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Electron scattering in graphene by impurities with electric and magnetic dipole moments

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ABSTRACT

The elastic electron scattering by impurities with electric and magnetic dipoles in graphene is studied with the help of Born approximation. Both types of scatterers give the nonzero cross section of backscattering. The scattering by the impurities with electric dipoles is more efficient even comparing to the scattering by the nanomagnets with anomalous magnetic moments. A comparison of the electron scattering transport cross sections by charged impurities and impurities with electric dipole moments shows that they can be comparable. The scattering by the impurities electric dipoles can be important in limiting the electron mobility in graphene along with the Coulomb scattering.

1. Introduction

The elastic electron scattering in graphene by different type of scatterers has been intensively studied since it was experimentally isolated (see [1], and references therein). It is known that the backscattering cross section of massless electrons by the impurities with radially symmetric potentials is equal to zero. But it is not true for the scattering by electric and magnetic dipoles that possess non-radially symmetric potentials. Nonzero backscattering can considerably increase the transport cross section that has a much larger effect on current than the small-angle scattering [2].

The electron scattering in graphene has been studied via scattering phases [1,3] and with the help of 2D Born approximation [3–6]. It is interesting that there are many different versions of 2D Born approximation proposed including the “self-consistent Born approximation” [7]. Various mechanisms of electron scattering of massless Dirac fermions have been discussed in Ref. [8].

To study the electron scattering cross section by electric and magnetic dipoles, we developed our version of the Born approximation for the one layer graphene based on results of Ref. [9]. The calculated cross sections are not zero for the backscattering in both cases. Our analysis shows that the scattering by electric dipoles is more efficient than the scattering by magnetic dipoles. But only very large nanomagnetic impurities with gigantic magnetic moments [10] can provide the scattering cross section comparable with that one by the electric dipoles. A comparison of the transport cross sections by Coulomb potential and by electric dipoles shows that they could be comparable.

The paper is designed as follows. In Section 2, we present the Born approximation for the scattering problems on the basis of 2D Dirac like equation of massless electrons. In Section 3, we calculate the electron cross section by an impurity with radially symmetric electrostatic potential to compare our result with the known results [3]. In Sections 4 and 5, we consider the electron scattering by the impurity with electric and magnetic dipole moments, respectively. In Section 6, we analyze and compare the obtained transport cross sections. The conclusion summarizes the results of the paper.

2. Born approximation

The Hamiltonian of 2D motion of the massless electron in graphene in the external field U can be written as [1]

$$\hat{H} = v_F \hat{\sigma} \cdot \left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A} \right) + U, \tag{1}$$

where v_F is the Fermi velocity, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ are the Pauli matrices, e and c are the electron charge and speed of light in vacuum, respectively; $\hat{\mathbf{p}}$ is the 2D momentum operator, $\mathbf{A}$ is the vector potential. The Schrodinger equation corresponding to the Hamiltonian (1)

$$\hat{H}\Psi = E\Psi, \tag{2}$$

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with

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \tag{3}$$

can be presented as a system of coupled equations

$$v_F \hat{\pi}_+ \psi_1 = (E-U)\psi_2,$$
$$v_F \hat{\pi}_- \psi_2 = (E-U)\psi_1, \tag{4}$$

where ψ_1, ψ_2 are the wave functions, $\hat{\pi}_\pm = \hat{p}_\pm - eA_\pm/c$, $\hat{p}_\pm = \hat{p}_x \pm i\hat{p}_y$, $A_\pm = A_x \pm iA_y$ with $\hat{p}_x$, $\hat{p}_y$ and A_x, A_y being the components of the momentum operator and the vector potential, respectively.

Substitution of ψ_2 from the first equation of (4) in the second one and vice versa allows one to decouple system (4)

$$\hat{\pi}_- \frac{1}{(E-U)} \hat{\pi}_+ \psi_1 = \frac{E-U}{v_F^2} \psi_1, \tag{5}$$

$$\hat{\pi}_+ \frac{1}{E-U} \hat{\pi}_- \psi_2 = \frac{E-U}{v_F^2} \psi_2. \tag{6}$$

In the scattering problems we are interested in the solutions of these equations far from the scattering center, where the energy of the incident electrons E is much greater than the average potential energy of the scattering center $\overline{U}$. For $|\overline{U}|/E < 1$, Eqs. (5) and (6) can be presented as follows:

$$\hat{\pi}_- \left\{ 1 + \frac{U}{E} + \frac{U^2}{(E)^2} + \cdots \right\} \hat{\pi}_+ \psi_1 = \frac{E^2}{v_F^2} \left(1 - \frac{U}{E} \right) \psi_1, \tag{7}$$

$$\hat{\pi}_+ \left\{ 1 + \frac{U}{E} + \frac{U^2}{(E)^2} + \cdots \right\} \hat{\pi}_- \psi_2 = \frac{E^2}{v_F^2} \left(1 - \frac{U}{E} \right) \psi_2. \tag{8}$$

Taking into account the explicit expressions of $\hat{\pi}_+$ and $A_\pm$ (see their definitions after system (4)), one can show that

$$\hat{\pi}_- \hat{\pi}_+ = \hat{p}^2 + \frac{e^2}{c^2} A^2 - \frac{e}{c} [2\mathbf{A} \cdot \hat{\mathbf{p}} + \hbar B_z],$$
$$[\hat{\pi}_+, \hat{\pi}_-] = 2\frac{e\hbar}{c} B_z, \tag{9}$$

where $B_z = (\nabla \times \mathbf{A})_z$ is the z component of the magnetic field and $[\hat{\pi}_+, \hat{\pi}_-]$ denotes a commutator. Here we chose the Coulomb gauge

$$\nabla \cdot \mathbf{A} = 0. \tag{10}$$

In the scattering problems, the terms containing the vector potential $\mathbf{A}$ and U are being small compared to the energy of electron E. We put them in the right hand side of Eqs. (7) and (8) keeping only terms linear on U/E and obtain the following equation for functions $\psi_{1,2}$:

$$(\nabla^2 + k^2)\psi_{1,2} = \hat{V}_{1,2} \psi_{1,2}. \tag{11}$$

Here we introduced the wave vector $k = E/(\hbar v_F)$ and operator

$$\hat{V}_{1,2} = \frac{1}{\hbar^2} \left\{ \frac{e^2}{c^2} A^2 - \frac{e}{c} [2\mathbf{A} \cdot \hat{p} \pm \hbar B_z] + \frac{EU}{v_F^2} + \hat{\pi}_\mp \frac{U}{E} \hat{\pi}_\pm \right\}. \tag{12}$$

It consists of two parts: terms associated with the vector potential $\mathbf{A}$ and the corresponding component of magnetic field B_z transversal to the graphene plane, and terms associated with the potential energy of electron U. It is worth noting that this part of $V_{1,2}$ contains the space derivatives of U. the two Eqs. in (11) are independent and specify the wave functions $\psi_{1,2}$ of electrons belonging to different sublattices of graphene.

At large distances from the scattering center due to the smallness of the operator $\hat{V}_{1,2}$, the functions $\psi_{1,2}$ can be presented as

$$\psi_{1,2} = \psi_{1,2}^{(0)} + \psi_{1,2}^{(1)}, \tag{13}$$

where $\psi_{1,2}^{(1)}$ are the small corrections to the functions $\psi_{1,2}^{(0)}$, which satisfy the two Eqs. in (11) with the zeroth right hand side. If the beam of incident electrons propagates along the x-axis, then $\psi_{1,2}^{(0)} = 1/\sqrt{2}\, \exp(ikx)$. The incident wave function can be written as

$$\Psi_{inc}(x) = \begin{pmatrix} \psi_1^{(0)} \\ \psi_2^{(0)} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \exp(ikx). \tag{14}$$

The factor $1/\sqrt{2}$ provides the normalization of the wave function (14) to unity. The wave functions $\psi_{1,2}^{(1)}$ satisfy the equation

$$(\nabla^2 + k^2)\psi_{1,2}^{(1)} = \hat{V}_{1,2} \psi_{1,2}^{(0)}. \tag{15}$$

At large distances from the scattering center, $\psi_{1,2}^{(1)}$ have the form

$$\Psi_{sc} = \begin{pmatrix} \psi_1^{(1)} \\ \psi_2^{(1)} \end{pmatrix} = \frac{\exp(ikr)}{\sqrt{r}} \begin{pmatrix} f_1(\varphi) \\ f_2(\varphi) \end{pmatrix}. \tag{16}$$

The functions $f_{1,2}(\varphi)$ are analogous to the scattering amplitudes with the scattering angle φ. They have dimension of the square root of length and are controlled by the scattering mechanism.

The 2D differential cross section or the differential cross length is a ratio of the scattered current J_{sc} through the elementary length dl (transversal to the radius vector $\mathbf{r}$) and the incident current J_{inc}

$$d\sigma(\varphi) = \frac{J_{sc}}{J_{inc}} dl. \tag{17}$$

The incident current is directed along the x-axis and equals to

$$J_{inc} = v_F \Psi_{inc}^+ \hat{\sigma}_x \Psi_{inc} = v_F. \tag{18}$$

The scattered current can be calculated as

$$J_{sc} = \sqrt{J_x^2 + J_y^2}, \tag{19}$$

where J_x and J_y are the components of the scattered current given by

$$J_x = v_F \Psi_{sc}^+ \hat{\sigma}_x \Psi_{sc},$$
$$J_y = v_F \Psi_{sc}^+ \hat{\sigma}_y \Psi_{sc}. \tag{20}$$

With the help of the wave functions (16), we obtain

$$J_x = \frac{2v_F}{r} Re[f_1(\varphi)^* f_2(\varphi)],$$
$$J_y = \frac{2v_F}{r} Im[f_1(\varphi)^* f_2(\varphi)]. \tag{21}$$

The differential cross (17) with account of Eqs. (19) and (21) can be presented as

$$\frac{d\sigma(\varphi)}{d\varphi} = 2|f_1(\varphi)^* f_2(\varphi)|. \tag{22}$$

This formula will be used below for obtaining the cross section of electron scattering in graphene by impurities with nonsymmetric scattering potentials.

3. Scattering by impurity with radially symmetric electrostatic potential

To check the obtained result, we calculate the electron scattering cross-section by a nonmagnetic impurity with the radially symmetric electrostatic potential $U(r)$. In this case, operator (12) with account of $\mathbf{A}=0$ takes the form

$$\hat{V}_{1,2} = \left(\frac{U}{E} k^2 + \frac{1}{\hbar^2} \hat{p}_\mp \frac{U}{E} \hat{p}_\pm \right). \tag{23}$$

It is convenient to use the rectangular coordinate system with the x-axis along the incident electron beam. With account of the