

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).

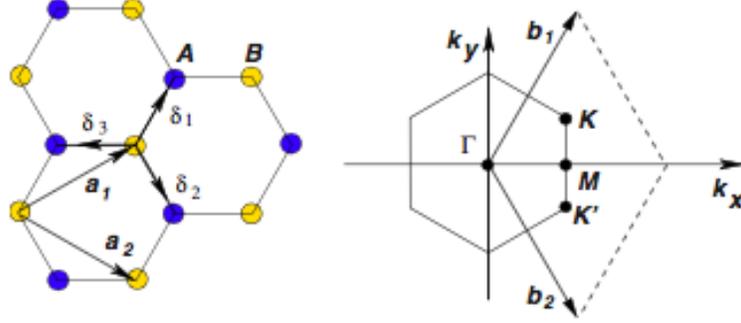


Figure 1: Honeycomb lattice and its Brillouin zone. Left: lattice structure of graphene, made out of two interpenetrating triangular lattices \mathbf{a}_1 and \mathbf{a}_2 are the lattice unit vectors, and δ_i , $i = 1, 2, 3$ are the nearest-neighbor vectors. Right: corresponding Brillouin zone. The 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:

$$\begin{aligned}
 \Delta_{\mathbf{k}} &= e^{i\mathbf{k}\cdot\delta_1} + e^{i\mathbf{k}\cdot\delta_2} + e^{i\mathbf{k}\cdot\delta_3} \\
 &= e^{i\mathbf{k}\cdot\delta_3} [1 + e^{i\mathbf{k}\cdot(\delta_1-\delta_3)} + e^{i\mathbf{k}\cdot(\delta_2-\delta_3)}] \\
 &= e^{-ik_x a} \left[1 + e^{i3k_x a/2} e^{i\sqrt{3}k_y a/2} + e^{i3k_x a/2} e^{-i\sqrt{3}k_y a/2} \right] \\
 &= e^{-ik_x a} \left[1 + e^{i3k_x a/2} (e^{i\sqrt{3}k_y a/2} + e^{-i\sqrt{3}k_y a/2}) \right] \\
 &= e^{-ik_x a} \left[1 + 2e^{i3k_x a/2} \cos\left(\frac{\sqrt{3}}{2}k_y a\right) \right].
 \end{aligned} \tag{11}$$

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 $E_{\pm}(\mathbf{k}) = 0$.

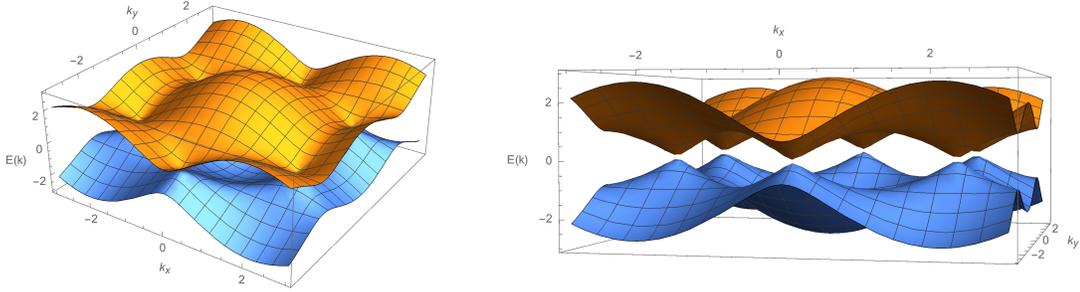


Figure 2: Energy bands for graphene from nearest-neighbor interactions. The bands meet at the Dirac points, at which the energy is zero.

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 σ_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 also have a σ_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 σ_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.

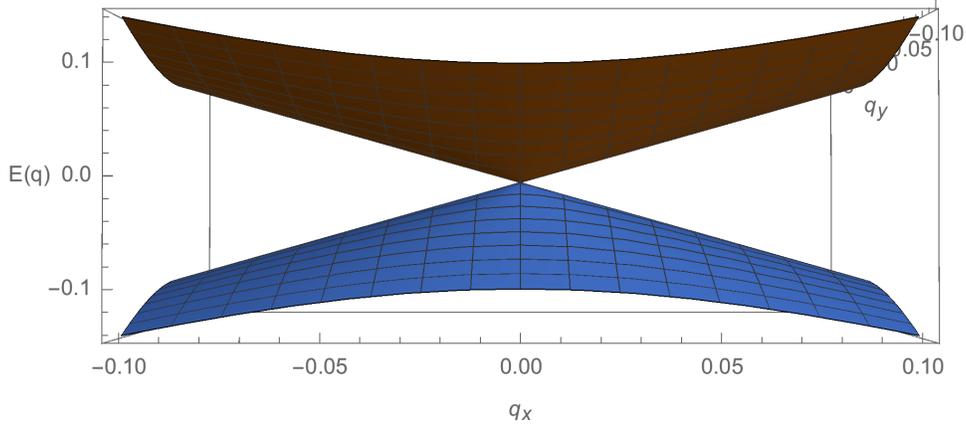


Figure 3: Conical behavior of the bands near a Dirac point, known as a Dirac cone, where the energy is linear in momentum.

3.4 σ_z term gapping

If we add the σ_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.

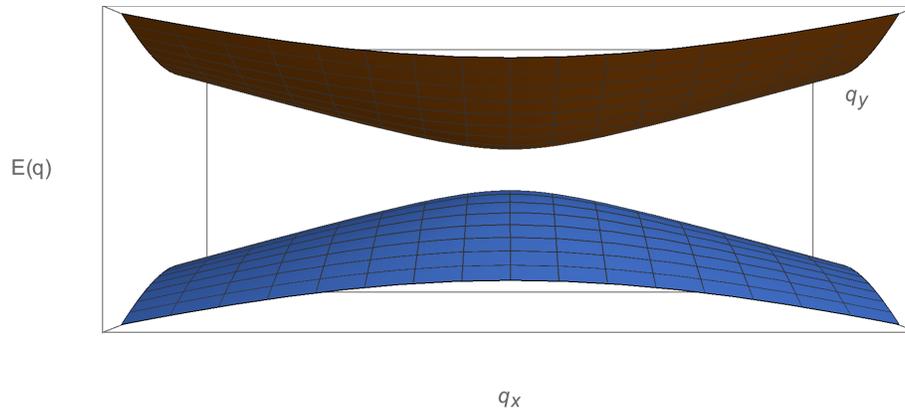


Figure 4: Energy gap near a Dirac point produced by a σ_z term. Compare to Fig. 3.

References

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- [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.