Electronic spectrum of Kekulé patterned graphene considering second neighbor-interactions

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Received 25 January 2021, revised 24 February 2021
Accepted for publication 17 March 2021
Published 4 May 2021

Abstract
The effects of second-neighbor interactions in Kekulé-Y patterned graphene electronic properties are studied starting from a tight-binding Hamiltonian. Thereafter, a low-energy effective Hamiltonian is obtained by projecting the high energy bands at the \( \Gamma \) point into the subspace defined by the Kekulé wave vector. The spectrum of the low energy Hamiltonian is in excellent agreement with the one obtained from a numerical diagonalization of the full tight-binding Hamiltonian. The main effect of the second-neighbour interaction is that a set of bands gains an effective mass and a shift in energy, thus lifting the degeneracy of the conduction bands at the Dirac point. This band structure is akin to a ‘pseudo spin-one Dirac cone’, a result expected for honeycomb lattices with a distinction between one third of the atoms in one sublattice. Finally, we present a study of Kekulé patterned graphene nanoribbons. This shows that the previous effects are enhanced as the width decreases. Moreover, edge states become dispersive, as expected due to second neighbors interaction, but here the Kek-Y bond texture results in an hybridization of both edge states. The present study shows the importance of second neighbors in realistic models of Kekulé patterned graphene, specially at surfaces.

Keywords: graphene, Kekule, nanoribbons, next-nearest-neighbors

(Some figures may appear in colour only in the online journal)

1. Introduction

The space-modulation of two-dimensional materials has opened avenues for new exciting physical phenomena and applications [1–10]. Several mechanisms allow to perform such modulations, these include interactions with substrates [11] as in Moiré patterns [12], strain [3, 13–15], adatoms [16, 17], magnetic fields [18–20], and time dependent electromagnetic fields [21–23].

Among such modulated systems, in graphene it has been experimentally observed that vacancies in a Cu substrate induce a spatial frequency modulation with the size of an hexagonal ring of carbon atoms [24]. This modulated system is known as Kekulé-distorted graphene [24–29]. As an example of its interest and importance, such Kekulé distortion has been proposed as a possible mechanism behind superconductivity in magic-angle twisted bilayer graphene [28, 30]. Also, strain in Kekulé distorted graphene can be used to perform valleytronics [26], a feature that recently has been experimentally confirmed [31]. Multiflavor Dirac fermions were predicted to emerge in Kekulé graphene bilayers [27], and it is even possible to produce such modulation in non-atomic systems, as with mechanical waves in solids [32] and acoustical lattices [29]. Kekulé modulations are also reachable via photonic [33], polaronic [34], magnonic [35, 36] and atomic systems [37].
Gamayun et al demonstrated the absence of a gap for a Kek-Y distortion and deduced the low energy Hamiltonian for Kekulé distortions by using a first-neighbor tight-binding Hamiltonian [25]. They show how the two Dirac cones merge at the center of the Brillouin zone, producing either a gap (Kek-O) or the superposition of two cones with different Fermi velocities (Kek-Y) [25].

Several works have been made using such first-neighbor tight-binding Hamiltonian, for example to study uniaxial strain [26, 31] and the electronic transport properties [38-41].

However, its is known that second-neighbors interactions in graphene are very important [42, 43]. They are fundamental to explain the electronic properties at graphene surface as in graphene nanoribbons (GNRs) [42]. This leads to the natural question of what are the effects of second neighbors interactions in a Kekulé patterns. Although density functional calculations already contains such effects, due to the involved energies and the low resolution of the mesh calculations near the Dirac cones, its is difficult to assert a detailed picture of the energy dispersion. In that sense, a tight-binding calculation can be very useful. Here we tackle this question by producing a low-energy Hamiltonian for a Kekulé patterned graphene which includes second-neighbor interactions. The resulting model is validated through a comparison with the numerical calculations.

The paper is organized as follows. In section 2 we introduce the Hamiltonian for a honeycomb lattice with a Kek-Y distortion up to next-nearest neighbors, and in section 3 we calculate an effective four band low-energy Hamiltonian, finally in section 4 we present our conclusions and remarks.

2. First and second neighbor Kekulé-Y graphene Hamiltonian

We can consider the Kek-Y bond modulation as a periodic strain which reduces the distance between one third of the atoms in one sublattice with its three nearest neighbors as shown in figure 1 panel (a). Thus the hopping integral gets modified by the change in the interatomic distances accordingly with strain theory [3]. However, this would also mean a change in the next-nearest neighbors hoppings. In figure 1 panel (c) we illustrate this point, by showing in red (pink) the stronger (weaker) bonds for the B sublattice. In blue we show the hoppings between the A sublattice atoms, which remain unaltered.

Assuming the Grüneisen parameter to be equal for both first and second neighbors we can consider that the bond changes with the same proportionality. Thus the Hamiltonian for graphene with Kek-Y distortion considering hopping up to next-nearest neighbors is,

\[
H = - \sum_{r} \sum_{j=1}^{3} \epsilon_{r}^{(0)} a_{r}^{\dagger} b_{r+j} + \text{h.c.} + \sum_{r \neq m} t_{2} a_{r}^{\dagger} a_{m} + \delta_{n} - \delta_{m} \\
+ \sum_{r \neq m} \epsilon_{r}^{(2)} b_{r}^{\dagger} b_{r+\delta_{n}} + \delta_{r} + \delta_{m},
\]

where \( r \) is the position vector that runs over the atomic positions of sites in sublattice A and its given by \( r = n_{1}a_{1} + n_{2}a_{2} \) where \( n_{1}, n_{2} \) are integers, \( a_{1} = a \left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \), \( a_{2} = a \left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \) are the lattice vectors and \( a \) is the distance between carbon atoms 1.42 \( \text{Å} \). The vectors \( \delta_{1} = a \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \), \( \delta_{2} = a \left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \) and \( \delta_{3} = a (0, 1) \) go from a site in the A sublattice towards its three nearest neighbors in the B sublattice as shown in figure 1 panel (b). From figure 1 panel (a), it can be seen that while the second neighbors A–A sublattice (black–black circles bonds) atom distances remain constant, the distances between second-neighbors in the B–B sublattice (white–white atoms distances) are modulated in the same proportion as the first-neighbors distances. Therefore,
and couples a wavevector $k$ with three simultaneous bands, defining the column vector $t$ in pristine graphene, and where $t$ is taken as the space dependent hopping parameters $J$. As a consequence, the two Dirac cones superlattice with a tripled unit cell (of the size of a hexagonal ring) is formed. As a consequence, the two Dirac cones are periodically modulated in the same proportion. By using the modulation proposed by Gamayun et al for the first-neighbours [25] we obtain,

$$\frac{iG(0)}{t_0} = \frac{iG(2)}{t_2} = 1 + 2\Delta \cos(G \cdot r) = 1 + 2\Delta \cos \left( \frac{2\pi}{3} (n_2 - n_1) \right),$$

(2)

where $t_0 = 2.8$ eV is the hopping parameter for first neighbors in pristine graphene, and $t_2$ for second neighbors which will be taken as $t_2 = 0.1t_0$ unless otherwise indicated. $\Delta$ is the Kekulé coupling amplitude and $G = \frac{2\pi}{3} \sqrt{3}(1, 0)$ is the Kekulé wave vector. Thus, one third of the hoppings are enhanced by a factor of $(1 + 2\Delta)$ while the other two thirds are diminished by $(1 - \Delta)$.

Since graphene is subject to a periodic perturbation, with a spatial periodicity associated with $G$ (Kekulé distortion), a superlattice with a tripled unit cell (of the size of a hexagonal ring) is formed. As a consequence, the two Dirac cones at opposite corners ($K$ and $K'$) are folded onto the center of the new hexagonal superlattice Brillouin zone [25]. The Fourier transform of our tight-binding Hamiltonian is then,

$$H(k) = -\epsilon(k)a^\dagger_k b_k - \Delta\epsilon(k + G)a^\dagger_{k-G} b_k - \Delta\epsilon(k-G)a^\dagger_{k-G} b_k + h.c.$$  

$$+ f(k)a^\dagger_k a_k + f(k)b^\dagger_k b_k + \Delta f^+(k)b^\dagger_{k-G} b_k + \Delta f^-(k)b^\dagger_{k+G} b_k,$$

(3)

where

$$\epsilon(k) = t_0 \sum_{j=1}^3 e^{ik \cdot d_j},$$

(4a)

$$f(k) = t_2 \sum_{m \neq n} e^{ik \cdot (\delta_m - \delta_n)},$$

(4b)

$$f^{\pm}(k) = t_2 \sum_{m \neq n} e^{ik \cdot (\delta_m - \delta_n)} e^{\mp G \delta_n},$$

(4c)

designing $\epsilon(k)$ and $f(k)$ are the dispersion relations for a honeycomb and a triangular lattice respectively, $f^{\pm}(k)$ is the dispersion relation for the triangular lattice which is modulated by the distortion, corresponding to the pink and red bonds in figure 1 panel (c). Some properties of $f^{\pm}(k)$ are:

$$f^{\pm}(k \pm G) = f^{\mp}(k \mp G), \quad f^{\pm}(k \pm G) = f^{\mp}(k).$$

(5)

Unlike graphene, where the two valleys can be described independently, here and due to the folding of the $K$ and $K'$ valleys onto the $\Gamma$ point, the Fourier transform now couples a wavevector $k$ with the Kekulé wavevectors $G$ and $-G$. Therefore we can use a reduced Brillouin zone with three simultaneous bands, defining the column vector

Figure 2. Comparison of the DOS for Kekulé patterned graphene with and without the second-neighbor interaction, where the zero energy corresponds to the Fermi energy. Notice the electron–hole asymmetry which is specially clear for the band widths.

Figure 3. Low-energy dispersion around the $\Gamma$ point with $\Delta = 0.1$ and $t_2/t_0 = 0.1$. The solid lines indicate our analytic results for both the conic (orange) and the bands with an effective mass (blue). The dots are the numerical calculations including second-neighbor interactions obtained by a direct diagonalization of the tight-binding Hamiltonian defined by the lattice presented in figure 1 panel (a).

$c_k = (ak, bk, ak_G, bk_G, ak_{-G}, bk_{-G})$, and the Hamiltonian in equation (3) results in a $6 \times 6$ matrix,

$$H(k) = c_k \begin{pmatrix} H_{\Gamma} & T \\ T^\dagger & H_G \end{pmatrix} c_k,$$

(6a)

made from the original second-neighbor $\Gamma$ point graphene Hamiltonian,

$$H_{\Gamma} = \begin{pmatrix} f(k) & -\epsilon(k) \\ -\epsilon(k) & f(k) \end{pmatrix}.$$
a matrix which represents a Hamiltonian that arises due to the folding of valleys onto the \( \Gamma \) point,

\[
H_G = \begin{pmatrix}
0 & -\Delta \epsilon (k + G) & f(k + G) \\
-\Delta \epsilon (k + G) & 0 & -\epsilon (k + G) \\
f(k + G) & -\epsilon (k + G) & 0 \\
\end{pmatrix},
\]

and the interaction between the \( \Gamma \) point and folded valleys,

\[
T = \begin{pmatrix}
0 & -\Delta \epsilon (k + G) & f(k + G) \\
-\Delta \epsilon (k + G) & 0 & -\Delta \epsilon (k - G) \\
-\Delta \epsilon (k - G) & -\Delta \epsilon (k + G) & 0 \\
\end{pmatrix}.
\]

In figure 2 we present the density of states (DOS) obtained from a numerical diagonalization of equation (6a). As expected, the main effect is the breaking of the electron–hole symmetry reflected in changes of the band widths. Also, around the Fermi energy there are changes that we explore in the following section, as we will develop a low-energy approximation and compare it with the numerical diagonalization of the Hamiltonian given in (6a).

\[
T \approx \begin{pmatrix}
0 & \Delta \nu \epsilon (k_i - ik_y) & \Delta \nu \epsilon (k_i + ik_y) \\
\Delta \nu \epsilon (k_i - ik_y) & 0 & -\Delta \nu \epsilon (k_i + ik_y) \\
\Delta \nu \epsilon (k_i + ik_y) & -\Delta \nu \epsilon (k_i - ik_y) & 0 \\
\end{pmatrix},
\]

where we defined two velocities, one is the usual Fermi velocity in pristine graphene,

\[
v_F = \frac{3a t_0}{2 \hbar}
\]

and the other is due to second neighbors,

\[
v_2 = \frac{9a t_2}{2 \hbar} = 3 \left( \frac{t_2}{t_0} \right) v_F.
\]

As we are interested in the spectrum at low energies, the relevant part is the one associated with the valleys \( K \) and \( K' \) which corresponds to the block matrix \( H_G \), and then we can add the effects from higher energy bands in the \( \Gamma \) point as a perturbation. We have verified that this is an essential step in order to recover the spectrum obtained from a direct diagonalization. We can obtain the effective Hamiltonian by projecting \( H_\Gamma \) into the subspace of \( H_G \). To do this, consider the Schrödinger equation applied to equation (6a),

\[
H_\Gamma \Psi_\Gamma + T \Psi_G = E \Psi_\Gamma.
\]

### 3. Low-energy Hamiltonian

Let us now build a low energy Hamiltonian starting with the full \( 6 \times 6 \) Hamiltonian given by equation (6a). Since we are interested in the low energy bands, we expand up to first order in \( k \) the functions that appear in equation (6a). We obtain the following results,

\[
\epsilon (k) \approx 3t_0, \quad \epsilon (k \pm G) \approx \frac{3}{2} t_0(\mp k_x + ik_y),
\]

\[
f(k) \approx 6t_2, \quad f (k \pm G) \approx -3t_2
\]

\[
f^{\pm}(k \pm G) \approx 0, \quad f^{\pm}(k \pm G) \approx \frac{9}{2} \frac{t_2}{t_0}(\pm k_x + ik_y),
\]

Using the previous approximations, the linearized components of the Hamiltonian equation (6a) are given by,

\[
H_\Gamma \approx \begin{pmatrix}
6t_2 & -3t_0 \\
-3t_0 & 6t_2
\end{pmatrix},
\]

\[
H_\Gamma = H_G + T^\dagger (E_1 - H_\Gamma )\dagger T.
\]

This Hamiltonian is exact but needs a self-consistent procedure to find \( E \). However, if we expand the term \( (E_1 - H_\Gamma )^{-1} \) and keep the first order term. We can make the approximation \( E \approx E_0 = -3t_2 \) which is the original energy dispersion in the \( \Gamma \) point. Now we write the Dirac-like equation for this system,

\[
\mathcal{H} \begin{pmatrix}
\Psi_{K'} \\
\Psi_K
\end{pmatrix} = E \begin{pmatrix}
\Psi_{K'} \\
\Psi_K
\end{pmatrix},
\]

\[
\Psi_{K'} = \begin{pmatrix}
-\psi_{\Lambda K'} \\
\psi_{\Lambda K'}
\end{pmatrix}, \quad \Psi_K = \begin{pmatrix}
\psi_{\Lambda K} \\
\psi_{\Lambda K}
\end{pmatrix},
\]

where the explicit form of the low-energy Hamiltonian is finally given by,
Figure 4. (a) A zoom of the energy dispersion around the Fermi energy of Kekulé patterned graphene including up to second-neighbor interactions obtained from the low-energy approximation. (b) The corresponding DOS showing how the cone with an effective mass produces two jumps in the DOS.

\[
H = \begin{pmatrix}
E_0 & v_F(1 - \Delta^2)(p_x - ip_y) & v_F\Delta(1 - \Delta)(p_x - ip_y) & 0 \\
v_F(1 - \Delta^2)(p_x + ip_y) & E_0 + \mu & v_F\Delta(1 - \Delta)(p_x + ip_y) & 0 \\
v_F\Delta(1 - \Delta^2)(p_x + ip_y) & E_0 + \mu & v_F(1 - \Delta^2)(p_x + ip_y) & v_F(1 - \Delta^2)(p_x - ip_y) \\
0 & E_0 + \mu & v_F(1 - \Delta^2)(p_x - ip_y) & E_0
\end{pmatrix},
\]

which can be compactly written as,

\[
\mathcal{H} = E_0 \sigma_0 \otimes \tau_0 + v_F(1 - \Delta^2)(p \cdot \sigma) \otimes \tau_0 + v_F\Delta(1 - \Delta)\sigma_0 \otimes (p \cdot \tau) + \frac{\mu}{2}(\sigma_0 \otimes \tau_0 + \sigma_x \otimes \tau_x + \sigma_y \otimes \tau_y - \sigma_z \otimes \tau_z),
\]

with \( \mu \) defined as,

\[
\mu = 9\Delta^2l_0^2t_2 \left/ \left( l_0^2 - 9t_2^2 \right) \right.
\]

The four low-energy bands are

\[
E_D^{\pm} = E_0 \pm v_D|p|,
\]
\[
E_M^{\pm} = E_0 + \mu \pm \sqrt{v_M^2p^2 + \mu^2},
\]

were we defined \( v_D = v_F(1 - \Delta) \) and \( v_M = v_F(1 - \Delta)(1 + 2\Delta) \).

Therefore, there is a mix of two-flavor Fermion gases. One with and effective Dirac Hamiltonian,

\[
H_D = E_0\sigma_0 + v_D p \cdot \sigma,
\]

and the other,

\[
H_M = (E_0 + \mu)\sigma_0 + v_M p \cdot \sigma + \mu\sigma_z.
\]

In figure 3 we compare our results from equation (3) with the numerical diagonalization of the tight-binding Hamiltonian given by equation (6a) and which represents the spectrum of the lattice presented in figure 1 panel (a). First we notice an excellent agreement within this regime. Without second neighbors interaction, the Kek-Y bond texture couples both valleys in the \( \Gamma \) point, resulting in two concentric cones with different velocities \[25\]. Turning on the interaction gives rise to two main effects: a set of bands gains an effective mass and a shift in energy. This last effect results in a particle–hole symmetry breaking, lifting the degeneracy of the conduction bands at the Dirac point, therefore only three bands intersect. This
Figure 5. Dispersion for zigzag GNRs with Kekulé-Y bond texture and hoppings up to next nearest neighbors. The amplitude of the bond texture is $\Delta = 0.1$ for all figures. (a)–(c) show the dispersion with $t_2/t_0 = 0, 0.1$ and 0.2 respectively for a ribbon with $W = 4.54$ nm, analogously (d)–(f) for a ribbon with $W = 13.06$ nm.

Structure is akin to a ‘pseudo spin-one Dirac cone’, expected for a honeycomb lattices with a distinction between one third of the atoms in one sublattice [44, 45]. We can see that the effect of adding next-nearest-neighbors interaction is equivalent to that of an on-site potential $\mu$ on the atom at which the Y deformation is centered [25].

From equation (3) we can easily calculate the DOS per unit cell. Considering spin degeneracy, it is given by,

$$D(E) = \frac{A}{\pi \hbar^2} \left[ \frac{|E - E_0|}{v^2_D} + \frac{E - (E_0 + \mu)}{v^2_M} \Theta(E - E_0 - 2\mu) \right.$$

$$+ \left. \frac{(E_0 + \mu) - E}{v^2_M} \Theta(E_0 - E) \right], \quad (19)$$

where $A = 9\sqrt{3}a^2/2$ is the unit cell area and $\Theta(E)$ is the Heaviside function. Although the DOS retains its linear behavior around the Dirac point, the massive bands produce a discontinuity shown in figure 4.

Second neighbors hoppings are particularly important for GNRs. We calculated numerically the band structure for zigzag edged GNR. In figure 5 our results are shown for different values of $t_2$ and width $W$. Due to the change in the periodicity produced by the Kekulé texture, the unit cell size $a_c$ is three times bigger, thus $a_c = 3\sqrt{3}a$. We can see that edge states become dispersive, which is a well known effect of second neighbors interaction [42], however the combination with the Kek-Y bond texture results in an hybridization of both edge states. The velocity induced in the edge states may indirectly close the small gap predicted for Kek-Y zigzag GNR [39].

4. Conclusions

The effects of second-neighbor interactions in Kekulé patterned graphene were studied starting from a tight-binding Hamiltonian. From there, a low-energy effective Hamiltonian was derived using a projection technique. This Hamiltonian was validated thorough a comparison with a numerical calculation obtained from the diagonalization of the full tight-binding Hamiltonian. We found that beyond the expected electron–hole symmetry breaking, the main effect of the second-neighbor interaction is that in one of the Dirac cones, the electron becomes massive when compared with the calculation made considering only first-neighbour interaction. As a result, the DOS near the Fermi energy contains a jump in the otherwise linear behavior. Finally, we considered the effects of second-neighbor interactions in Kekulé patterned GNRs, as it is known that such effects are essential to reproduce a minimally realistic behavior at the edges. As expected, the same mass effect is seen in the nanoribbons and in fact is amplified as the width is decreased.

Thus, we expect that such second-neighbor effects to be important in the electronic and optical properties of Kekulé bond textures.
Acknowledgments

We thank UNAM DGAPA Project IN102620 and CONACyT Project 1564464. E Andrade thanks an scholarship from CONACyT.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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