Why Dirac points in graphene are where they are?

E. Kogan

Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel

(Dated: February 13, 2012)

We present a simple group theory explanation of the fact that the energy bands merge in the corners of the Brillouin zone for graphene and for two particular cases of Kagome lattice for arbitrary tight–binding Hamiltonian. We connect the linearity of the spectrum in the vicinity of these points for monolayer graphene, bilayer graphene for AA stacking and Kagome lattice with the properties of the conical points of the surface, known from geometry.

INTRODUCTION

The contacts of energy bands have been studied from the early days of quantum solid state physics [1, 2]. The early classical papers in the field are reprinted in Ref. [3]. The existence of such points of contact in graphene was also known since the early quantum mechanical studies of graphite. When graphene was first isolated experimentally [4], these points were immediately brought into the focus of attention of both theorists and experimentalists. The reason is very simple: for undoped and ungated graphene these points lie on the Fermi surface, and many physical properties of such graphene are determined by the electron states in the vicinity of these points. In addition, the electron spectrum in the vicinity of these points is linear (in a monolayer graphene), and these states are effectively described by the Dirac equation [5]. This is why these points of contact in monolayer graphene (and other materials showing similar properties) are called the Dirac points.

Graphene is traditionally considered within the tight–binding approximation. The approximation starts from mentioning that in isolated form, carbon has six electrons in the orbital configuration 1s²2s²2p². When arranged in the honeycomb crystal, two electrons remain in the core 1s orbital, while the other orbitals hybridize, forming three sp² bonds and one pz orbital. The sp² orbitals form the σ band, which contains three localized electrons. The bonding configuration among the p orbitals of different lattice sites generates a valence band, or π-band, containing one electron, whereas the antibonding configuration generates the conduction band (π⁺), which is empty [5].

The early classical papers consider merging of Brillouin zones [3]. On the other hand, in the framework of the tight-binding approximation there exists only a single Brillouin zone. However, this zone contains the number of energy bands, equal to the number of atoms in the elementary cell (more exactly, the number of orbitals per elementary cell considered), which emulate a finite number of Brillouin zones.

The structure of graphene can be seen as a triangular lattice with a basis of two atoms per unit cell. For a model tight–binding Hamiltonian, taking into account only nearest–neighbor and next–nearest–neighbor hopping, it can be easily shown that the energy bands neither overlap, nor have a finite gap between them, but touch each other in two points in momentum space, both for monolayer and bilayer graphene. [6]. We show in the framework of group theory that taking into account hopping between more distant neighbors does not shift these points of contact; their positions are determined only by the point symmetry of the honeycomb lattice. The linearity of the spectrum of the electrons in the vicinity of the points of contact in monolayer and bilayer graphene with the AA stacking also remains for the general tight–binding Hamiltonian.

In addition we prove the existence of the Dirac points in the corners of the bands for the isotropic Kagome and Lieb lattices, described in the framework of the general tight–binding Hamiltonian.

THE GENERAL TIGHT–BINDING
HAMILTONIAN

The structure of graphene can be seen as a triangular lattice with a basis of two atoms per unit cell, displaced from each other by any one (fixed) vector connecting two sites of different sub-lattices, say \( \delta = -a (1, 0) \). The general Hamiltonian for the π bands is

\[
H = -\left( \sum_a t'(a) e^{i k \cdot a} + \sum_a t'(a + \delta) e^{-i k \cdot (a + \delta)} + \sum_a t'(a) e^{i k \cdot a} \right),
\]

where \( a \) is an arbitrary lattice vector, that is a linear combination of \( a_1 = \frac{a}{3} (3, \sqrt{3}) \), \( a_2 = \frac{a}{3} (3, -\sqrt{3}) \).

The selection rule for matrix elements [6] gives

\[
\sum_a t(a + \delta) e^{i K \cdot (a + \delta)} = 0,
\]

where \( K \) is a the corner of the Brillouin zone. In fact, we are dealing with the product of two functions: \( t(a + \delta) \) realizes the unit representation of the point symmetry group \( C_3 \) (the full symmetry group of the inter–sublattice hopping is \( C_{3v} \), but the restricted symmetry \( C_3 \) will be enough to prove the cancelation). As far as the function \( e^{i K \cdot (a + \delta)} \) is concerned, rotation of the lattice by the angle \( 2\pi/3 \), say anticlockwise, is equivalent to rotation of
the vector $K$ in the opposite direction, that is to substitution of the three equivalent corners of the Brillouin zone: $K_1 \rightarrow K_2 \rightarrow K_3 \rightarrow K_1$, where $K_1 = \left( \frac{2\pi}{3\alpha}, \frac{2\pi}{3\sqrt{3}\alpha} \right)$, $K_2 = \left( 0, -\frac{4\pi}{3\sqrt{3}\alpha} \right)$ and $K_3 = \left( \frac{2\pi}{3\alpha}, \frac{2\pi}{3\sqrt{3}\alpha} \right)$. Thus due to the rotation $e^{iK(a+\delta)}$ is multiplied by the factor $e^2$ and realizes $x - iy$ representation of the group $C_3$. Because each of multipliers in Eq. $2$ realizes different irreducible representation of the symmetry group, the matrix element is equal to zero. Simply speaking, at a point $K$ the sublattices become decoupled, and this explains the degeneracy of the electron states in this point (these points) or, in other words, merging of the two branches of the single Brillouin zone.

On the other hand, generally

$$\sum_a t'(a)e^{iK \cdot a} \neq 0.$$  (3)

To understand this statement consider the maximum symmetry group of the intra–lattice hopping; $C_{6v}$. The function $t'(a)$ realizes the $A_1$ representation of the group. Applying Eq. (2) we see that reducible representation of the group $C_{6v}$, realized by the two functions $e^{iK \cdot a}$ and $e^{iK' \cdot a}$ can be decomposed as $A_1 + B_2$.

In addition, the tight–binding model provides us with a simple explanation why the dispersion law in the vicinity of the merging points is linear, that is why these points are Dirac points. The dispersion law for the Hamiltonian is given by equation

$$F(E, k) = 0,$$  (4)

where

$$F(E, k) = \left| \sum_a t'(a)e^{iK \cdot a} \sum_a t(a + \delta)e^{iK(\cdot a + \delta)} \right|.$$  (5)

In mathematics the Dirac points, we are dealing with, are called conical points of the surface; if the surface is given by Eq. (4), the conditions for the conical points are [7]

$$\frac{\partial F}{\partial E} = 0, \quad \frac{\partial F}{\partial k} = 0.$$  (6)

Recalling the rule for differentiating of a determinant, we realize that Eq. 2 guarantees that the conditions for $k = K$. This explains linearity of the spectrum in the vicinity of the points $K(K')$. The axis of the cone is perpendicular to the $k_x, k_y$ plane, and the cone is a circular one, because any vector in the $k_x, k_y$ plane compatible with the symmetry $C_{6v}$ is identically equal to zero, and any tensor of rank two compatible with the symmetry is proportional to the unity tensor.

The important role played by discrete symmetries in protecting a $k$–linear dispersion in graphene was pointed out in Ref. [9]. The appearance of massless Dirac fermions under conditions of hexagonal symmetry was considered in Ref. [10]. Group theory was used to derive an invariant expansion of the Hamiltonian for electron states near the K points of the graphene Brillouin zone in Ref. [11].

**BILAYER GRAPHENE**

The same selection rule for matrix elements, we applied for the case of monolayer graphene, can be applied to bilayer graphene.

![Figure 1: Top view of a graphene bilayer; white and black circles: top layer carbon atoms; gray and red: bottom layer. [Adapted from Ref. [13]]](image)

The general tight–binding Hamiltonian for the AB stacking has the form

$$H = -\left( \sum_a t'(a)e^{iK \cdot a} \sum_a t(a + \delta)e^{iK(\cdot a + \delta)} - \sum_a t'_1(a)e^{iK \cdot a} \sum_a t'_1(a)e^{iK(\cdot a + \delta)} - \sum_a t'_2(a)e^{iK \cdot a} \sum_a t'_2(a)e^{iK(\cdot a + \delta)} - \sum_a t'_3(a)e^{iK \cdot a} \sum_a t'_3(a)e^{iK(\cdot a + \delta)} - \sum_a t'_4(a)e^{iK \cdot a} \sum_a t'_4(a)e^{iK(\cdot a + \delta)} \right).$$  (7)

where $t'$ and $t$ are the intra– and inter–sublattice intra–layer hopping integrals respectively, and $t_1, t_3$ and $t_4$ are
the $A-A$, $B-B$, and $A-B$ inter–layer hopping integrals respectively [12].

For $k = K(K)'$, the terms containing $t$, $t_3$ and $t_4$ are zero, due to symmetry reasons mentioned above. Hence, at the corner of the Brillouin zone the Hamiltonian takes the form

$$H = - \begin{pmatrix}
\sum_a t'(a)e^{iK\cdot a} & 0 & \sum_a t'(a)e^{iK\cdot a} & 0 \\
0 & \sum_a t'(a)e^{-iK\cdot a} & 0 & \sum_a t'(a)e^{iK\cdot a} \\
0 & \sum_a t'(a)e^{-iK\cdot a} & 0 & \sum_a t'(a)e^{iK\cdot a} \\
0 & 0 & 0 & \sum_a t'(a)e^{iK\cdot a}
\end{pmatrix}.$$  \hfill (8)

We again have merging of the energy band. Of course, in this case the points of contact are not the Dirac points.

$$H = - \begin{pmatrix}
\sum_a t'(a)e^{ik\cdot a} & \sum_a t(a + \delta)e^{i(k\cdot a + \delta)} & \sum_a t(a + \delta)e^{-i(k\cdot a + \delta)} & \sum_a t'(a)e^{iK\cdot a} \\
\sum_a t'(a)e^{-i(k\cdot a + \delta)} & \sum_a t'(a)e^{iK\cdot a} & \sum_a t'(a)e^{-i(k\cdot a + \delta)} & \sum_a t'(a)e^{iK\cdot a} \\
\sum_a t'(a)e^{-i(k\cdot a + \delta)} & \sum_a t'(a)e^{iK\cdot a} & \sum_a t'(a)e^{-i(k\cdot a + \delta)} & \sum_a t'(a)e^{iK\cdot a} \\
\sum_a t'(a)e^{iK\cdot a} & \sum_a t'(a)e^{-iK\cdot a} & \sum_a t'(a)e^{iK\cdot a} & \sum_a t'(a)e^{-iK\cdot a}
\end{pmatrix}.$$

The general tight–binding Hamiltonian for the AA stacking has the form

$$H = - \begin{pmatrix}
\sum_a t'(a)e^{iK\cdot a} & 0 & \sum_a t'(a)e^{iK\cdot a} & 0 \\
0 & \sum_a t'(a)e^{-iK\cdot a} & 0 & \sum_a t'(a)e^{iK\cdot a} \\
0 & \sum_a t'(a)e^{-iK\cdot a} & 0 & \sum_a t'(a)e^{iK\cdot a} \\
0 & 0 & 0 & \sum_a t'(a)e^{iK\cdot a}
\end{pmatrix}.$$  \hfill (9)

where $t_1$ and $t_4$ are the $A-A(B-B)$ and $A-B$ inter–layer hopping integrals respectively. At the corner of the Brillouin zone the Hamiltonian takes the form

$$H = - \begin{pmatrix}
\sum_a t'(a)e^{iK\cdot a} & 0 & \sum_a t'(a)e^{iK\cdot a} & 0 \\
\sum_a t'(a)e^{-iK\cdot a} & 0 & \sum_a t'(a)e^{iK\cdot a} & 0 \\
\sum_a t'(a)e^{-iK\cdot a} & 0 & \sum_a t'(a)e^{iK\cdot a} & 0 \\
\sum_a t'(a)e^{iK\cdot a} & \sum_a t'(a)e^{-iK\cdot a} & \sum_a t'(a)e^{iK\cdot a} & \sum_a t'(a)e^{-iK\cdot a}
\end{pmatrix}.$$  \hfill (10)

and we again have merging of two bands. However, for the AA stacking, in distinction from the AB stacking the function

$$F(E, k) = |EI - H|,$$

where $I$ is the unity matrix, satisfies Eq. (6). Hence the points of contact are the Dirac points.

$$H = \begin{pmatrix}
\sum_a t(a)e^{iK\cdot a} & \sum_a t(a + a_1/2)e^{iK\cdot (a + a_1/2)} & \sum_a t(a + a_1/2)e^{iK\cdot (a + a_1/2)} \\
\sum_a t'(a + a_1/2)e^{-iK\cdot (a + a_1/2)} & \sum_a t(a)e^{iK\cdot a} & \sum_a t(a + a_1/2)e^{iK\cdot (a + a_1/2)} \\
\sum_a t'(a + a_1/2)e^{-iK\cdot (a + a_1/2)} & \sum_a t'(a)e^{iK\cdot a} & \sum_a t(a + a_1/2)e^{iK\cdot (a + a_1/2)} \\
\sum_a t(a + a_1/2)e^{iK\cdot (a + a_1/2)} & \sum_a t'(a)e^{iK\cdot a} & \sum_a t(a + a_1/2)e^{iK\cdot (a + a_1/2)}
\end{pmatrix}.$$  \hfill (12)

where $a_1$ and $a_2$ are the elementary lattice vectors, and $a_3 = a_1 - a_2$.

KAGOME LATTICE

Kagome lattice has three sublattices. The general anisotropic tight–binding Hamiltonian for such lattice is characterized by three sets of exchange integrals. We consider general tight–binding Hamiltonian for two particular cases. First consider isotropic case $t_1 = t_2 = t_3 = t$. The Hamiltonian in this case is given by equation

$$H = \begin{pmatrix}
V(k) & T(k)\cos\left(\frac{k_0a_1}{2}\right) & T(k)\cos\left(\frac{k_0a_2}{2}\right) \\
T(k)\cos\left(\frac{k_0a_1}{2}\right) & V(k) & T(k)\cos\left(\frac{k_0a_2}{2}\right) \\
T(k)\cos\left(\frac{k_0a_2}{2}\right) & T(k)\cos\left(\frac{k_0a_2}{2}\right) & V(k)
\end{pmatrix}.$$  

Eq. (12) can be presented as

$$H = \begin{pmatrix}
\sum_a t^* \cdot (a + a_1/2)e^{-iK\cdot (a + a_1/2)} & \sum_a t^* \cdot (a + a_1/2)e^{-iK\cdot (a + a_1/2)} & \sum_a t^* \cdot (a + a_1/2)e^{-iK\cdot (a + a_1/2)} \\
\sum_a t^* \cdot (a + a_1/2)e^{-iK\cdot (a + a_1/2)} & \sum_a t^* \cdot (a + a_1/2)e^{-iK\cdot (a + a_1/2)} & \sum_a t^* \cdot (a + a_1/2)e^{-iK\cdot (a + a_1/2)} \\
\sum_a t^* \cdot (a + a_1/2)e^{-iK\cdot (a + a_1/2)} & \sum_a t^* \cdot (a + a_1/2)e^{-iK\cdot (a + a_1/2)} & \sum_a t^* \cdot (a + a_1/2)e^{-iK\cdot (a + a_1/2)}
\end{pmatrix}.$$  

where $a_1$ and $a_2$ are the elementary lattice vectors, and $a_3 = a_1 - a_2$. 
with obvious expressions for $V(k)$ and $T(k)$. We see, that the dispersion law for a general tight-binding Hamiltonian can be presented as

$$E(k) = V(k) + T(k)\tilde{E}(k)$$  \quad (14)

where $\tilde{E}(k)$ is the dispersion law given by the Hamiltonian taking into account only the nearest–neighbor hopping \footnote{C.-H. Park and S. G. Louie, Nano Lett. 9, 82 (2009).}

$$\tilde{H} = \begin{pmatrix} 0 & \cos\left(\frac{k\cdot a_1}{2}\right) & \cos\left(\frac{k\cdot a_2}{2}\right) \\ \cos\left(\frac{k\cdot a_1}{2}\right) & 0 & \cos\left(\frac{k\cdot a_3}{2}\right) \\ \cos\left(\frac{k\cdot a_2}{2}\right) & \cos\left(\frac{k\cdot a_3}{2}\right) & 0 \end{pmatrix}. \quad (15)$$

One branch of the spectrum we find by inspection:

$$\tilde{E}_1(k) = -1. \quad (16)$$

The other two branches are given by the reduced Hamiltonian

$$\tilde{H} = \frac{1}{2} \left( \sum_{i=1}^{3} e^{-i k \cdot a_i} \right). \quad (17)$$

At the point $K(K')$ the non–diagonal matrix elements of the Hamiltonian \footnote{R. Winkler, U. Zlicke, Phys. Rev. B 86, 174515 (2014).} are equal to zero due to the reasons presented above, and we have merging of the bands. In addition, at the point $K(K')$ the function $F$, defined by

$$F(\tilde{E}, k) = \left| \begin{array}{c} 1 - \tilde{E} \\ \sum_{i=1}^{3} e^{-i k \cdot a_i} \end{array} \right|, \quad (18)$$

satisfies conditions \footnote{Eugene.Kogan@biu.ac.il}. Thus we have two Dirac points in the corners of the Brillouin zone. Note also, that at $\Gamma$ point one of the branches given by Eq. (17) touches the branch $\tilde{E}_1$.

Now consider particular case of the Kagome lattice $t_1 = t_2 = t$, $t_3 = 0$. In this case, called isotropic Lieb lattice, we recover Eq. (12), the role of the Hamiltonian \footnote{K.-H. Park and S. G. Louie, Nano Lett. 9, 1793 (2009).} being played by the Hamiltonian

$$\tilde{H} = \begin{pmatrix} 0 & \cos\left(\frac{k\cdot a_1}{2}\right) & 0 \\ \cos\left(\frac{k\cdot a_1}{2}\right) & 0 & \cos\left(\frac{k\cdot a_3}{2}\right) \\ 0 & \cos\left(\frac{k\cdot a_3}{2}\right) & 0 \end{pmatrix}. \quad (19)$$

The spectrum is

$$\tilde{E}_1(k) = 0, \quad \tilde{E}_{2,3}(k) = \cos^2\left(\frac{k \cdot a_1}{2}\right) + \cos^2\left(\frac{k \cdot a_3}{2}\right). \quad (20)$$