Tight-Binding Model for Graphene

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1 Introduction

The unit cell of graphene’s lattice consists of two different types of sites, which we will call $A$ sites and $B$ sites (see Fig. 1).

![Figure 1: Honeycomb lattice and its Brillouin zone. Left: lattice structure of graphene, made out of two interpenetrating triangular lattices $a_1$ and $a_2$ are the lattice unit vectors, and $\delta_i$, $i = 1, 2, 3$ are the nearest-neighbor vectors. Right: corresponding Brillouin zone. The Dirac cones are located at the $K$ and $K'$ points.]

Note: This figure and caption are from Castro et al. [2].

These vectors are given by

\[
\begin{align*}
    a_1 &= \frac{a}{2} (3, \sqrt{3}) \\
    a_2 &= \frac{a}{2} (3, -\sqrt{3}) \\
    \delta_1 &= \frac{a}{2} (1, \sqrt{3}) \\
    \delta_2 &= \frac{a}{2} (1, -\sqrt{3}) \\
    \delta_3 &= -a (1, 0) \\
    K &= \frac{2\pi}{3\sqrt{3}a} (\sqrt{3}, 1) \\
    K' &= \frac{2\pi}{3\sqrt{3}a} (\sqrt{3}, -1),
\end{align*}
\]

where $K, K'$ are the corners of graphene’s first Brillouin zone, or Dirac points.

2 Tight-binding Hamiltonian

Considering only nearest-neighbor hopping, the tight-binding Hamiltonian for graphene is

\[
\hat{H} = -t \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i),
\]
where \( i \) (\( j \)) labels sites in sublattice \( A \) (\( B \)), the fermionic operator \( \hat{a}_i^\dagger (\hat{a}_i) \) creates (annihilates) an electron at the \( A \) site whose position is \( \mathbf{r}_i \), and similarly for \( \hat{b}_j^\dagger, \hat{b}_j \). We can rewrite the sum over nearest neighbors as

\[
\sum_{(ij)} (\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i) = \sum_{i \in A} \sum_{\delta} (\hat{a}_i^\dagger \hat{b}_{i+\delta} + \hat{b}_{i+\delta}^\dagger \hat{a}_i),
\]

where the sum over \( \delta \) is carried out over the nearest-neighbor vectors \( \delta_1, \delta_2, \) and \( \delta_3 \), and the operator \( \hat{b}_{i+\delta} \) annihilates a fermion at the \( B \) site whose position is \( \mathbf{r}_i + \delta \). Using

\[
\hat{a}_i^\dagger = \frac{1}{\sqrt{N/2}} \sum_{k} e^{i\mathbf{k} \cdot \mathbf{r}_i} \hat{a}_k^\dagger,
\]

where \( N/2 \) is the number of \( A \) sites, and similarly for \( \hat{b}_i^\dagger \), we can write the tight-binding Hamiltonian for graphene (Eq. 2) as

\[
\hat{H} = -\frac{t}{N/2} \sum_{i \in A} \sum_{\delta,k,k'} [e^{i(k-k') \cdot \mathbf{r}_i} e^{-i\mathbf{k'} \cdot \delta} \hat{a}_k^\dagger \hat{b}_{k'} + \text{H.c.}]
\]

\[
= -t \sum_{\delta,k} (e^{-i\mathbf{k} \cdot \delta} \hat{a}_k^\dagger \hat{b}_k + \text{H.c.})
\]

\[
= -t \sum_{\delta,k} (e^{-i\mathbf{k} \cdot \delta} \hat{a}_k^\dagger \hat{b}_k + e^{i\mathbf{k} \cdot \delta} \hat{b}_k^\dagger \hat{a}_k),
\]

where in the second line we have used

\[
\sum_{i \in A} e^{i(k-k') \cdot \mathbf{r}_i} = \frac{N}{2} \delta_{kk'}.
\]

We can therefore express the Hamiltonian as

\[
\hat{H} = \sum_{\mathbf{k}} \Psi^\dagger \mathbf{h}(\mathbf{k}) \Psi,
\]

where

\[
\Psi \equiv \begin{pmatrix} \hat{a}_k \\ \hat{b}_k \end{pmatrix}, \quad \Psi^\dagger = \begin{pmatrix} \hat{a}_k^\dagger & \hat{b}_k^\dagger \end{pmatrix},
\]

and

\[
\mathbf{h}(\mathbf{k}) \equiv -t \begin{pmatrix} 0 & \Delta_k \\ \Delta_k^* & 0 \end{pmatrix}
\]

is the matrix representation of the Hamiltonian and

\[
\Delta_k \equiv \sum_{\delta} e^{i\mathbf{k} \cdot \delta}.
\]
2.1 Energy bands

The eigenvalues of this matrix are $E_\pm = \pm t \sqrt{\Delta_k \Delta_k^*}$. We can compute this by writing $\Delta_k$ out more explicitly:

$$\Delta_k = e^{ik\cdot\delta_1} + e^{ik\cdot\delta_2} + e^{ik\cdot\delta_3}$$

$$= e^{ik\cdot\delta_1}[1 + e^{ik\cdot(\delta_2-\delta_3)}]$$

$$= e^{-ikx_0} \left[ 1 + e^{i3k_xa/2}e^{i\sqrt{3}k_ya/2} + e^{i3k_xa/2}e^{-i\sqrt{3}k_ya/2} \right]$$

$$= e^{-ikx_0} \left[ 1 + e^{i3k_xa/2}(e^{i\sqrt{3}k_ya/2} + e^{-i\sqrt{3}k_ya/2}) \right]$$

$$= e^{-ikx_0} \left[ 1 + 2e^{i3k_xa/2} \cos \left( \frac{\sqrt{3}}{2}k_ya \right) \right]. \quad (11)$$

The energy bands are therefore given by

$$E_\pm(k) = \pm t \sqrt{1 + 4 \cos \left( \frac{3}{2}k_xa \right) \cos \left( \frac{\sqrt{3}}{2}k_ya \right) + 4 \cos^2 \left( \frac{\sqrt{3}}{2}k_ya \right)}, \quad (12)$$

or, as it is sometimes written,

$$E_\pm(k) = \pm t \sqrt{3 + f(k)}, \quad (13)$$

where

$$f(k) = 2 \cos(\sqrt{3}k_ya) + 4 \cos \left( \frac{3}{2}k_xa \right) \cos \left( \frac{\sqrt{3}}{2}k_ya \right). \quad (14)$$

These are two gapless bands that touch at the Dirac points $K$ and $K'$ (see Fig. 2). In other words, the Dirac points are the points in $k$-space for which $E_\pm(k) = 0$.

![Figure 2: Energy bands for graphene from nearest-neighbor interactions. The bands meet at the Dirac points, at which the energy is zero.](image-url)

2.2 Hamiltonian in terms of Pauli matrices

We can express the Hamiltonian

$$h(k) = -t \begin{pmatrix} 0 & \Delta_k \\ \Delta_k^* & 0 \end{pmatrix} \quad (15)$$
in terms of Pauli matrices by expressing $\Delta_k$ as
\[
\Delta_k = \sum_{\delta} e^{i k \cdot \delta} = \sum_{\delta} \left[ \cos(k \cdot \delta) + i \sin(k \cdot \delta) \right],
\]
so the Hamiltonian reads
\[
h(k) = -t \sum_{\delta} \begin{pmatrix} 0 & \cos(k \cdot \delta) + i \sin(k \cdot \delta) \\ \cos(k \cdot \delta) - i \sin(k \cdot \delta) & 0 \end{pmatrix}.
\]
In terms of Pauli matrices, the Hamiltonian is then
\[
h(k) = -t \sum_{\delta} [\cos(k \cdot \delta) \sigma_x - \sin(k \cdot \delta) \sigma_y].
\]

2.3 $\sigma_z$ term

Writing the Hamiltonian in the form
\[
h(k) = -t \sum_{\delta} [\cos(k \cdot \delta) \sigma_x - \sin(k \cdot \delta) \sigma_y]
\]
it is natural to ask whether we can have also have a $\sigma_z$ term. Let’s see what happens when we do:
\[
h_M(k, M) = -t \sum_{\delta} [\cos(k \cdot \delta) \sigma_x - \sin(k \cdot \delta) \sigma_y + M \sigma_z]
\]
\[
= -t \sum_{\delta} \begin{pmatrix} M & \cos(k \cdot \delta) + i \sin(k \cdot \delta) \\ \cos(k \cdot \delta) - i \sin(k \cdot \delta) & -M \end{pmatrix}.
\]
From the matrix form of the Hamiltonian we can see that this additional $\sigma_z$ term raises the energy of $A$ sites and lowers the energy of $B$ sites, thereby gapping the bands. We can think of this as being caused by on-site potential terms of the form
\[
\hat{H}_{\text{potential}} = M \left( \sum_{\{A \text{ sites}\}} \hat{n}_{a,\alpha} - \sum_{\{B \text{ sites}\}} \hat{n}_{b,\beta} \right),
\]
where $\hat{n}_{a,\alpha} = \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha}$ and $\hat{n}_{b,\beta} = \hat{b}_{\beta}^{\dagger} \hat{b}_{\beta}$. This could arise when there are two different types of atoms on the $A$ and $B$ sites, such as in boron nitride, which has the same lattice structure as graphene, but whose $A$ and $B$ sites correspond to boron atoms and nitrogen atoms.
3 Behavior near the Dirac points

3.1 Near K

Let’s look at the behavior of \( \Delta_k \) about the Dirac point \( K \). Defining the relative momentum \( q \equiv k - K \), we can write \( \Delta_k \) in terms of \( q \) as

\[
\Delta_{K+q} = e^{-iK_x a} e^{-iK_y a} \left[ 1 + 2e^{i3(K_x + q_x)a/2} \cos\left(\frac{\sqrt{3}(K_y + q_y)a}{2}\right) \right]
\]

\[
= e^{-iK_x a} e^{-iK_y a} \left[ 1 - 2e^{3iaq_x/2} \cos\left(\frac{\pi}{3} + \frac{\sqrt{3}a}{2}q_y\right) \right].
\]

(22)

Now, expanding this about \( q = 0 \) to first order, we have

\[
\Delta_{K+q} = -ie^{-iK_x a} \frac{3a}{2}(q_x + iq_y).
\]

(23)

The phase of \( \Delta_{K+q} \) carries no physical significance (since, for example, the energy bands are given by \( E_{\pm}(K + q) = \pm t\sqrt{\Delta_{K+q}\Delta_{K+q}^*} \)), so it is convenient to ignore the phase of \( ie^{-iK_x a} \). We thus have

\[
\Delta_{K+q} = -\frac{3a}{2}(q_x + iq_y).
\]

(24)

About the Dirac point \( K \), the Hamiltonian is thus

\[
h(K + q) = v_F \begin{pmatrix} 0 & q_x + iq_y \\ q_x - iq_y & 0 \end{pmatrix},
\]

(25)

where

\[
v_F = \frac{3at}{2}
\]

(26)

is the Fermi velocity. We can express this in terms of Pauli matrices as

\[
h(K + q) = v_F (q_x \sigma_x - q_y \sigma_y),
\]

(27)

or, defining the vector

\[
\bar{q} \equiv \begin{pmatrix} q_x \\ -q_y \end{pmatrix},
\]

(28)

we can express \( h(K + q) \) more naturally as

\[
h(K + q) = v_F \bar{q} \cdot \sigma.
\]

(29)

3.2 Near \( K' \)

Similarly, defining the relative momentum \( q \equiv k - K' \) and expanding \( \Delta_k \) about the Dirac point \( K' \), we find

\[
\Delta_{K'+q} = -\frac{3a}{2}(q_x - iq_y),
\]

(30)
so the Hamiltonian about this Dirac point is

\[ h(K' + q) = v_F \begin{pmatrix} 0 & q_x - i q_y \\ q_x + i q_y & 0 \end{pmatrix} = v_F (q_x \sigma_x + q_y \sigma_y) = v_F \mathbf{q} \cdot \mathbf{\sigma}. \]  (31)

### 3.3 Linear dispersion relation

From the matrix form of the Hamiltonian near the Dirac points (Eqs. 25, 31) we find that the energy bands near the Dirac points are given by

\[ E_{\pm}(q) = v_F |q|. \]  (32)

Near a Dirac point, the dispersion relation is therefore linear in momentum, so the energy bands form cone (called a Dirac cone; see Fig. 3) with the vertex lying on the Dirac point.

**Figure 3:** Conical behavior of the bands near a Dirac point, known as a Dirac cone, where the energy is linear in momentum.

### 3.4 \( \sigma_z \) term gapping

If we add the \( \sigma_z \) term that we introduced in Section 2.3, the Hamiltonian near the Dirac points will be of the form

\[ h_M = v_F (q_x \sigma_x + q_y \sigma_y + M \sigma_z) = v_F \begin{pmatrix} M & q_x - i q_y \\ q_x + i q_y & -M \end{pmatrix}. \]  (33)

As we saw, this additional term gaps the energies, so that near the Dirac points, the energies become

\[ E_{M,\pm} = \pm \sqrt{q_x^2 + q_y^2 + M^2}, \]  (34)

See Fig. 4 for a plot of the band gap near a Dirac point.
Figure 4: Energy gap near a Dirac point produced by a $\sigma_z$ term. Compare to Fig. 3.

References
