

# Tight-Binding Model for Graphene

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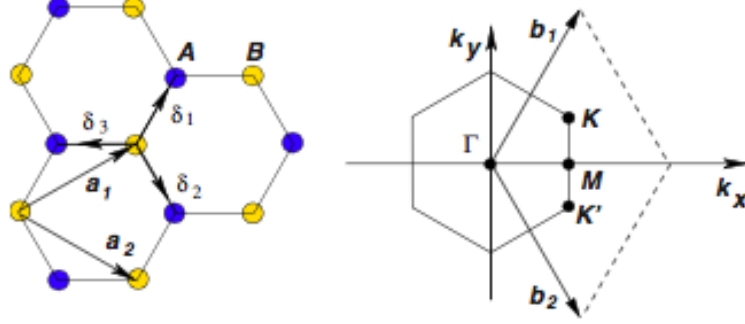
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## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Tight-binding Hamiltonian</b>	<b>2</b>
2.1	Energy bands . . . . .	4
2.2	Hamiltonian in terms of Pauli matrices . . . . .	4
2.3	$\sigma_z$ term . . . . .	5
<b>3</b>	<b>Behavior near the Dirac points</b>	<b>6</b>
3.1	Near $\mathbf{K}$ . . . . .	6
3.2	Near $\mathbf{K}'$ . . . . .	6
3.3	Linear dispersion relation . . . . .	7
3.4	$\sigma_z$ term gapping . . . . .	7

# 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  $\mathbf{a}_1$  and  $\mathbf{a}_2$  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  $\mathbf{K}$  and  $\mathbf{K}'$  points.

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

These vectors are given by

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{a}{2}(3, \sqrt{3}) \\
 \mathbf{a}_2 &= \frac{a}{2}(3, -\sqrt{3}) \\
 \delta_1 &= \frac{a}{2}(1, \sqrt{3}) \\
 \delta_2 &= \frac{a}{2}(1, -\sqrt{3}) \\
 \delta_3 &= -a(1, 0) \\
 \mathbf{K} &= \frac{2\pi}{3\sqrt{3}a}(\sqrt{3}, 1) \\
 \mathbf{K}' &= \frac{2\pi}{3\sqrt{3}a}(\sqrt{3}, -1),
 \end{aligned} \tag{1}$$

where  $\mathbf{K}, \mathbf{K}'$  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

$$\hat{H} = -t \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i), \tag{2}$$

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

$$\sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i) = \sum_{i \in A} \sum_{\boldsymbol{\delta}} (\hat{a}_i^\dagger \hat{b}_{i+\boldsymbol{\delta}} + \hat{b}_{i+\boldsymbol{\delta}}^\dagger \hat{a}_i), \quad (3)$$

where the sum over  $\boldsymbol{\delta}$  is carried out over the nearest-neighbor vectors  $\boldsymbol{\delta}_1, \boldsymbol{\delta}_2$ , and  $\boldsymbol{\delta}_3$ , and the operator  $\hat{b}_{i+\boldsymbol{\delta}}$  annihilates a fermion at the  $B$  site whose position is  $\mathbf{r}_i + \boldsymbol{\delta}$ . Using

$$\hat{a}_i^\dagger = \frac{1}{\sqrt{N/2}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} \hat{a}_{\mathbf{k}}^\dagger, \quad (4)$$

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

$$\begin{aligned} \hat{H} &= -\frac{t}{N/2} \sum_{i \in A} \sum_{\boldsymbol{\delta}, \mathbf{k}, \mathbf{k}'} [e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_i} e^{-i\mathbf{k}' \cdot \boldsymbol{\delta}} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'} + \text{H.c.}] \\ &= -t \sum_{\boldsymbol{\delta}, \mathbf{k}} (e^{-i\mathbf{k} \cdot \boldsymbol{\delta}} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} + \text{H.c.}) \\ &= -t \sum_{\boldsymbol{\delta}, \mathbf{k}} (e^{-i\mathbf{k} \cdot \boldsymbol{\delta}} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} + e^{i\mathbf{k} \cdot \boldsymbol{\delta}} \hat{b}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}), \end{aligned} \quad (5)$$

where in the second line we have used

$$\sum_{i \in A} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_i} = \frac{N}{2} \delta_{\mathbf{k}\mathbf{k}'}. \quad (6)$$

We can therefore express the Hamiltonian as

$$\hat{H} = \sum_{\mathbf{k}} \boldsymbol{\Psi}^\dagger \mathbf{h}(\mathbf{k}) \boldsymbol{\Psi}, \quad (7)$$

where

$$\boldsymbol{\Psi} \equiv \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{b}_{\mathbf{k}} \end{pmatrix}, \quad \boldsymbol{\Psi}^\dagger = (\hat{a}_{\mathbf{k}}^\dagger \quad \hat{b}_{\mathbf{k}}^\dagger), \quad (8)$$

and

$$\mathbf{h}(\mathbf{k}) \equiv -t \begin{pmatrix} 0 & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & 0 \end{pmatrix} \quad (9)$$

is the matrix representation of the Hamiltonian and

$$\Delta_{\mathbf{k}} \equiv \sum_{\boldsymbol{\delta}} e^{i\mathbf{k} \cdot \boldsymbol{\delta}}. \quad (10)$$

## 2.1 Energy bands

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

$$\begin{aligned}
 \Delta_{\mathbf{k}} &= e^{i\mathbf{k} \cdot \boldsymbol{\delta}_1} + e^{i\mathbf{k} \cdot \boldsymbol{\delta}_2} + e^{i\mathbf{k} \cdot \boldsymbol{\delta}_3} \\
 &= e^{i\mathbf{k} \cdot \boldsymbol{\delta}_3} [1 + e^{i\mathbf{k} \cdot (\boldsymbol{\delta}_1 - \boldsymbol{\delta}_3)} + e^{i\mathbf{k} \cdot (\boldsymbol{\delta}_2 - \boldsymbol{\delta}_3)}] \\
 &= e^{-ik_x a} \left[ 1 + e^{i3k_x a/2} e^{i\sqrt{3}k_y a/2} + e^{i3k_x a/2} e^{-i\sqrt{3}k_y a/2} \right] \\
 &= e^{-ik_x a} \left[ 1 + e^{i3k_x a/2} (e^{i\sqrt{3}k_y a/2} + e^{-i\sqrt{3}k_y a/2}) \right] \\
 &= e^{-ik_x a} \left[ 1 + 2e^{i3k_x a/2} \cos\left(\frac{\sqrt{3}}{2}k_y a\right) \right].
 \end{aligned} \tag{11}$$

The energy bands are therefore given by

$$E_{\pm}(\mathbf{k}) = \pm t \sqrt{1 + 4 \cos\left(\frac{3}{2}k_x a\right) \cos\left(\frac{\sqrt{3}}{2}k_y a\right) + 4 \cos^2\left(\frac{\sqrt{3}}{2}k_y a\right)}, \tag{12}$$

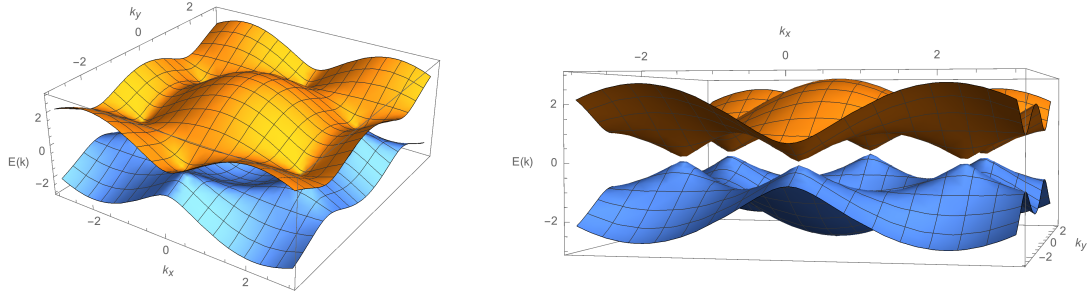
or, as it is sometimes written,

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

where

$$f(\mathbf{k}) = 2 \cos(\sqrt{3}k_y a) + 4 \cos\left(\frac{3}{2}k_x a\right) \cos\left(\frac{\sqrt{3}}{2}k_y a\right). \tag{14}$$

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



**Figure 2:** Energy bands for graphene from nearest-neighbor interactions. The bands meet at the Dirac points, at which the energy is zero.

## 2.2 Hamiltonian in terms of Pauli matrices

We can express the Hamiltonian

$$\mathbf{h}(\mathbf{k}) = -t \begin{pmatrix} 0 & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & 0 \end{pmatrix} \tag{15}$$

in terms of Pauli matrices by expressing  $\Delta_{\mathbf{k}}$  as

$$\Delta_{\mathbf{k}} = \sum_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}} = \sum_{\boldsymbol{\delta}} [\cos(\mathbf{k}\cdot\boldsymbol{\delta}) + i \sin(\mathbf{k}\cdot\boldsymbol{\delta})], \quad (16)$$

so the Hamiltonian reads

$$\mathbf{h}(\mathbf{k}) = -t \sum_{\boldsymbol{\delta}} \begin{pmatrix} 0 & \cos(\mathbf{k}\cdot\boldsymbol{\delta}) + i \sin(\mathbf{k}\cdot\boldsymbol{\delta}) \\ \cos(\mathbf{k}\cdot\boldsymbol{\delta}) - i \sin(\mathbf{k}\cdot\boldsymbol{\delta}) & 0 \end{pmatrix}. \quad (17)$$

In terms of Pauli matrices, the Hamiltonian is then

$$\mathbf{h}(\mathbf{k}) = -t \sum_{\boldsymbol{\delta}} [\cos(\mathbf{k}\cdot\boldsymbol{\delta})\sigma_x - \sin(\mathbf{k}\cdot\boldsymbol{\delta})\sigma_y]. \quad (18)$$

### 2.3 $\sigma_z$ term

Writing the Hamiltonian in the form

$$\mathbf{h}(\mathbf{k}) = -t \sum_{\boldsymbol{\delta}} [\cos(\mathbf{k}\cdot\boldsymbol{\delta})\sigma_x - \sin(\mathbf{k}\cdot\boldsymbol{\delta})\sigma_y] \quad (19)$$

it is natural to ask whether we can have also have a  $\sigma_z$  term. Let's see what happens when we do:

$$\begin{aligned} \mathbf{h}_M(\mathbf{k}, M) &= -t \sum_{\boldsymbol{\delta}} [\cos(\mathbf{k}\cdot\boldsymbol{\delta})\sigma_x - \sin(\mathbf{k}\cdot\boldsymbol{\delta})\sigma_y + M\sigma_z] \\ &= -t \sum_{\boldsymbol{\delta}} \begin{pmatrix} M & \cos(\mathbf{k}\cdot\boldsymbol{\delta}) + i \sin(\mathbf{k}\cdot\boldsymbol{\delta}) \\ \cos(\mathbf{k}\cdot\boldsymbol{\delta}) - i \sin(\mathbf{k}\cdot\boldsymbol{\delta}) & -M \end{pmatrix}. \end{aligned} \quad (20)$$

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

$$\hat{H}_{\text{potential}} = M \left( \sum_{\substack{\alpha \\ \{A \text{ sites}\}}} \hat{n}_{a,\alpha} - \sum_{\substack{\beta \\ \{B \text{ sites}\}}} \hat{n}_{b,\beta} \right), \quad (21)$$

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 $\mathbf{K}$

Let's look at the behavior of  $\Delta_{\mathbf{k}}$  about the Dirac point  $\mathbf{K}$ . Defining the relative momentum  $\mathbf{q} \equiv \mathbf{k} - \mathbf{K}$ , we can write  $\Delta_{\mathbf{k}}$  in terms of  $\mathbf{q}$  as

$$\begin{aligned}\Delta_{\mathbf{K}+\mathbf{q}} &= e^{-iK_x a} e^{-iq_x a} \left[ 1 + 2e^{i3(K_x+q_x)a/2} \cos\left(\frac{\sqrt{3}(K_y+q_y)a}{2}\right) \right] \\ &= e^{-iK_x a} e^{-iq_x a} \left[ 1 - 2e^{3iaq_x/2} \cos\left(\frac{\pi}{3} + \frac{\sqrt{3}a}{2}q_y\right) \right].\end{aligned}\quad (22)$$

Now, expanding this about  $\mathbf{q} = \mathbf{0}$  to first order, we have

$$\Delta_{\mathbf{K}+\mathbf{q}} = -ie^{-iK_x a} \frac{3a}{2} (q_x + iq_y). \quad (23)$$

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

$$\Delta_{\mathbf{K}+\mathbf{q}} = -\frac{3a}{2} (q_x + iq_y). \quad (24)$$

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

$$\mathbf{h}(\mathbf{K} + \mathbf{q}) = v_F \begin{pmatrix} 0 & q_x + iq_y \\ q_x - iq_y & 0 \end{pmatrix}, \quad (25)$$

where

$$v_F = \frac{3at}{2} \quad (26)$$

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

$$\mathbf{h}(\mathbf{K} + \mathbf{q}) = v_F (q_x \sigma_x - q_y \sigma_y), \quad (27)$$

or, defining the vector

$$\bar{\mathbf{q}} \equiv \begin{pmatrix} q_x \\ -q_y \end{pmatrix}, \quad (28)$$

we can express  $\mathbf{h}(\mathbf{K} + \mathbf{q})$  more naturally as

$$\mathbf{h}(\mathbf{K} + \mathbf{q}) = v_F \bar{\mathbf{q}} \cdot \boldsymbol{\sigma}. \quad (29)$$

#### 3.2 Near $\mathbf{K}'$

Similarly, defining the relative momentum  $\mathbf{q} \equiv \mathbf{k} - \mathbf{K}'$  and expanding  $\Delta_{\mathbf{k}}$  about the Dirac point  $\mathbf{K}'$ , we find

$$\Delta_{\mathbf{K}'+\mathbf{q}} = -\frac{3a}{2} (q_x - iq_y), \quad (30)$$

so the Hamiltonian about this Dirac point is

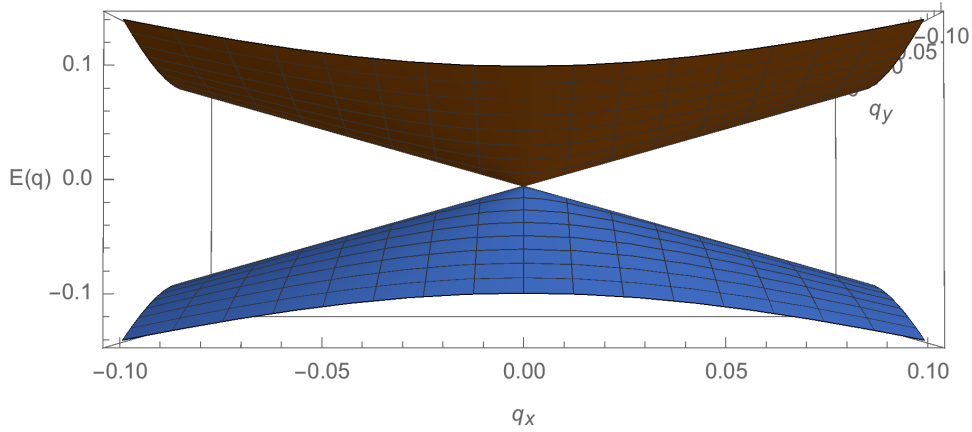
$$\mathbf{h}(\mathbf{K}' + \mathbf{q}) = v_F \begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix} = v_F(q_x\sigma_x + q_y\sigma_y) = v_F \mathbf{q} \cdot \boldsymbol{\sigma}. \quad (31)$$

### 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

$$E_{\pm}(\mathbf{q}) = v_F |\mathbf{q}|. \quad (32)$$

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

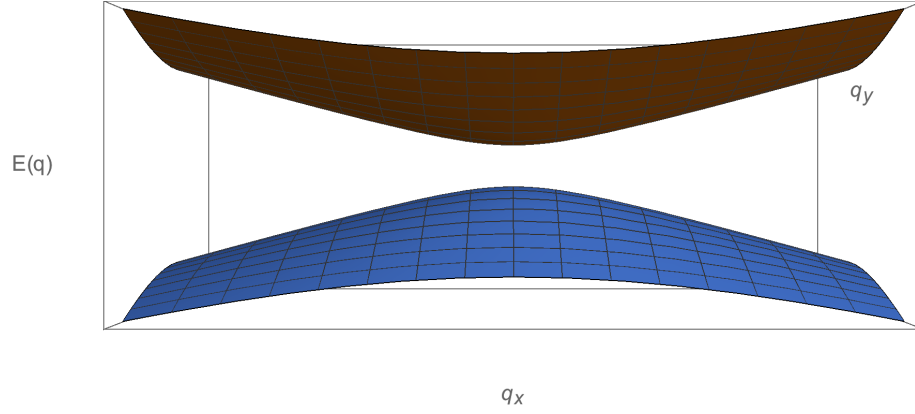
If we add the  $\sigma_z$  term that we introduced in Section 2.3, the Hamiltonian near the Dirac points will be of the form

$$\mathbf{h}_M = v_F(q_x\sigma_x + q_y\sigma_y + M\sigma_z) = v_F \begin{pmatrix} M & q_x - iq_y \\ q_x + iq_y & -M \end{pmatrix}. \quad (33)$$

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

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

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

- [1] Anthony J. Leggett. Lecture 5: Graphene: Electronic band structure and Dirac fermions. <http://web.physics.ucsb.edu/~phys123B/w2015/leggett-lecture.pdf>, 2010.
- [2] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim. The electronic properties of graphene. <https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.81.109>, 2009.