Berry-Phase Induced Dynamical Instability and Minimum Conductivity in Graphene

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Abstract

Single-layer carbon, or graphene, demonstrates amazing transport properties, such as the minimum conductivity near \( \frac{4e^2}{h} \) independent of shapes and mobility of samples. This indicates there exist some unusual effects due to specific Dirac dispersion relation of fermion in two dimensions. By deriving fermion-lattice interaction Hamiltonian we show that Berry phases can be produced in fermion states around two Dirac points by relative rotations of two sublattices. The Berry phases in turn remove the degeneracies of energies for states near the Fermi surface, leading to a dynamical instability of the lattice with respect to the rotations. By considering the Berry phases emerging in an uncertain way on fermion wavefunctions in vicinities of the Fermi surface, the conductivity is calculated by using the Landauer-Büttiker formula together with the transfer-matrix technique, verifying \( \sim \frac{4e^2}{h} \) quantized minimum conductivity as observed in experiments independent of shapes and sizes. The relationship between the chaotic structure of fermions due to the Berry phases and the classical transport properties are discussed. The physical meaning is profound as this relationship provides an excellent example to elucidate the mechanism of quantum-classical transition.

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As a potential candidate material for carbon-based electronics, the graphene, a two-dimensional (2D) honeycomb lattice of carbon atoms, has attracted much attention [1, 2, 3, 4, 5]. It is found that both the type (electrons or holes) and the number of carriers can be tuned by changing the gate voltage [3, 6]. Such tunability originates from the specific dispersion relation of the massless Dirac fermions in graphene [7, 8]. The Fermi level of the system can be varied by changing the gate voltage. Particularly, there exists a universal maximal resistivity of the order of 6.5kΩ for all samples with the Fermi level near the Dirac points, independent of their mobility. By increasing the Fermi level the conductivity linearly increases [3]. The value of the minimal resistivity ($\frac{h}{4e^2} \sim 6.5k\Omega$) [3] implies the existence of at least 4 channels (including spin degrees of freedom) in a square of unit area and the number of channels increases with increasing the sample width. Although there are 4 ballistic channels at a node of the Dirac dispersion relation in a graphene lattice, the experimental fact of constant conductivity is inconsistent with the quantum-mechanical description from which all states are localized by extremely weak disorder in 2D [9]. The non-zero minimal conductivity has been investigated by several theoretical studies using different methods [10, 11, 12, 13]. The minimum conductivity was correctly demonstrated, but as to the reason for it and as to its exact value being $e^2/h$ or $e^2/\pi h$ there is no consensus at the present. By carefully examining the interaction between Dirac fermions and lattice motions, we show that the Berry phases produced by relative rotations of two sublattices can induce dynamical instability and cause constant conductivity $\frac{4e^2}{h}$.

The main features of the band structure in graphene can be well described by a tight-binding Hamiltonian with one $\pi$ orbital per site on the graphene lattice [7]:

$$H = \sum_{\langle n, n' \rangle} t_{nn'}(a_n^\dagger a_{n'} + a_{n'}^\dagger a_n), \quad (1)$$

where $a_n^\dagger$ ($a_n$) creates (annihilates) an electron at site $n$, $\langle \ldots \rangle$ denotes the nearest-neighbor (NN) sites, and $t_{nn'}$ is the NN hopping. Here, we omit the diagonal terms by shifting the energy zero as no diagonal disorder is considered, and the spin indices are not explicitly included. The hopping integral $t_{nn'}$ depends on distance between NN sites. Considering a relative displacement $\mathbf{d} \equiv (d_x, d_y)$ between two sublattices as shown in Fig. 1, the lengths of three bonds in a cell become

$$l_i = \sqrt{(d \sin(\theta - \alpha_i))^2 + (l_0 - d \cos(\theta - \alpha_i))^2}, \quad (2)$$
where $\theta$ is the angle of $\mathbf{d}$ related to $x$ axis, $l_0$ is the original bond length, and $\alpha_i = 0, \frac{2\pi}{3}, -\frac{2\pi}{3}$ for $i = 1, 2, 3$. For small displacement, we only keep the first-order terms of $d$ and obtain $l_i \sim l_0 - d \cos(\theta - \alpha_i)$. Then the corresponding hopping integrals can be written as

$$t_i = t_0 + \lambda d \cos(\theta - \alpha_i),$$

(3)

where $t_0$ is the original hopping and $\lambda$ is a coefficient describing the linear dependence of $t_i$ on $l_i$ in the case of small $d$. On the other hand, the elastic energy trends to keep $d = 0$. The in-plane displacements occur in two vibrational modes along $x$ and $y$ directions. We adopt variables $d_x$ and $d_y$ to express these two vibration modes. Using the Bloch transformation for graphene lattice and keeping terms of the first orders of $d_x, d_y$, and electron wave vector $\mathbf{k}$ related to the Dirac points, the Hamiltonian becomes

$$H = \frac{3}{2} \sum_{\mathbf{k}} \left[ (t_0 k_y \hat{\tau}_z + \lambda d_x \hat{1}) \otimes \hat{\sigma}_x - (t_0 k_x \hat{1} - \lambda d_y \hat{\tau}_z) \otimes \hat{\sigma}_y \right],$$

(4)

where $\hat{1}$ and $\hat{\tau}_z$ are unit and Pauli matrices acting on two irreducible Dirac points, and $\hat{\sigma}_{x,y}$ are Pauli matrices on two sublattices. So the dispersion relations around two Dirac points are

$$E_1^{(\pm)} = \pm \frac{3}{2} |t_0 (k_y + i k_x) + \lambda(d_x - id_y)|, \quad E_2^{(\pm)} = \pm \frac{3}{2} |t_0 (-k_y + i k_x) + \lambda(d_x + id_y)|.$$  

(5)

It is interesting to note that the diabolical points of the dispersion relations are moved by sublattice displacements. The dependence of energies on real $\mathbf{d}$ for a given $\mathbf{k}$ also has a diabolical point determined by $(d_x = -t_0 k_y/\lambda, d_y = t_0 k_x/\lambda)$ for $E_1^{(\pm)}$ and by $(d_x = t_0 k_y/\lambda, d_y = -t_0 k_x/\lambda)$ for $E_2^{(\pm)}$ as shown in Fig. 2.

From the Berry theorem a circle of rotation in a parameter space can cause a Berry phase $\pm \pi$ in a wavefunction whose eigenenergy has a diabolical point enclosed in this circle. If there exists a circular vibration with amplitude $d_f = t_0 k_f/\lambda$ with $k_f$ being the magnitude of the Fermi wave vector, in every circle of the vibration the states inside the Fermi circle change sign due to the acquired Berry phases but the states outside the Fermi circle do not. Now we consider an inside state $|\psi_1\rangle$ and an outside state $|\psi_2\rangle$ situated in an infinitesimal vicinity of a $\mathbf{k}$ point at the Fermi circle. They can be degenerate because of the continuity of the band. So we can construct a $\psi_+ - \psi_-$ basis to represent these two states:

$$|\psi_{\pm}\rangle = \frac{1}{\sqrt{2}} (|\psi_1\rangle \pm |\psi_2\rangle).$$

(6)
FIG. 1: Sublattices A (red points) and B (blue points) on graphene lattice. With relative displacement \( \mathbf{d} \), sublattice A is moved to positions marked with light magenta circles.

The asymmetric acquirement of a \( \pm \pi \) Berry phase in \( |\psi_{1,2}\rangle \) during a circle of circular vibration \( d_f \) leads to a hybridization of \( \psi_{\pm}(k) \) and removes the degeneracy. This can be described by an effective Hamiltonian

\[
H_B = \sum_{\alpha = \pm} |\psi_\alpha\rangle \epsilon_f \langle \psi_\alpha | + g (|\psi_+\rangle \langle \psi_-| + \text{H.c.}),
\]

where \( \epsilon_f \) is the Fermi energy and \( g \) is the hybridization strength depending on the rotation rates. Hamiltonian \( H_B \) raises one level to \( \epsilon_f + g \) and lowers the other to \( \epsilon_f - g \). Since the former is empty and the latter is occupied by fermion, this leads to the lowering of the fermion energy by \( g \). Thus, the energy gain per cell of the fermion system due to the vibration \( d_f \) is \( E_g \sim 2\pi k_f g D \) where \( D \) is the width of a narrow stripe around the Fermi circle in which the fermion energies are affected by \( g \). At the same time the energy per cell of the circular vibration \( d_f \) is proportional to \( d_f^2 \) and can be written as \( E_v \sim cd_0^2 \) with \( c \) being a prefactor. So, if \( E_v \leq E_g \), viz.

\[
k_f \leq k_v \equiv \frac{2\pi gD\lambda^2}{cd_0^2},
\]
a dynamical instability occurs with undamped fluctuations of rotations and Berry phases.

The condition (8) for the dynamical instability can be easily satisfied since $k_v$ is finite and positive while $k_f \to 0$ for the Fermi level situated at the Dirac points. It could still be satisfied even by slightly shifting the Fermi level with the gate voltage $V_g$. The value of $k_v$ can be estimated as follows: From the Harrison formula, the hopping integral of NN sites $n$ and $n'$ is $t_{nn'} = t_0 \left( \frac{l_0}{l_{nn'}} \right)^2$. So $\lambda \sim \frac{2t_0}{l_0} \sim 1.4l_0 \text{Å}^{-1}$. $c$ is related to the elastic coefficient $s_e$ of the C-C bonds by $c \sim \frac{3}{4}s_e$, and $s_e \sim 43.37 \text{eV Å}^{-2}$. $g$ is related to the vibration frequency $\omega_0$ by $g \sim \hbar \omega_0$, and $D$ is mainly due to the uncertainty of the Fermi energy in the vibration and can be expressed as $W \sim \frac{2\hbar \omega_0}{3t_0}$. From the value of $s_e$ and the mass of carbon atom we have $\hbar \omega_0 \sim 0.1 \text{eV}$. All these can give $k_v \sim 10^{-3}$ in units of $l_0^{-1}$. This value is considerable as the whole Dirac dispersion relation is valid for small $k$.

The circular vibrations could also propagate in the space with different wavelengths longer than the lattice spacing (long-wavelength limit) and cause mesoscopic inhomogeneity of the
created Berry phases. The spatial and temporal uncertainty of Berry phases attached on fermion states by such circular vibrations has radical effects on the basic structure of fermions in graphene. To illustrate this we adopt a model with random signs of NN hoppings $t_{nn'} = t_0$ or $-t_0$ to mimic the fluctuations of Berry phases $\pm \pi$ and calculate the conductivity for a rectangular sheet with different width $W$ and length $L$ connecting to two reservoirs with Fermi energy at the Dirac points ($E_f = 0$) by using the Landauer-Büttiker formula:

$$\sigma = \frac{2Le^2}{Wh} \sum_l \frac{1}{\cosh^2(\gamma_l L)},$$  \hspace{1cm} (9)

where $\gamma_l$ is the Lyapunov exponent of the $l$th channel in the system with width $W$ calculated with the transfer-matrix technique. The prefactor 2 is from contributions of two spins. The obtained conductivity as a function of $W/L$ for different sizes is shown in Fig. 3. Except for small values of $W/L$, the conductivity has almost a constant value near $\frac{4e^2}{h}$ independent of $W/L$ and $W$, in consistence with the experimental findings. Surprisingly, this value is even larger than $\frac{4e^2}{\pi h}$ obtained in ballistic graphene \[17\] in spite of the disorder introduced by random signs of hoppings. In a perfect 2D Dirac fermion gas, the difference between two successive Lyapunov exponents in Eq. (9) is $\delta \gamma = 2\pi/W$ due to the Dirac fermion dispersion relation \[17\]. In the present model the values of $W\delta \gamma$ are distributed within $[1, 2.5]$, smaller than that in the perfect case by a factor about $\pi$, leading to the $\pi$ times of the conductivity as can be derived from the expansion of Eq. (9). Thus, the $\pi$ factor difference in the conductivity is not trivial and reflects an essential change of the fermion properties due to the Berry-phase induced instability.

Besides the phase fluctuation, there are complicated level crossings in the dependence of energy on $k$ and $d$. The energy degeneracies at crossings can be easily modified by slight disturbing, resulting in chaotic energy structure. Thus, the global quantum-mechanical description of the Dirac fermions could be modified with a semi-classical scenario: The whole sheet can be divided into areas of size $b_0$ which are classically connected together as there is no quantum coherence among them. This is equivalent to an ohmic network of small conductors each of which represents an area of size $b_0$. Thus, the conductivity of the whole system is determined by the conductivity of every area which can be quantized. For the Fermi energy $E_f = 0$ there are only two transmission channels in an area providing minimum conductivity $\sigma = \frac{4e^2}{h}$. By applying the gate voltage $V_g$ the Fermi energy is shifted as $E_f = \beta V_g$ with $\beta$ being a prefactor and the number of transmission channels in an area is
\[ \frac{2\beta V_g b_0}{3\pi \hbar} \], producing a conductivity \( \sigma \sim \frac{4e^2 \beta b_0 |V_g|}{3\pi \hbar} \). The experiments show a linear dependence of \( \sigma \) on the gate voltage \( V_g \) with a finite slope, suggesting a finite coherent size \( b_0 \). From the slope one could estimate \( \frac{\beta b_0}{3\pi \hbar} \sim 0.2V^{-1} \).

In summary, we show the specific coupling between the Dirac fermions and the circular vibrations in graphene which can lead to a dynamical instability due to the produced Berry phases. The calculations from this scenario provide a constant conductivity consistent with the experiments. The results indicate that a picture of an ohmic network consisting of small quantum conductors is suitable to account for the peculiar transport properties in graphene.

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FIG. 3: Calculated conductivity as a function of ratio $W/L$ for rectangular sheets with different transverse sizes $W$. Inset in the lower panel: Distribution function $P(W\delta\gamma)$ of $W\delta\gamma$. The green dashed line indicates the $\delta$-function distribution at $2\pi$ in the case of perfect sheet. Units of $W$ and $L$ are cell sizes of graphene lattice.