Conductance enhancement due to atomic potential fluctuations in graphene

Dima Bolmatov1 and D. V. Zavialov2,3

1 School of Physics, Queen Mary University of London, Mile End Road, London, E1 4NS, UK
2 Volgograd State Social-Pedagogical University, Volgograd, 400005, Russia and
3 Volgograd State Technical University, Volgograd, 400005, Russia

We solve the Dirac equation, which describes charge massless chiral relativistic carriers in a two-dimensional graphene. We have identified and analysed a novel pseudospin-dependent scattering effect. We compute the tunneling conductance and generalize the analytical result in the presence of the tunable atomic potential of a graphene strip. The absence of back scattering in graphene is shown to be due to Berry’s phase which corresponds to a sign change of the wave function under a spin rotation of a particle. We use the transfer matrix approach and find that the electric conductance of doped graphene increases due to atomic potential fluctuations.

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I. INTRODUCTION

Graphene is a single layer of carbon atoms densely packed in a honeycomb lattice. This material was found in its free state only recently, when individual graphene samples of a few microns in size were isolated by micromechanical cleavage of graphite [1]. The current intense interest in graphene is driven by both the unusual physics involved and a realistic promise of device applications. Among relativistic like phenomena observed in graphene so far, there are two new types of the integer quantum Hall effect and the presence of minimal metallic conductivity of about one conductivity quantum [2]. Transport properties of graphene are interesting because of their unique topological structure [3, 4]. There have been some reports on experimental study of transport in graphene [5]. Various calculations have been performed to understand energy bands of graphene [6, 7]. It has been successful in the study of various properties including the Aharonov-Bohm effect [10], optical absorption spectra [11], quantum tunneling in graphene-based structures [12, 13], ferromagnetism [14] and instabilities in the presence and absence of a magnetic field [15].

In a two-dimensional world, there are two basic motions: forward and backward. Random scattering can cause them to mix, which leads to resistance. Just as we have learned from the basic traffic control, it would be much better if we could spatially filter the counter-flow directions. This effect could be used to produce a valley-polarized current out of an unpolarized stream of electrons due to line defect particularly in graphene [17–20].

The electronic transport properties of graphene with defects and impurities exhibit pronounced differences from those of conventional two dimensional electron systems investigated in the past. The basic question that we seek to answer is what happens to the tunneling as we approach the Dirac point of zero carrier concentration with the presence of electrically charged scatters. In the present work we consider the effects of atomic potential fluctuations in the setup depicted in fig. 1. At low doping the conductance is determined by quasiparticle tunneling, which is independent of the boundary conditions in the y-direction if $L \ll W$.

II. BACK SCATTERING IN GRAPHENE

A. General consideration

The quasiparticle excitation spectrum of the graphene-based junction consists of the positive eigenvalues of the Dirac equation. The Dirac equation has the form of two equations for electron $u(r)_{A,B}$ and hole wavefunctions $v(r)_{A,B}$. In this study we restrict ourselves to the single-valley Dirac equation for graphene

$$-i\hbar v_F \sigma \nabla u + Vu = \varepsilon u$$

where $u$ is a spinor of wave amplitudes for two nonequivalent sites of the honeycomb lattice. The Fermi energy $\varepsilon$ and the impurity potential $V(x, y)$ in the graphene sample $(0 < x < L)$ are considered to be much smaller than the Fermi energy $E_F$ in the ideal metallic leads $(x < 0$
and \( x > L \). For zero doping the conductance is determined by the states at the Dirac point, \( \varepsilon = 0 \). Transport properties at finite energies determine the conductance of doped graphene.

Since for aspect ratios \( W \gg L \) the boundary conditions in the \( y \)-direction are irrelevant, so we take periodic boundary conditions for simplicity. Different wave vectors \( q_n = 2\pi n/W \) (with \( n = 0, \pm 1, \pm 2, \ldots \) ) in the \( y \)-direction parallel to the interfaces (at the points \( x = 0 \) and \( x = L \)) and not coupled, so we can consider each transverse mode separately. Without impurity in the bulk at a given energy \( \varepsilon \) and transverse wave vector \( q \) we have up to two basis states

\[
u^\pm(x) = \frac{1}{\sqrt{\cos \alpha}} \chi_n(y) \exp \pm i k x \exp \pm i \alpha/2
\]

with the definitions

\[
\alpha(\varepsilon) = \arcsin [\hbar v_F q / (\varepsilon + E_F)], \quad k(\varepsilon) = (\hbar v_F)^{-1} (\varepsilon + E_F) \cos(\alpha)
\]

The angle \( \alpha \in (-\pi/2, \pi/2) \) is the angle between the initial and final wave vectors \( k_i = (k, q) |_{x=0} \) and \( k_f = (k, q) |_{x=L} \). With this sign convention the state \( u^+ \) move in the +x, while \( u^- \) move in the −x direction. The factor \( 1/\sqrt{\cos \alpha} \) ensure that two states carry the same particle current.

Considering a back scattering process \( k \rightarrow -k \) in an arbitrary external potential we will confine ourselves to states in the vicinity of the K point, but the extension to states near a K' point is straightforward. We have \( \alpha(k) = 0 \) and \( \alpha(-k) = \pi \). Rotation in spin space can be obtained through the replacement \((s, k_i) \rightarrow (s, -k_f)\) corresponding to the electron motion of a time-reversal path. When the wave vector \( k \) is rotated in the anticlockwise direction adiabatically as a function of time \( t \) around the origin for a time interval \( 0 < t < T \), the wavefunction is changed into \( u_i(k) \exp(-i \phi) \), where \( u_i(k) \) is the "spin" part of an eigenfunction of the Eq. \( \text{II} \) and \( \phi \) is Berry's phase. Choosing \( \phi(k) = \alpha(k)/2 \) in such a way that the wave function becomes continuous as a function of \( \alpha(k) \) and given by

\[
\phi = -i \int_0^T dt (u_s(k(t)) \left| \frac{d}{dt} u_s(k(t)) \right| = \pi
\]

This shows that the rotation in the \( k \) space by \( 2\pi \) leads to the change in the phase by +\( \pi \), i.e., a sign change. A similar phase change of back scattering process is the origin of the so-called anti-localization effect in systems with strong spin-orbit scattering [27]. This anti-localization effect was observed experimentally [28, 29]. The absence of back scattering can be destroyed by various effects. When the potential range becomes shorter than the lattice constant, the back scattering appears two reasons. The first is the appearance of inter-valley matrix elements between \( K \) and \( K' \) points [30]. The second, which we investigate in this work, is that the effective potential of an impurity for \( A \) and \( B \) sites in honeycomb lattice can be different. This causes mixing of the spin space and the momentum space.

### III. TRANSFER MATRIX APPROACH

We first determine the transfer matrix \( M_n(x, 0) \) of the \( n \)th mode \( u_n(x)e^{i\phi_n(y)} \) through the undoped graphene ribbon. The evolution of \( u_n(x) \) inside the graphene sample can be written as \( u_n(x) = M_n(x, 0)u_n(0) \), where the transfer matrix \( M_n(x) \) should satisfy a generalized unitarity condition

\[
M^{-1} = \sigma_x M^\dagger \sigma_x
\]

In general Eq[I] (ignoring an irrelevant scalar phase factor) restricts \( M \) to a three-parameter form

\[
M = e^{i\alpha_1 \sigma_y} e^{i\alpha_2 \sigma_x} e^{i\alpha \sigma_z}
\]

The real parameters \( \alpha_1, \alpha_2, \alpha \) depend on the boundary at the scale of the lattice constant and they cannot be determined from the Dirac equations. In this work we consider the ideal interfaces \( x = 0 \) and \( x = L \) case, when \( \alpha_1 = 0 = \alpha_2 \). From the Dirac Eq[I] we obtain the differential equation

\[
\frac{d}{dx} M_n(x, 0) = \left( \frac{i\varepsilon}{\hbar v_F} \sigma_z + q_n \sigma_x \right)
\]

with solution for \( V(x, y) = 0 \)

\[
M_n(x, 0) = \cos k_n x + \frac{\sin k_n x}{k_n} \left( \frac{i\varepsilon}{\hbar v_F} \sigma_x + q_n \sigma_z \right)
\]

where \( k_n = \sqrt{(\varepsilon/m)^2 - q_n^2} \) is the longitudinal wave vector, \( q_n \) is the transversal wave vector. The total transfer matrix through the impurity-free graphene ribbon \( (0 < x < L) \) is

\[
M_{\text{tot}} = M(L, 0)e^{i\alpha \sigma_z} M(0, 0)
\]
potential given by a diagonal matrix, i.e.,
\[ V = \begin{pmatrix} \gamma_A \delta(x-x_0) & 0 \\ 0 & \gamma_B \delta(x-x_0) \end{pmatrix} \]  
(12)

where \( \gamma_A, \gamma_B \) is the corresponding microscopic potential and smooth on atomic scales, which is localized along a line \( x = x_0 \) and placed in the zone corner \( K (K') \) of sublattice \( A (B) \). The Fermi-energy \( \varepsilon \) and impurity potential \( V \) (Eq.12) in graphene sample \( 0 < x < L \) are considered to be much smaller than the Fermi-energy \( E_F \) in the ideal metallic leads \( x < 0 \) and \( x > L \). For zero doping the conductance is determined by the states at the Dirac point, \( \varepsilon = 0 \). Transport properties at finite energies determine the conductance of doped graphene.

The great physical and analytical advantage of the \( M \) matrix is that it is multiplicative. In order to obtain transfer matrix for disorder region (along line \( x = x_0 \)) graphene \( M_d \), we integrate Eq. 1

\[ \lim_{\nu \to 0} \int_{x_0 - \nu}^{x_0 + \nu} (-i \hbar v_F \sigma \cdot \nabla u + Vu) dx = \lim_{\nu \to 0} \int_{x_0 - \nu}^{x_0 + \nu} \varepsilon u dx \]

Making use of well-known algebraic property for Pauli matrices

\[ \sigma_x^2 = \sigma_y^2 = \sigma_z^2 = -i \sigma_x \sigma_y \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]  
(13)

we easily obtain the final form for total transfer matrix \( M \) in disorder graphene sample

\[ M_{tot} = M(L,0)e^{i \widetilde{\varepsilon}_A \sigma_z} M_d e^{i \Phi \sigma_x} M(0,0) \]  
(14)

where

\[ M_d = \begin{pmatrix} 1 & \tilde{\gamma}_A \\ \tilde{\gamma}_B & 1 \end{pmatrix} \]  
(15)

and \( \tilde{\gamma}_{A(B)} = -i \gamma_{A(B)}/\hbar v_F \). The transfer matrix of the whole sample is straightforwardly related to the matrices of transmission and reflection amplitudes

\[ M \equiv M_{tot} = \begin{pmatrix} 1/t^{\dagger} & -r^{\dagger}/t^{\dagger} \\ -r/\tilde{t} & 1/t \end{pmatrix} \]  
(16)

The conductance of the graphene strip is expressed through the transmission amplitudes by the Landauer
formula

\[ G = g_0 \sum_{n=0}^{N-1} T_n, \quad g_0 = \frac{4e^2}{h} \]  \hspace{1cm} (17)

where \( T = \text{Tr}[t^\dagger t] \). At the Dirac point \( V_{\text{gate}} = 0 \) the transmission probability for the case \( N \gg W/L \) reads

\[ T_n = \frac{1}{(\cos \frac{\alpha}{2} + P \sin \frac{\alpha}{2})^2 \cosh^2 \left[ \pi (n + \frac{1}{2}) \frac{L}{W} \right]} \]  \hspace{1cm} (18)

When parameters \( P = 0 \) and \( \alpha = 0 \) the Eq.18 reduces to equation \( 4 \), derived in the paper \[31\]. Parameter \( P = |\gamma_A - \gamma_n| \) represents atomic potential fluctuations, when finite \( P \ll h v_F \).

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