \rangle$: Interaction between A and A.
2. $\langle A, 0 | H | B, \mathbf{R} \rangle$: Interaction between A and B.
3. $\langle B, 0 | H | A, \mathbf{R} \rangle$: Interaction between B and A.
4. $\langle B, 0 | H | B, \mathbf{R} \rangle$: Interaction between B and B.

Block 1: Intra-cell Coupling ($H_{0,0}$)

This block describes interactions where both atoms are located within the reference unit cell ($\mathbf{R} = 0$).

- **Element (1,1)** $\langle A, 0 | H | A, 0 \rangle$: The distance is $|\mathbf{d}_A - \mathbf{d}_A| = 0$. By definition, this is the on-site energy:

$$H_{AA} = E_z^0.$$

- **Element (1,2)** $\langle A, 0 | H | B, 0 \rangle$: The vector connecting these atoms is $\boldsymbol{\delta}_1 = \mathbf{d}_B - \mathbf{d}_A = \mathbf{d}_B$, so the distance is $|\mathbf{d}_B| = a_{cc}$. This corresponds to the first nearest neighbor (Neighbor B_0), and therefore:

$$H_{AB} = t.$$

- **Element (2,1)** $\langle B, 0 | H | A, 0 \rangle$: The vector is $\mathbf{d}_A - \mathbf{d}_B = -\boldsymbol{\delta}_1$, and the distance is a_{cc} , so:

$$H_{BA} = t^*.$$

(Note that since this is an intra-cell block, the matrix must be Hermitian, so $H_{BA} = H_{AB}^*$).

- **Element (2,2)** $\langle B, 0 | H | B, 0 \rangle$: The distance is 0. This is the on-site energy for atom B:

$$H_{BB} = E_z^0.$$

$$\boxed{H_{0,0} = \begin{pmatrix} E_z^0 & t \\ t^* & E_z^0 \end{pmatrix}}. \quad (8)$$

Block 2: Coupling to Cell $-\mathbf{a}_1$ ($H_{0,-\mathbf{a}_1}$)

We now evaluate the interactions between orbitals in the reference cell (0) and the cell shifted by $-\mathbf{a}_1$. Note that unlike the intra-cell block, this matrix is not required to be Hermitian, since it represents hopping in a specific direction.

- **Element (1,1)** $\langle A, 0 | H | A, -\mathbf{a}_1 \rangle$: The distance corresponds to the lattice vector magnitude $|\mathbf{a}_1| = a$. Since $a > a_{cc}$, there is no 1NN hopping between A atoms, and:

$$H_{AA} = 0.$$

- **Element (1,2)** $\langle A, 0 | H | B, -\mathbf{a}_1 \rangle$: The position of atom B in this cell is

$$\delta_2 = \mathbf{d}_B - \mathbf{a}_1 = \frac{2\mathbf{a}_1 + \mathbf{a}_2}{3} - \frac{3\mathbf{a}_1}{3} = \frac{\mathbf{a}_2 - \mathbf{a}_1}{3},$$

whose magnitude is $a/\sqrt{3} = a_{cc}$, corresponding to Neighbor B_1 . Therefore:

$$H_{AB} = t.$$

- **Element (2,1)** $\langle B, 0 | H | A, -\mathbf{a}_1 \rangle$: The distance between B at \mathbf{d}_B and A at $-\mathbf{a}_1$ is given by the magnitude of vector $-\mathbf{a}_1 - \mathbf{d}_B$, which can be checked that it is larger than a_{cc} (either by explicitly computing the magnitude, or visually in the lattice structure displayed in Figure 1). Therefore, in the 1NN approximation, we get:

$$H_{BA} = 0.$$

- **Element (2,2)** $\langle B, 0 | H | B, -\mathbf{a}_1 \rangle$: The distance is $|\mathbf{d}_B - (\mathbf{d}_B - \mathbf{a}_1)| = |\mathbf{a}_1| = a > a_{cc}$, which is too far for 1NN hopping:

$$H_{BB} = 0.$$

$$\boxed{H_{0,-\mathbf{a}_1} = \begin{pmatrix} 0 & t \\ 0 & 0 \end{pmatrix}}. \quad (9)$$

Block 3: Coupling to Cell $-\mathbf{a}_1 - \mathbf{a}_2$ ($H_{0,-\mathbf{a}_1 - \mathbf{a}_2}$)

We now evaluate the interactions with the cell shifted by $-\mathbf{a}_1 - \mathbf{a}_2$.

- **Element (1,1)** $\langle A, 0 | H | A, -\mathbf{a}_1 - \mathbf{a}_2 \rangle$: The distance is given by the magnitude of the vector connecting the NN unit cells: $|\mathbf{a}_1 + \mathbf{a}_2| = a > a_{cc}$, so:

$$H_{AA} = 0.$$

- **Element (1,2)** $\langle A, 0 | H | B, -\mathbf{a}_1 - \mathbf{a}_2 \rangle$: The vector connecting these two orbitals is

$$\delta_3 = \mathbf{d}_B - \mathbf{a}_1 - \mathbf{a}_2 = \frac{-\mathbf{a}_1 - 2\mathbf{a}_2}{3},$$

whose magnitude is $|\delta_3| = a_{cc}$. This corresponds to Neighbor B_2 , and therefore:

$$H_{AB} = t$$

- **Element (2,1)** $\langle B, 0 | H | A, -\mathbf{a}_1 - \mathbf{a}_2 \rangle$: Similar to Block 2, this vector points to a distant neighbor significantly farther than a_{cc} , so:

$$H_{BA} = 0.$$

- **Element (2,2)** $\langle B, 0 | H | B, -\mathbf{a}_1 - \mathbf{a}_2 \rangle$: The distance is $|\mathbf{a}_1 + \mathbf{a}_2| = a > a_{cc}$. Therefore:

$$H_{BB} = 0.$$

$$\boxed{H_{0,-\mathbf{a}_1 - \mathbf{a}_2} = \begin{pmatrix} 0 & t \\ 0 & 0 \end{pmatrix}}. \quad (10)$$

Other Blocks

So far, we have calculated the blocks where atom A acts as the "Receiver" (the Bra $\langle A, 0|$). However, the Hamiltonian must be Hermitian. Physically, this means that if an electron can hop from atom B in a neighbor cell to atom A in the origin, the reverse process must also be possible: an electron must be able to hop from atom A in a neighbor cell to atom B in the origin.

From the translational invariance of the crystal, we know that:

$$H_{0,\mathbf{R}} = H_{\mathbf{R},0} = (H_{0,-\mathbf{R}})^\dagger. \quad (11)$$

This relation implies that for every non-zero block $H_{0,-\mathbf{R}}$ we just calculated, there exists a corresponding block $H_{0,\mathbf{R}}$ describing the inverse process:

- **Block 4: Coupling to Cell $+\mathbf{a}_1$ (H_{0,\mathbf{a}_1})** This block represents the "inverse" of Block 2: if in Block 2, A(0) received an electron from B($-\mathbf{a}_1$), here in this block, B(0) must receive an electron from A($+\mathbf{a}_1$).

Using the property $H_{0,\mathbf{a}_1} = (H_{0,-\mathbf{a}_1})^\dagger$:

$$H_{0,\mathbf{a}_1} = \begin{pmatrix} 0 & t \\ 0 & 0 \end{pmatrix}^\dagger = \begin{pmatrix} 0 & 0 \\ t^* & 0 \end{pmatrix}. \quad (12)$$

- **Block 5: Coupling to Cell $+\mathbf{a}_1 + \mathbf{a}_2$ ($H_{0,\mathbf{a}_1+\mathbf{a}_2}$)** This block represents the "inverse" of Block 3, in which B(0) now interacts with A($+\mathbf{a}_1 + \mathbf{a}_2$).

Using the property $H_{0,\mathbf{a}_1+\mathbf{a}_2} = (H_{0,-\mathbf{a}_1-\mathbf{a}_2})^\dagger$:

$$H_{0,\mathbf{a}_1+\mathbf{a}_2} = \begin{pmatrix} 0 & t \\ 0 & 0 \end{pmatrix}^\dagger = \begin{pmatrix} 0 & 0 \\ t^* & 0 \end{pmatrix}. \quad (13)$$

Finally, in the 1NN approximation, the boxed block matrices are the only interactions that satisfy the bond length distance condition. Any other lattice vector \mathbf{R} (such as $-\mathbf{a}_2$, $2\mathbf{a}_1$, etc.) corresponds to atomic distances significantly larger than a_{cc} . Therefore, all other blocks $H_{0,\mathbf{R}}$ are strictly zero.

2 Bulk Hamiltonian in Reciprocal space

We now move to reciprocal space to construct the bulk Hamiltonian $H(\mathbf{k})$.

According to the Bloch theorem, the Hamiltonian can be written in the basis of Bloch sums constructed from the localized orbitals [1]:

$$|\phi_\alpha, \mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_m} e^{i\mathbf{k}\cdot\mathbf{R}_m} |\phi, \mathbf{R}_m\rangle. \quad (14)$$

It can be shown that the Hamiltonian matrix elements between any two Block sums is:

$$H(\mathbf{k}) = \langle \phi, \mathbf{k} | H | \psi, \mathbf{k} \rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \underbrace{\langle \phi, 0 | H | \psi, \mathbf{R} \rangle}_{H_{0,\mathbf{R}}} \quad (15)$$

where the summation runs over all lattice vectors \mathbf{R} for which the coupling is non-zero. From the previous section, we identified exactly five non-zero blocks:

1. $H_{0,0}$ (Intra-cell coupling)
2. $H_{0,-\mathbf{a}_1}$ and $H_{0,-\mathbf{a}_1-\mathbf{a}_2}$ (Coupling to neighbors where atom A receives)
3. H_{0,\mathbf{a}_1} and $H_{0,\mathbf{a}_1+\mathbf{a}_2}$ (Coupling to neighbors where atom B receives)

Substituting these into the sum, we get:

$$H(\mathbf{k}) = H_{0,0}e^{i\mathbf{k}\cdot\mathbf{0}} + H_{0,-\mathbf{a}_1}e^{-i\mathbf{k}\cdot\mathbf{a}_1} + H_{0,-\mathbf{a}_1-\mathbf{a}_2}e^{-i\mathbf{k}\cdot(\mathbf{a}_1+\mathbf{a}_2)} + \text{h.c. terms} \quad (16)$$

We now calculate the four components of the 2×2 matrix $H(\mathbf{k})$ explicitly:

Diagonal elements (H_{AA} and H_{BB})

- $H_{AA}(\mathbf{k})$: In order to compute it, we simply need to sum the (1,1) entry of every block and multiply it by the corresponding phase factor (which in this case is always equal to 1). The only non-zero element is in the intra-cell block $H_{0,0}$, so:

$$H_{AA}(\mathbf{k}) = E_z^0 \cdot e^{i\mathbf{k} \cdot \mathbf{0}} + 0 + \dots = E_z^0. \quad (17)$$

- $H_{BB}(\mathbf{k})$: Similarly, summing the (2,2) entry of every block we find that, again, only the block $H_{0,0}$ contributes. Therefore:

$$H_{BB}(\mathbf{k}) = E_z^0. \quad (18)$$

Off-Diagonal elements (H_{AB} and H_{BA})

- $H_{AB}(\mathbf{k})$: We now sum the non-zero (1,2) entry of every block and multiply then by the corresponding phase factor $e^{i\mathbf{k} \cdot \mathbf{R}}$:

$$\begin{aligned} H_{AB}(\mathbf{k}) &= e^{i\mathbf{k} \cdot \mathbf{0}} \underbrace{\langle A, 0 | H | B, 0 \rangle}_t + e^{i\mathbf{k} \cdot (-\mathbf{a}_1)} \underbrace{\langle A, 0 | H | B, -\mathbf{a}_1 \rangle}_t + e^{i\mathbf{k} \cdot (-\mathbf{a}_1 - \mathbf{a}_2)} \underbrace{\langle A, 0 | H | B, -\mathbf{a}_1 - \mathbf{a}_2 \rangle}_t \\ &= t \cdot 1 + t \cdot e^{-i\mathbf{k} \cdot \mathbf{a}_1} + t \cdot e^{-i\mathbf{k} \cdot (\mathbf{a}_1 + \mathbf{a}_2)} \\ &= t \left(1 + e^{-i\mathbf{k} \cdot \mathbf{a}_1} + e^{-i\mathbf{k} \cdot (\mathbf{a}_1 + \mathbf{a}_2)} \right) \\ &= t f(\mathbf{k}), \end{aligned} \quad (19)$$

where we have defined the so-called geometric structure factor $f(\mathbf{k})$ as:

$$f(\mathbf{k}) = 1 + e^{-i\mathbf{k} \cdot \mathbf{a}_1} + e^{-i\mathbf{k} \cdot (\mathbf{a}_1 + \mathbf{a}_2)}. \quad (20)$$

- $H_{BA}(\mathbf{k})$: For this element, we could compute it in a similar way as we did with $H_{AB}(\mathbf{k})$. However, it is much faster to notice that, since the Hamiltonian must be Hermitian, it satisfies $H_{BA}(\mathbf{k}) = (H_{AB}(\mathbf{k}))^*$. Therefore,

$$H_{BA}(\mathbf{k}) = t^* \left(1 + e^{i\mathbf{k} \cdot \mathbf{a}_1} + e^{i\mathbf{k} \cdot (\mathbf{a}_1 + \mathbf{a}_2)} \right) = t^* f^*(\mathbf{k}). \quad (21)$$

All things considered, the bulk Tight-Binding Hamiltonian for graphene is finally given by:

$$H(\mathbf{k}) = \begin{pmatrix} E_z^0 & t f(\mathbf{k}) \\ t^* f^*(\mathbf{k}) & E_z^0 \end{pmatrix} \quad (22)$$

The energy eigenvalues (band structure) are obtained by diagonalizing this matrix:

$$E(\mathbf{k}) = E_z^0 \pm |t| |f(\mathbf{k})| \quad (23)$$

Note that the term E_z^0 is usually set to zero.

3 Expansion of Bulk Hamiltonian around K point

We now study the behavior of the Hamiltonian near the Brillouin zone corners, the so-called K -points [2].

3.1 Gap Closing at the Dirac Point (\mathbf{K})

Let us verify first that the energy gap indeed closes at the K-point. The K-point is defined as:

$$\mathbf{K} = \frac{1}{3}(\mathbf{b}_1 + \mathbf{b}_2), \quad (24)$$

where \mathbf{b}_i are the reciprocal basis vectors. These vectors satisfy the relation $\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$. Then, at the K-point, the phases involved in the structure factor $f(\mathbf{k})$ are:

$$\mathbf{K} \cdot \mathbf{a}_1 = \frac{2\pi}{3}, \quad \mathbf{K} \cdot (\mathbf{a}_1 + \mathbf{a}_2) = \frac{4\pi}{3}.$$

Substituting these into the expression for the structure factor:

$$\begin{aligned} f(\mathbf{K}) &= 1 + e^{-i\frac{2\pi}{3}} + e^{-i\frac{4\pi}{3}} = 1 + \omega + \omega^2 \\ &= 1 + \left(-\frac{1}{2} - i\frac{\sqrt{3}}{2}\right) + \left(-\frac{1}{2} + i\frac{\sqrt{3}}{2}\right) = 0, \end{aligned} \quad (25)$$

where we have defined $\omega = e^{-i2\pi/3}$, and used the Euler's relations.

Since the energy eigenvalues are $E(\mathbf{K}) = \pm|t||f(\mathbf{K})|$ (after setting $E_z^0 = 0$), this implies $E(\mathbf{K}) = 0$, proving that the valence and conduction bands touch and the gap closes exactly at this point.

3.2 Taylor Expansion around \mathbf{K}

We now study the physics of small momenta \mathbf{q} around the K-point. We define $\mathbf{k} = \mathbf{K} + \mathbf{q}$, where $|\mathbf{q}| \ll |\mathbf{K}|$, and substitute it into the structure factor:

$$\begin{aligned} f(\mathbf{K} + \mathbf{q}) &\equiv f(\mathbf{q}) = 1 + e^{-i(\mathbf{K}+\mathbf{q})\cdot\mathbf{a}_1} + e^{-i(\mathbf{K}+\mathbf{q})\cdot(\mathbf{a}_1+\mathbf{a}_2)} \\ &= 1 + (e^{-i\mathbf{K}\cdot\mathbf{a}_1}) e^{-i\mathbf{q}\cdot\mathbf{a}_1} + (e^{-i\mathbf{K}\cdot(\mathbf{a}_1+\mathbf{a}_2)}) e^{-i\mathbf{q}\cdot(\mathbf{a}_1+\mathbf{a}_2)}. \end{aligned}$$

Using the definition $\omega = e^{-i2\pi/3}$, and the Taylor expansion $e^{-ix} \approx 1 - ix$, we arrive to

$$\begin{aligned} f(\mathbf{q}) &\approx 1 + \omega(1 - i\mathbf{q} \cdot \mathbf{a}_1) + \omega^2(1 - i\mathbf{q} \cdot (\mathbf{a}_1 + \mathbf{a}_2)) \\ &= \underbrace{(1 + \omega + \omega^2)}_{=0} - i[\omega(\mathbf{q} \cdot \mathbf{a}_1) + \omega^2(\mathbf{q} \cdot (\mathbf{a}_1 + \mathbf{a}_2))]. \end{aligned}$$

Explicitly calculating the remaining term using the lattice vectors $\mathbf{a}_1 = (\frac{a}{2}, -\frac{a\sqrt{3}}{2})$ and $\mathbf{a}_1 + \mathbf{a}_2 = (a, 0)$, we get:

$$\begin{aligned} f(\mathbf{q}) &\approx -i \left[\left(-\frac{1}{2} - i\frac{\sqrt{3}}{2}\right) \left(\frac{a}{2}q_x - \frac{a\sqrt{3}}{2}q_y\right) + \left(-\frac{1}{2} + i\frac{\sqrt{3}}{2}\right) (aq_x) \right] = \dots \\ &= -i \left[\left(-\frac{3a}{4}q_x + \frac{a\sqrt{3}}{4}q_y\right) + i \left(\frac{a\sqrt{3}}{4}q_x + \frac{3a}{4}q_y\right) \right] = \dots \\ &= \underbrace{\frac{3a}{4} \left[\frac{1}{\sqrt{3}} + i\right]}_{C_x} q_x + \underbrace{\frac{3a}{4} \left[1 - \frac{i}{\sqrt{3}}\right]}_{C_y} q_y. \end{aligned}$$

Noticing that $C_y = -iC_x$:

$$f(\mathbf{q}) \approx C_x(q_x - iq_y).$$

Taking the absolute value of this function and using $|C_x| = \frac{\sqrt{3}}{2}a$, we get:

$$|f(\mathbf{q})| = \frac{\sqrt{3}a}{2}|\mathbf{q}| \quad (26)$$

Therefore, the energy dispersion near the Dirac point in our Tight-Binding model is:

$$E_{TB}(\mathbf{q}) = \pm |t| |f(\mathbf{q})| = \pm |t| \frac{\sqrt{3}a}{2} |\mathbf{q}|. \quad (27)$$

Comparing this to the standard continuum Dirac dispersion relation for massless fermions, defined by the Fermi velocity v_F [2]:

$$E_{Dirac}(\mathbf{q}) = \pm \hbar v_F |\mathbf{q}|, \quad (28)$$

it is straightforward to arrive to:

$$\boxed{v_F = \frac{\sqrt{3}a|t|}{2\hbar} = \frac{3a_{cc}|t|}{2\hbar}}. \quad (29)$$

References

- [1] Neil W. Ashcroft and N. David Mermin. *Solid State Physics*. Holt, Rinehart and Winston, New York, 1976.
- [2] M. I. Katsnelson. *The Physics of Graphene*. Cambridge Univ. Press, Cambridge, 2020.