Shift of Dirac points and strain induced pseudo-magnetic field in graphene

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We propose that the strain induced effective pseudo-magnetic field in graphene can also be explained by a curl movement of the Dirac points, if the Dirac points can be regarded as a slowly varying function of position. We also prove that the Dirac points must be confined within two triangles, each one has 1/8 the area of the Brillouin zone.

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The discovery of graphene, a monolayer carbon atom sheet [1], and the development of experimental technique to manipulate this two-dimensional (2D) material have ignited intense interest in this system [2,3]. One of the most attractive characters of graphene is that its low energy excitation satisfies a massless 2D Dirac equation [6], and the chemical potential crosses its Dirac points (or Fermi points) in neutral graphene. These special characters lead to many unusual properties and new phenomena [5,7,8], such as the anomalous integer quantum Hall effect (QHE) [8,9]. Recently, experiments have confirmed another remarkable effect that mechanical strain can induce a very strong effective pseudo-magnetic field, leading to a pseudo-QHE, which can be observed in zero magnetic field [10,11]. In this paper we propose that the strain induced effective pseudo-magnetic field in graphene can also be explained by a curl movement of the Dirac points, if the Dirac points can be regarded as a slowly varying function of position. We also prove that the Dirac points must be confined within two triangles, each one has 1/8 the area of the Brillouin zone (BZ).

Firstly, consider a tight-binding Hamiltonian describing a uniformly deformed honeycomb lattice with three different nearest-neighbor hopping energies $t_1,t_2,t_3$ [13-15]:

$$
\hat{H} = - \sum_{\langle i,j \rangle} t_{i\alpha,j\beta} c_{i\alpha}^\dagger c_{j\beta} + h.c.,
$$

where $c_{j\beta}$ ($c_{i\alpha}^\dagger$) are annihilation (creation) operators, $i(j)$ are position vectors of unit cells, $a(b)$ denote two inequivalent atoms in a unit cell, $t_{i\alpha,j\beta}$ is the electronic hopping energy from the $j$th unit cell $b$ atom to $i$th unit cell $a$ atom. Suppose that the deformed lattice remains invariant under spatial translation, i.e., $t_{i\alpha,j\beta}$ only depends on $i-j$, but the three nearest-neighbor hopping energies $t_{1,2,3}$ may be different owing to anisotropy of strains, as shown in Fig. 1. The hopping parameters can be written as some $2 \times 2$ matrices $t(i-j)$, whose elements are defined by $[t(i-j)]_{a,b} ≡ t_{i\alpha,j\beta}$. For this nearest-neighbor tight-binding Hamiltonian, the non-vanishing hopping matrixes are

$$
t(0) = \begin{pmatrix} 0 & t_1 \\ t_2 & 0 \end{pmatrix}, t(a_1) = \begin{pmatrix} 0 & t_2 \\ t_3 & 0 \end{pmatrix}, t(a_2) = \begin{pmatrix} 0 & t_3 \\ t_1 & 0 \end{pmatrix},
$$

and $t(-a_1) = t(a_1)^\dagger$, $t(-a_2) = t(a_2)^\dagger$. By Fourier transformation

$$
c_{j,a(b)} = \frac{1}{\sqrt{N}} \sum_k c_{k,a(b)} \exp(ik \cdot j),
$$

with $N$ a normalization constant, the Hamiltonian (1) can be cast into the form

$$
\hat{H} = - \sum_k \left[ c_{k,a}^\dagger c_{k,b}^\dagger \right] \left[ \begin{array}{cc} h_{aa}(k) & h_{ab}(k) \\ h_{ba}(k) & h_{bb}(k) \end{array} \right] \left[ \begin{array}{c} c_{k,a} \\ c_{k,b} \end{array} \right],
$$

where $h_{aa}(k) = h_{bb}(k) = 0$, $h_{ab}(k) = h_{ba}^*(k)$, and

$$
h_{ba}(k) = t_1 + t_2 \exp(ik \cdot a_1) + t_3 \exp(ik \cdot a_2),
$$

with $a_1,a_2$ the lattice unit vectors. The energy bands obtained by diagonalizing this Hamiltonian are [16]

$$
E_k^\pm(k) = \pm \left[ t_1 + \tilde{t}_2(k) + \tilde{t}_3(k) \right],
$$

where $\tilde{t}_2(k) = t_2 e^{ik \cdot a_1}$, $\tilde{t}_3(k) = t_3 e^{ik \cdot a_2}$, the plus sign corresponds to the upper($\pi$) and minus to the lower($\pi^*$) band respectively. From Eq. (5) we notice that if $K$ is a zero point of $h_{ba}(K)$, i.e.,

$$
t_1 + \tilde{t}_2(K) + \tilde{t}_3(K) = 0,
$$

FIG. 1: Unit cell and hopping parameters for deformed graphene.
then \( E_+(\mathbf{k}) \) and \( E_-(\mathbf{k}) \) will meet at \( \mathbf{K} \), i.e., \( E_+(\mathbf{K}) = E_-(\mathbf{K}) = 0 \), this \( \mathbf{K} \) is known as the Dirac point. The Hamiltonian (3) can be expanded up to a linear order in \( \mathbf{p} = \mathbf{k} - \mathbf{K} \) in a neighborhood of point \( \mathbf{K} \)

\[
\begin{bmatrix}
    h_{aa}(\mathbf{k}) & h_{ab}(\mathbf{k}) \\
    h_{ba}(\mathbf{k}) & h_{bb}(\mathbf{k})
\end{bmatrix} \approx 
\begin{bmatrix}
    0 & \alpha^- \cdot \mathbf{p} \\
    \alpha^- \cdot \mathbf{p} & 0
\end{bmatrix} = v_{\mu\nu} \sigma^\mu p^\nu,
\]

(7)

where \( \mu, \nu \) denote two components of a 2D vector and a sum over the repeated indices \( \mu, \nu \) is implied, \( \alpha \) is a complex vector with \( \text{Re}(\alpha) = (v_{11}, v_{12}), \text{Im}(\alpha) = (v_{21}, v_{22}) \), \( \sigma^{1,2} \) are Pauli matrices acting on the sublattice degree of freedom, tensor \( v_{\mu\nu} \) represents the anisotropy of the dispersion near the Dirac points, it only occurs noticeable departure from \( \mathbf{p} = \delta \mathbf{K} \) in a strongly deformed graphene[12]. However, after this modification the strain induced effective vector potential will acquire a direct physical meaning. For a graphene under nonuniform but slowly varying strain, \( t_1(\mathbf{x}) \) and hence the Dirac point \( \mathbf{K}(\mathbf{x}) \) as well as \( v_{\mu\nu}(\mathbf{x}) \) can be regarded as some smooth functions of position \( \mathbf{x} \), the local linearized Hamiltonian \( v_{\mu\nu}(\mathbf{x}) \sigma^{\mu}(p^\nu - \delta K^{\nu}(\mathbf{x})) \) on the RHS of Eq.(7) can be cast into

\[
v_{\mu\nu}(\mathbf{x})\sigma^{\mu}(p^\nu - \delta K^{\nu}(\mathbf{x})),
\]

(8)

where \( \mathbf{p} = \delta \mathbf{K}(\mathbf{x}) \equiv \mathbf{k} - \mathbf{K}(\mathbf{x}) \), \( \delta \mathbf{K}(\mathbf{x}) \equiv \mathbf{K}(\mathbf{x}) - \mathbf{K}_f \) with \( \mathbf{K}_f \) the corresponding Dirac point in strain-free graphene. Unlike the usual explanation of the strain induced gauge field in graphene[13,17], where the effective vector potential is an auxiliary quantity and describes the mixed effects of both anisotropy of \( v_{\mu\nu} \) and the shift of Dirac point, here the vector potential only represents the relative translation of the Dirac points, \( (e/c)A(\mathbf{x}) = \delta \mathbf{K}(\mathbf{x}) \), its pseudo-magnetic field \( \mathbf{B}(\mathbf{x}) = (c/e) \nabla \times \mathbf{K}(\mathbf{x}) \), and the physical effects are mainly determined by the pseudo-magnetic flux through a loop \( (c/e) \oint_s \mathbf{K}(\mathbf{x}) \cdot d\mathbf{x} \).

In the following sections we shall discuss the properties of \( \mathbf{K}(\mathbf{x}) \), and illustrate how a curl field \( \mathbf{K}(\mathbf{x}) \) is induced by a strain.

From Eq.(6) we know that the vectors representing \( t_1, t_2(\mathbf{K}), t_3(\mathbf{K}) \) in the complex plane can form a direct triangle for a Dirac point \( \mathbf{K} \), as illustrated in Fig.2a.

According to the triangle inequality, we have the following necessary and sufficient conditions for the existence of the Dirac points[13]:

\[
t_1 + t_2 \geq t_3, \quad t_2 + t_3 \geq t_1, \quad t_3 + t_1 \geq t_2.
\]

(9)

These conditions define a pyramidal domain in the \((t_1, t_2, t_3)\) space, shown in Fig.2b. If \( t_1, t_2, t_3 \) satisfy inequalities [15], then there exists two directed triangles with the same edges \( t_1, t_2, t_3 \) but different possible orientations, which determine two angles \( \theta_1, \theta_2 \) satisfying \( t_1 e^{i\theta_1} + t_2 e^{i\theta_2} = 0 \), where \( \theta_1, \theta_2 \) are given by the law of cosine

\[
\begin{align*}
\theta_{\pm 1} &= \pm \arccos \left( \frac{t_1^2 + t_3^2 - t_2^2}{2t_1 t_3} \right), \\
\theta_{\pm 2} &= \pm \arccos \left( \frac{t_2^2 + t_3^2 - t_1^2}{2t_2 t_3} \right) - \pi.
\end{align*}
\]

(10)

Thus the Dirac points \( \mathbf{K} \) can be determined by letting

\[
\exp(i\mathbf{K} \cdot \mathbf{a}_1) = \exp(i\theta_1), \quad \exp(i\mathbf{K} \cdot \mathbf{a}_2) = \exp(i\theta_2),
\]

(11)

so we have

\[
\mathbf{K} = \frac{1}{2\pi} (\theta_1 \mathbf{b}_1 + \theta_2 \mathbf{b}_2) + \mathbf{K}_0,
\]

(12)

with \( \mathbf{b}_1, \mathbf{b}_2 \) the reciprocal lattice vectors defined by \( \mathbf{a}_1 \cdot \mathbf{b}_2 = 2\pi\delta_{ij} \), and \( \mathbf{K}_0 = n\mathbf{b}_1 + m\mathbf{b}_2 \) with \( n, m \) are arbitrary integers. Notice that if \( t_1 + t_2 + t_3 = 0 \), then \( t_1 + t_2^* + t_3 = 0 \), this implies that there exists two Dirac points \( \mathbf{K}(\mathbf{x}) \) and \(-\mathbf{K}(\mathbf{x})\). However, if \( t_1, t_2, t_3 \) exactly locates on the boundary surface of the pyramid, e.g., \( t_1 = t_2 + t_3 \), then the two triangles will mutually coincide and \( t_2 = t_2^*, t_3 = t_3^* \) (see Fig.2b), hence \( \mathbf{K}(\mathbf{x}) \) and \(-\mathbf{K}(\mathbf{x})\) become equivalent, and \( \delta \) is \( i(t_2 \mathbf{a}_1 + t_3 \mathbf{a}_2) \) becomes a pure imaginary vector, so the Fermi velocity in the directions perpendicular to \( \delta \) vanishes(Fig.3a and 3b)[14,15,18]. If \( (t_1, t_2, t_3) \) goes beyond the domain defined by Eq.(9), e.g., \( t_1 > t_2 + t_3 \), Eq.(11) will have no any root, an energy gap with magnitude \( E_g = 2(t_1 - t_2 - t_3) \) will occur at the corresponding points \( K_\pm = \pm 1/2(\mathbf{b}_1 + \mathbf{b}_2) \)(see Fig.3b), and the effective Hamiltonian [15,18,19] must be further modified by adding a mass term and some second order terms.

Another important property is the range of \( \mathbf{K}(\mathbf{x}) \). We shall prove that the Dirac points must be confined within some special regions of the BZ. To this end, notice that if a Dirac point \( \mathbf{K} = (1/2\pi)(\theta_1, \theta_2) \) is given, then its associated \( t_{1,2,3} \) can also be determined up to an arbitrary factor, except six special cases of \( \theta_1, \theta_2 = 0, \pm \pi \)(see Fig.2b). If \( \theta_1, \theta_2 \neq 0, \pm \pi \). According to the law of sines we have

\[
\begin{align*}
t_2 &= \frac{\sin \theta_2}{\sin(\theta_1 - \theta_2)} , \quad t_3 = \frac{\sin \theta_1}{\sin(\theta_2 - \theta_1)},
\end{align*}
\]

(13)
regularity, here we have ignored the variations of pseudo-magnetic field. In order to show the underlying the Dirac points for the Dirac points. This confinement also limits the remaining hexagon (blue in Fig.4) is a forbidden region.

FIG. 3: (color online) (a) Energy band when two Dirac points are very close, where $t_1 = 2.8, t_{2,3} = 1.45$, (b), (d) $t_1 = 2.8, t_{2,3} = 1.4$, two Dirac points are equivalent (superposed), (c) $t_1 = 2.8, t_{2,3} = 1.35$, an energy gap occurs.

or

$$(t_1, t_2, t_3) \propto (\sin(\theta_2 - \theta_1), -\sin \theta_2, \sin \theta_1).$$

For the six special cases we have: if $(\theta_1, \theta_2) = (\pm(\pi, \pi)$, $t_1 = t_2 + t_3$; if $(\theta_1, \theta_2) = (\pm(\pi, 0)$, $t_2 = t_1 + t_3$; if $(\theta_1, \theta_2) = (\pm(0, \pi)$, $t_3 = t_1 + t_2$. From Eq.14 we can find that the $\theta_1, \theta_2$ must satisfy some constrain conditions to guarantee $t_{1,2,3} \geq 0$, as illustrated in Fig.2. For an arbitrary $t_2$ and a fixed $\theta_1$ (direction of $\tilde{t}_2$), $t_3$ must point in a direction between the directions of $-\tilde{t}_2$ and negative real axis, i.e., argument $\theta_1, \theta_2$ must satisfy

$$\theta_1 + \pi < \theta_2 < \pi, \quad \theta_1 \in (\pi, 0),$$

$$-\pi < \theta_2 < \theta_1 - \pi, \quad \theta_1 \in (0, \pi).$$

These two inequalities respectively determine the range of $K(x)$ and $-K(x)$. They describe two open triangles $\Delta MM'_1M''_1$ and $\Delta M'M_1M''_1$ in reciprocal space, as shown in Fig.4 each one has $1/8$ the area of a unit cell of the reciprocal space (the parallelogram $M''M'_1M''_1M'_1$), and each Dirac point is confined within a triangle, so, the Dirac points $K$ and $-K$ can meet (become equivalent) only at the vertexes of $\Delta MM'_1M''_1$ and $\Delta M'M_1M''_1$. The remaining hexagon (blue in Fig.4) is a forbidden region for the Dirac points. This confinement also limits the order of magnitude of $\nabla \times K(x)$, i.e., the strain induced pseudo-magnetic field. In order to show the underlying regularity, here we have ignored the variations of $b_1, b_2$ with the deformation of lattice, and simply sketch all $K = (k_1, k_2)$ in the same affine frame. After translating to the first BZ of graphene, $\Delta MM'_1M''_1$ and $\Delta M'M_1M''_1$ are equivalent to a ringlike region consists of six triangles $\Delta MM'_1, \Delta M'_1K_2M''_2, \Delta M''K'_1M', \Delta M'_1K'_2M''_2, \Delta M''K_1M', \Delta M'_1K_2M''_1$ etc.

FIG. 4: (color inline) Rand of the Dirac points consists of six triangles in first BZ, or $\Delta MM'_1M''_1$ and $\Delta M'M_1M''_1$. In order to illustrate how a non-vanishing $\nabla \times K$ is induced by strain, we only need to analyze three ideal cases, in which only one $t_i$ is slightly changed, $t_i \rightarrow t_0 + \delta t_i$, while the other two $t_{j,k}$ remain constant, $t_j = t_k = t_0$, which can also be roughly regarded as that the bond $c_i$ is elongated (or compressed) while the other two bonds $c_j, c_k$ and their directions remain fixed (see Fig.2b). Notice that the Dirac points only depend on the relative proportions of $t_1, t_2, t_3$, so, as an equivalent case, we can always assume that $t_1$ remains constant and only $t_2, t_3$ are variables. Moreover, in these equivalent cases the $t_2$ and $\tilde{t}_3$ can be determined by the end of the vector $t_1 + \tilde{t}_2 = -\tilde{t}_3$, denoted by $P$ in Fig.a. So, we can represent the variation of the Dirac points by the shift of the point $P$. To this end, we have to determine the corresponding $P$ of the three classes of characteristic points in the range of the Dirac points: (1) $K$ (or $K'$) etc., (2) critical points $M(M'_1) = (\pm 1/2, 0), M'(M'_1) = (0, \pm 1/2)$, and $M''(M''_1) = (\pm 1/2, \pm 1/2)$, in these cases there exist only one Dirac point since the points $K$ and $-K$ are equivalent, their corresponding $(t_1, t_2, t_3)$ are located on the boundary of the pyramidal domain, while their corresponding $P$ are located at the real axis in Fig.3; (3) $O, O', O''$ etc., their corresponding $P$ are the centers of two circles and the infinite limit points of the straight line $KK'$ in Fig.4, which respectively correspond to the limits of $t_2 \rightarrow 0$, $t_3 \rightarrow 0$ and $t_1 \rightarrow 0$ (equivalent to $t_2 = t_3 \rightarrow \infty$). Now we analyze the shifts of the Dirac points in the three ideal situations. (1) $t_1, t_2$ remain constant and $t_2 = t_1$, only $t_3$ is variable, the trajectory of the corresponding $P$ is a circle with radius $t_1$ and centered.
at the point \((t_1, 0)\) in Fig.5a, so the arguments \((\theta_1, \theta_2)\) satisfy
\[
\theta_1 - 2\theta_2 - 2\pi = 0, \quad \theta_1 \in (-\pi, 0), \\
\theta_1 - 2\theta_2 + 2\pi = 0, \quad \theta_1 \in (0, \pi).
\] (16)
They describe line segments \(M'O_1\) and \(M'O_2\) in Fig.5 (2) \(t_3(-=t_1)\) remain constant while \(t_2\) is variable, the trajectory of corresponding \(P\) is another circle with radius \(t_1\) centered at the origin, its associated \((\theta_1, \theta_2)\) satisfy
\[
\theta_2 - 2\theta_1 + 2\pi = 0, \quad \theta_2 \in (-\pi, 0), \\
\theta_2 - 2\theta_1 - 2\pi = 0, \quad \theta_2 \in (0, \pi),
\] (17)
which describe \(M'O'\) and \(M'O_2'\) in Fig.4 (3) \(t_1\) remains constant while \(t_2, t_3\) are variable but \(t_2 = t_3\) (or vice versa, \(t_1\) is variable, \(t_2(-=t_3)\) remain constant), the trajectory of \(P\) is straight line \(KK'\), \((\theta_1, \theta_2)\) satisfy
\[
\theta_1 + \theta_2 = 0, \quad \frac{\pi}{2} < |\theta_1| < \pi,
\] (18)
which describe \(M'O''\) and \(M'O_2''\) in Fig.4. Summarizing Eqs.(16)(17)(18) and comparing with Fig.3 we observe that if a band, e.g., \(c_1\) is slightly elongated (or compressed) along its direction, \(c_1 \rightarrow (1 + \delta)c_1\), while the other two bonds \(c_2, c_3\) remain fixed, then \(t_1\) will be slightly changed while \(t_2\)\((=t_3)\) remain constant, the Dirac point \(K\) will be slightly moved in the direction perpendicular to \(c_1\), i.e., \(\delta K_y \neq 0\)(see Fig.3) \(K\) moves towards \(O''\) if \(t_1\) decreases, towards \(M'_c\) if \(t_1\) increases, \(K'\)(=\(-K\)) is moved in the opposite direction. Thus, if the elongation of \(c_1\) is slowly varying in the \(x\)-direction, i.e., \(\partial t_1/\partial x \neq 0\), then \(\partial K_y/\partial x \neq 0\), the other two cases are similar. So, a nonuniform strain as schematically shown in Fig.5b can induce a curl field \(K(x), \nabla \times K \neq 0\).

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