Dirac cones on the generalized honeycomb lattice

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Abstract.
We study the tight-binding model on the generalized honeycomb lattice, where nearest-neighbor and next-nearest-neighbor transfer integrals and the on-site potentials are taken as parameters. We obtain the condition for the untilted Dirac cone. We discuss the effects of the uniaxial strain on the opening of the gap and the tilting of the Dirac cone.

1. Introduction
It is well-known that "massless Dirac fermions" are realized in graphene [1, 2, 3], the organic conductor α-(BEDT-TTF)₂I₃ [4, 5, 6, 7, 8] and iron-based superconductors, BaFe₂As₂[9]. The massless Dirac fermions are the origin of anomalous phenomena such as temperature-independent conductivity and unusual quantum Hall effect[2].

The electron band of graphene is obtained by fully first-principles band calculations[10, 11, 12]. It can be reproduced by a tight-binding model on a honeycomb lattice with nearest-neighbor transfer integrals[13, 14, 15, 16]. As the electrons are half-filled, a lower band is fully occupied. The energy gap between two bands is zero at the points, \( k^* = (k_x^*, k_y^*) \)[13, 14]. The linearized energy dispersion is called the Dirac cone, as seen in Fig. 1 (a).

The opening of the gap has been observed on an epitaxial graphene on a SiC substrate[17]. The finite gap is necessary for the application in electronic devices. When only the nearest-neighbor transfer integrals are present, the condition for the zero gap is obtained as \( |t_b| \leq |t_a| \leq |t_c| \) (1).

The large asymmetry (for example, \( t_c > 2t_a \) when \( t_b = t_a \)) is necessary to open the gap. The band calculations[16] have shown that the deformation of the order of 20% is indispensable to open the gap.

We consider the next-nearest-neighbor transfer integrals \( (t'_a, t'_b, t'_c, t''_a, t''_b, t''_c) \), where \( t'_a, t'_b \) and \( t'_c \) are transfer integrals within sublattice A and \( t''_a, t''_b \) and \( t''_c \) are those within sublattice B and the on-site potentials \( \epsilon_A \) and \( \epsilon_B \) on sublattices A and B as seen in Fig. 1 (b). Then, the condition of the zero gap is given by Eq. (1) and Eq. (12) in this paper[18, 19]. If \( t_a = t_b = t_c \), the gap is opened due to at least one of the inequalities, \( t'_a \neq t''_a, t'_b \neq t''_b, t'_c \neq t''_c \) or \( \epsilon_A \neq \epsilon_B \).

Thus, even if the asymmetries of next-nearest-neighbor transfer integrals or on-site potentials
creation operators for A (B) sites, respectively, and transition due to the tilting of the Dirac cone in lattice symmetry, the tilted Dirac cone is realized\[4, 5, 6, 7\]. The anomalous Kosterlitz-Thouless Dirac cone means the anisotropy of the Fermi velocity. In α-(BEDT-TTF) Dirac cone of graphene is shown to be tilted\[6\] as in the right figure in Fig. 1 (a). The tilted Hamiltonian is given by

\[
H = \sum_{\mathbf{k}} A_{\mathbf{k}}^\dagger \sum_{\mu=0,1,2,3} \epsilon_{\mu}(\mathbf{k}) \sigma_\mu \mathbf{A}_\mathbf{k},
\]

where \( A_{\mathbf{k}} = (a_{\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger, \sigma_0 \) is the 2 × 2 unit matrix, \( \sigma_j \) (j = 1, 2, 3) are Pauli matrices, \( a_{\mathbf{k}}^\dagger(t_{\mathbf{k}}^\dagger) \) are creation operators for A (B) sites, respectively, and

\[
\epsilon_0(\mathbf{k}) = \frac{\epsilon_A + \epsilon_B}{2} - (t'_c + t''_c) \cos(\mathbf{a}_1 \cdot \mathbf{k}) - (t'_b + t''_b) \cos(\mathbf{a}_2 \cdot \mathbf{k}) - (t'_c + t''_c) \cos((\mathbf{a}_2 - \mathbf{a}_1) \cdot \mathbf{k}),
\]

\[
\epsilon_1(\mathbf{k}) = -t_a \cos\left(\frac{\mathbf{a}_1 + \mathbf{a}_2}{3} \cdot \mathbf{k}\right) - t_b \cos\left(\frac{1}{3}(2\mathbf{a}_1 - \mathbf{a}_2) \cdot \mathbf{k}\right) - t_c \cos\left(\frac{1}{3}(2\mathbf{a}_2 - \mathbf{a}_1) \cdot \mathbf{k}\right),
\]

\[
\epsilon_2(\mathbf{k}) = -t_a \sin\left(\frac{\mathbf{a}_1 + \mathbf{a}_2}{3} \cdot \mathbf{k}\right) + t_b \sin\left(\frac{1}{3}(2\mathbf{a}_1 - \mathbf{a}_2) \cdot \mathbf{k}\right) + t_c \sin\left(\frac{1}{3}(2\mathbf{a}_2 - \mathbf{a}_1) \cdot \mathbf{k}\right),
\]

\[
\epsilon_3(\mathbf{k}) = \frac{\epsilon_A - \epsilon_B}{2} - (t'_c - t''_c) \cos(\mathbf{a}_1 \cdot \mathbf{k}) - (t'_b - t''_b) \cos(\mathbf{a}_2 \cdot \mathbf{k}) - (t'_c - t''_c) \cos((\mathbf{a}_2 - \mathbf{a}_1) \cdot \mathbf{k}),
\]

where the unit vectors are given by

\[
a_1 = \left(\frac{\sqrt{3}}{2}a, -\frac{1}{2}a\right), \quad a_2 = \left(\frac{\sqrt{3}}{2}a, \frac{1}{2}a\right),
\]
and \(a\) is the lattice constant. The off-diagonal elements of \(\epsilon_1(\mathbf{k})\) and \(\epsilon_2(\mathbf{k})\) contain the nearest-neighbor transfer integrals, and the diagonal elements of \(\epsilon_0(\mathbf{k})\) and \(\epsilon_3(\mathbf{k})\) contain the next-nearest-neighbor transfer integrals, which connect sublattice A (B) and A (B). We show in this paper that the tilting of the Dirac cone is caused by \(\epsilon_0(\mathbf{k})\) and that the deformation of the Dirac cone from a circle to an ellipsoid is caused by \(\epsilon_1(\mathbf{k}), \epsilon_2(\mathbf{k})\) and \(\epsilon_3(\mathbf{k})\). While the nearest-neighbor transfer integrals, \(t_a, t_b\) and \(t_c\) for graphene are estimated to be \(2.7 \sim 3.1\) eV\(^{-1}\), the values of the next-nearest-neighbor transfer integrals are not known. In some studies \([15, 22]\), the values of \(t_a', t_b', t_c', t_a'', t_b''\) and \(t_c''\) have been taken to be the order of 0.1 \(t_a\).

### 3. Eigenvalues

Eigenvalues of Eq. (2) are obtained as

\[
E^{\pm}(k_x, k_y) = \epsilon_0(\mathbf{k}) \pm \Delta_{\mathbf{k}}, \tag{7}
\]

where

\[
\Delta_{\mathbf{k}} = \sqrt{\sum_{j=1}^{3} (\epsilon_j(\mathbf{k}))^2}. \tag{8}
\]

One of the authors\([14]\) has obtained that \((\epsilon_1(\mathbf{k}^*)^2 + (\epsilon_2(\mathbf{k}^*))^2\) becomes zero when the following three equations are satisfied,

\[
\cos(a_1 \cdot \mathbf{k}^*) = \frac{t_a^2 - t_a'^2 - t_b^2}{2 t_a t_b}, \tag{9}
\]
\[
\cos(a_2 \cdot \mathbf{k}^*) = \frac{t_a^2 - t_a'^2 - t_c^2}{2 t_a t_c}, \tag{10}
\]
\[
\cos((a_1 - a_2) \cdot \mathbf{k}^*) = \frac{t_a^2 - t_a'^2 - t_c^2}{2 t_b t_c}. \tag{11}
\]

In general, there exist \(\mathbf{k}^*\) and \(-\mathbf{k}^*\), which are located at the positions of inversion symmetry and time reversal symmetry. These points are merged when one of the equalities in Eq. (1) is satisfied\([14]\).

When \(\epsilon_3(\mathbf{k}^*)\) becomes zero, the energy gap, \(\Delta_{\mathbf{k}^*}\), is zero. Thus, by putting Eqs. (9), (10) and (11) into Eq (6), we obtain the condition for the zero gap at \(\mathbf{k}^*\) as following\([18, 19]\):

\[
\epsilon_A - \epsilon_B - (t_a' - t_a'') \left( \frac{t_a^2 - t_b^2 - t_c^2}{t_a t_c} \right) - (t_b' - t_b'') \left( \frac{t_a^2 - t_a'^2 - t_c^2}{t_a t_c} \right) - (t_c' - t_c'') \left( \frac{t_a^2 - t_a'^2 - t_b^2}{t_a t_b} \right) = 0. \tag{12}
\]

We call the condition given in Eq. (12) the averaged inversion symmetry. When only the nearest-neighbor integrals are considered, the system is invariant with respect to inversion. On the other hand, when the next-nearest-neighbor integrals are finite, the gap is not opened as long as the averaged inversion symmetry is conserved, even if the inversion symmetry is broken\([18, 19]\).

### 4. Linearization for eigenvalues near \(\mathbf{k}^*\)

In this section we study the energy around \(\mathbf{k}^*\) when Eqs. (1) and (12) are satisfied, i.e., \(\Delta_{\mathbf{k}^*} = 0\).

\[
\epsilon_0(\mathbf{k}) \simeq \epsilon_0(\mathbf{k}^*) + v_{0x}(\mathbf{k}^*)q_x + v_{0y}(\mathbf{k}^*)q_y + O(q_x^2, q_y^2), \tag{13}
\]
\[
\epsilon_j(\mathbf{k}) \simeq v_{jx}(\mathbf{k}^*)q_x + v_{jy}(\mathbf{k}^*)q_y + O(q_x^2, q_y^2), \quad j = 1, 2, 3 \tag{14}
\]
where \( q_x = k_x - k_x^* \), \( q_y = k_y - k_y^* \) and \( v_{\mu}(k^*) = \frac{\partial E_{\mu}(k)}{\partial k_{\mu}} \mid_{k=k^*} \) \( (\mu = 0, 1, 2, 3, i = x, y) \). For example, we obtain
\[
\begin{align*}
v_{0x}(k^*) &= \frac{\sqrt{3}a}{2} \left\{ (t'_c + t'_c) \sin(a_1 \cdot k^*) + (t'_b + t'_b) \sin(a_2 \cdot k^*) \right\}, \\
v_{0y}(k^*) &= -\frac{a}{2} \left\{ (t'_c + t'_c) \sin(a_1 \cdot k^*) - (t'_b + t'_b) \sin(a_2 \cdot k^*) - 2(t'_a + t''_a) \sin((a_2 - a_1) \cdot k^*) \right\}.
\end{align*}
\]
(15) (16)
We get from Eqs. (8) and (14)
\[
\Delta^2_k \approx (q_x, q_y) \left( \begin{array}{c|c}
|\vec{v}_x(k^*)|^2 & (\vec{v}_x(k^*) \cdot \vec{v}_y(k^*)) \\
(\vec{v}_x(k^*) \cdot \vec{v}_y(k^*)) & |\vec{v}_y(k^*)|^2
\end{array} \right) \left( \begin{array}{c}
q_x \\
q_y
\end{array} \right),
\]
(17)
where \( \vec{v}_i(k^*) = (v_{1i}(k^*), v_{2i}(k^*), v_{3i}(k^*)) \). The \( 2 \times 2 \) matrix in Eq. (17) can be diagonalized by the rotation\([6, 23]\) in the \( q_x, q_y \) plane, i.e.
\[
\left( \begin{array}{c}
q_x \\
q_y
\end{array} \right) = U \left( \begin{array}{c}
\tilde{q}_x \\
\tilde{q}_y
\end{array} \right),
\]
(18)
with the unitary matrix
\[
U = \left( \begin{array}{cc}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{array} \right),
\]
(19)
where \( \theta \) is given by
\[
\tan \theta = \frac{2(\vec{v}_x(k^*) \cdot \vec{v}_y(k^*))}{|\vec{v}_x(k^*)|^2 - |\vec{v}_y(k^*)|^2}.
\]
(20)
Then we obtain
\[
E^\pm(k) \approx \epsilon_0(k^*) + w_{0x} \tilde{q}_x + w_{0y} \tilde{q}_y \pm \sqrt{w_{0x}^2 \tilde{q}_x^2 + w_{0y}^2 \tilde{q}_y^2},
\]
(21)
where
\[
\begin{align*}
w_{x}^2 &= \frac{|\vec{v}_x(k^*)|^2 + |\vec{v}_y(k^*)|^2}{2} + \sqrt{\left( \frac{|\vec{v}_x(k^*)|^2 - |\vec{v}_y(k^*)|^2}{2} \right)^2 + (\vec{v}_x(k^*) \cdot \vec{v}_y(k^*))^2}, \\
w_{y}^2 &= \frac{|\vec{v}_x(k^*)|^2 + |\vec{v}_y(k^*)|^2}{2} - \sqrt{\left( \frac{|\vec{v}_x(k^*)|^2 - |\vec{v}_y(k^*)|^2}{2} \right)^2 + (\vec{v}_x(k^*) \cdot \vec{v}_y(k^*))^2},
\end{align*}
\]
(22) (23)
and
\[
(w_{0x}, w_{0y}) = (v_{0x}(k^*) v_{0y}(k^*))U.
\]
(24)
Note that \( w_{x}^2 \geq w_{y}^2 \geq 0 \) and we obtain \( w_y = 0 \) only when \( \vec{v}_x(k^*) \parallel \vec{v}_y(k^*) \). When \( w_y = 0 \), the Dirac cone is not formed. The conditions for the isotropic (\(|w_x| = |w_y|\)) and untilted (\(w_{0x} = w_{0y} = 0\)) Dirac cone are obtained as follows. The Dirac cone is isotropic, if and only if the vectors \( \vec{v}_x(k^*) \) and \( \vec{v}_y(k^*) \) are perpendicular each other and have the same length. If these conditions are not satisfied, the cross-section of the Dirac cone at the constant energy is elliptic. The Dirac cone is untilted, if and only if
\[
v_{0x}(k^*) = v_{0y}(k^*) = 0.
\]
(25)
Since the nearest-neighbor transfer integrals ($t_a$, $t_b$, and $t_c$) do not appear in $\epsilon_0(\mathbf{k})$ of Eq. (3), the next-nearest-neighbor transfer integrals are required to tilt the Dirac cone[6]. The equations for untitled Dirac cone (Eq. (25)) can be written as

$$ (t'_a + t''_a) \sin((a_2 - a_1) \cdot \mathbf{k}^*) = -(t'_b + t''_b) \sin(a_2 \cdot \mathbf{k}^*) = (t'_c + t''_c) \sin(a_1 \cdot \mathbf{k}^*). $$

By taking square of each terms and inserting Eqs. (9), (10) and (11), we obtain the condition for the untitled Dirac cone as

$$ t_a(t'_a + t''_a) = t_b(t'_b + t''_b) = t_c(t'_c + t''_c). $$

5. Discussion

Here, we discuss the effects of strain on graphene. When there is no strain, $t_a = t_b = t_c$, $t'_a = t'_b = t'_c = t''_a = t''_b = t''_c$, and $\epsilon_A = \epsilon_B$. In this case the energy gap is zero and the Dirac cone is untitled. If the uniaxial strain is applied, transfer integrals are changed, but the parallel pairs of the next-nearest-neighbor transfer integrals are the same, i.e., $t'_a - t''_a = t'_b - t''_b = t'_c - t''_c = 0$. In that case, the energy gap is zero, since Eq. (12) is satisfied. On the other hand, Eq. (27) is not satisfied, i.e., the Dirac cone is tilted.

6. Conclusion

We obtain the band dispersion near $\mathbf{k}^*$ in the tight-binding model on generalized honeycomb lattice, Eq. (21). The condition for the untitled Dirac cone is given by Eq. (27). The tilted Dirac cone of graphene is realized in the weak uniaxial strain although the gap is not opened. In that case, the peculiar property of $\alpha$-(BEDT-TTF)$_2$I$_3$ such as Kosterlitz-Thouless transition at lower temperature[8] may also be observed in graphene.

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