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THE HALL CONDUCTIVITY OF A DOPED GRAPHENE IN A QUANTIZING MAGNETIC FIELD

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In this paper we study the electron energy spectrum corresponding to Landau levels in doped graphene when an external magnetic field is applied in the direction normal to the graphene planar sheet. The derived dispersion relation for the electrons in the doped graphene allows us to determine the dependence of the electrical conductivity on the applied magnetic field. This relationship between electrical conductivity and applied magnetic field is further analyzed for different characteristics of the impurities; specifically the potential of hybridization and the energy of the adsorbed atom.

Keywords: Hall conductivity; Landau levels; graphene.

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1. Introduction

Graphene is of great scientific interest not only because of the prospects for future use in microelectronics,[1,2] but also because of the wealth of nonclassical, surprising and unusual effects evidenced experimentally and awaiting to be explained theoretically. The uniqueness of the physical characteristics of graphene is well epitomized by the Hall effect, caused by an unusual relativistic dispersion of quasiparticles driving an electric current. For instance, fractional and integer quantum Hall effects in graphene show different features in comparison with the effects obtained with a classical two-dimensional electron gas.

It is well known that the application of a magnetic field to conductors forces the conduction electrons to move — within the semiclassical framework — in a limited region of space with a discrete and uniformly distributed set of energy levels. Such quantized orbits are called the Landau levels. In graphene, these levels

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are nonuniformly distributed since the conduction electrons behave as massless fermions, whose speed does not depend on their energy. Recently, experimental evidences confirmed the theoretical predictions about the unusual properties of the Landau levels in graphene.[3] One has however to note that in practice, most likely, a manufactured graphene will contain a certain level of impurities. Moreover, the inclusion of specific impurities can enrich the number of surprising graphene properties. Thus, the present study is devoted to shedding some light on the impact of impurities on the electron energy spectrum of doped graphene layers.

2. Model for the Graphene Layer

The Hamiltonian for graphene in the long-wave approximation reads

$$H = v_{\mathrm{F}}(\sigma_x p_x + \sigma_y p_y)\,, \tag{1}$$

where v_{F} is the Fermi velocity, σ_x and σ_y stand for Pauli matrices, p_x and p_y the quasi-momentum components.[4] Note that the Hamiltonian (1) is appropriate near one of the Dirac points K and acts in the space of wave functions $\psi = (\psi_A, \psi_B)$ which correspond to the wave functions of electrons localized on A and B sublattices, respectively. Consider that next to the atoms of the sublattices A and B, the localized impurities can be present, and the corresponding Hamiltonian in the space of wave functions can be written as $\psi = (\psi_A, \psi_B, \phi_A, \phi_B)$, where ϕ_A and ϕ_B correspond to the wave functions of electrons localized on the impurity, which is located near the graphene atom of A and B sublattices, respectively. In this space, the Hamiltonian has the form

$$H = \begin{pmatrix} 0 & v_{\mathrm{F}}(p_x - ip_y) & V & 0 \\ v_{\mathrm{F}}(p_x + ip_y) & 0 & 0 & V \\ V & 0 & \epsilon_a & 0 \\ 0 & V & 0 & \epsilon_a \end{pmatrix}, \tag{2}$$

where V is the hybridization potential, and ϵ_a is the energy of the absorbed atom with respect to the Fermi level. Let us now turn to an external magnetic field B directed perpendicular to the graphene plane. In this study, we chose the gauge $\mathbf{A} = (-B_y, 0, 0)$, with $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$. Note that in the presence of the electromagnetic field, momentum must be replaced by the generalized momentum, $p \to p - qA/c$, where q is the electron charge, and c is the speed of light in vacuum. Thereafter we set $c = \hbar = 1$ unless explicitly stated otherwise, so that $p_\alpha = i\partial_\alpha$. By making the substitution

$$\psi \to \phi \exp(ikx)\,, \tag{3}$$

and introducing the dimensionless coordinate $y = l_m \bar{y}$ ($l_m = 1/\sqrt{qB}$ being the "magnetic length"), we define the operators

$$a = \frac{1}{\sqrt{2}}\left(\bar{y} + \frac{\partial}{\partial \bar{y}}\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(\bar{y} - \frac{\partial}{\partial \bar{y}}\right),$$

which satisfy the commutation relations $[a, a^\dagger] = 1$. With the above notations, the Hamiltonian takes the form

$$H = \begin{pmatrix} 0 & \omega_c a & V & 0 \\ \omega_c a^\dagger & 0 & 0 & V \\ V & 0 & \epsilon_a & 0 \\ 0 & V & 0 & \epsilon_a \end{pmatrix}, \tag{4}$$

where $\omega_c = v_{\mathrm{F}}\sqrt{2qB}$ is the cyclotron frequency.[5,6] Note that a and $a^\dagger$ are the creation (annihilation) operators, and hence, the Hamiltonian (4) can be diagonalized in the basis of wave functions $\phi = (a_1|n\rangle, a_2|n-1\rangle), a_3|n\rangle, a_4|n-1\rangle$, where $|n\rangle$ is the eigenfunction of a harmonic oscillator corresponding to the nth energy level, and $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$. With this choice of eigenfunctions, the problem of finding the energy spectrum, is reduced to finding the eigenvalues of the Hamiltonian

$$H = \begin{pmatrix} 0 & \omega_c\sqrt{n} & V & 0 \\ \omega_c\sqrt{n} & 0 & 0 & V \\ V & 0 & \epsilon_a & 0 \\ 0 & V & 0 & \epsilon_a \end{pmatrix}. \tag{5}$$

It is easy to prove that the energy spectrum of the problem is given by the following relations, which correspond to the four Landau levels in a doped graphene

$$E_n = \begin{pmatrix} \frac{1}{2}\epsilon_a + \frac{1}{2}h_n + \frac{1}{2}\sqrt{(\epsilon_a - h_n)^2 + 4V^2} \\ \frac{1}{2}\epsilon_a + \frac{1}{2}h_n - \frac{1}{2}\sqrt{(\epsilon_a - h_n)^2 + 4V^2} \\ \frac{1}{2}\epsilon_a - \frac{1}{2}h_n + \frac{1}{2}\sqrt{(\epsilon_a + h_n)^2 + 4V^2} \\ \frac{1}{2}\epsilon_a - \frac{1}{2}h_n - \frac{1}{2}\sqrt{(\epsilon_a + h_n)^2 + 4V^2} \end{pmatrix}, \tag{6}$$

where $h_n = \omega_c\sqrt{n}$ $(n = 0, 1, 2\ldots)$.

Kubo formula for the calculation of the conductivity has the form[8]

$$\sigma_{ij} = \frac{e^2\hbar}{\Omega}\sum_{n\neq n'}\frac{(f_{pn} - f_{pn'})\,\mathrm{Im}[\langle pn|v_i|pn'\rangle\langle pn'|v_j|pn\rangle]}{(E_{pn} - E_{pn'})(E_{pn} - E_{pn'} + i\delta^+)}, \tag{7}$$

where $\delta^+ \to 0^+$, Ω is the Berry surface, and f_{pn} is the Dirac distribution function:

$$f_{pn} = \frac{1}{\exp[\beta(E_{pn} - \mu) + 1]}, \tag{8}$$

and μ is the chemical potential. Note that E_{pn} in Eq. (7) refers to any energy level in the system (not necessarily the Landau level). In the Heisenberg representation the velocity operator has the form

$$v_j = \frac{1}{i\hbar}[r_j, H], \quad (j = x, y, z). \tag{9}$$

The matrix form of the operators of velocities v_x and v_y is as follows:

$$v_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad v_y = i \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{10}$$

3. Results of the Numerical Analysis

The derived expressions for the off-diagonal conductivity σ_{xy} [see Eq. (7)] have been analyzed numerically. Figure 1 shows a typical dependence of conductivity on the magnitude of the magnetic field for different values ϵ_a of the energy of the impurity atoms. Note that such a behavior of the conductivity is associated with the movement of electrons in a magnetic field given the complex nature of the Landau levels (6) and the presence of the Fermi distribution function in Eq. (7). This leads to a decrease in susceptibility when the magnetic field becomes large enough, since most of the electrons will occupy the lowest Landau level. In other words, the effective size of the region of localization of electrons becomes rather small, which leads to a decrease in the transport characteristics. The region of negative conductivity, in our opinion, is associated with transitions between Landau levels similarly to semiconductor systems.[10,11] To demonstrate the strong influence of the hybridization potential on the Hall conductivity we present in Fig. 2 similar dependences for a value of V almost three times smaller than the one considered in Fig. 1. To be even more transparent at this point, we would like to refer to Fig. 3, where the conductivity is plotted for different values of hybridization potential. It is important

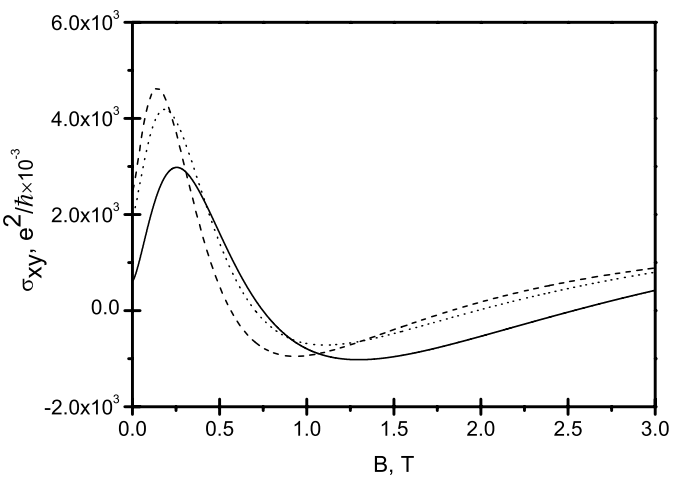

Fig. 1. The dependence of conductivity on the magnetic field for different values of the energy of the impurity atoms ($V = -1.43$ eV): (i) solid line, $\epsilon_a = -4$ eV; (ii) dotted line, $\epsilon_a = -5$ eV; (iii) dashed line, $\epsilon_a = -6$ eV.

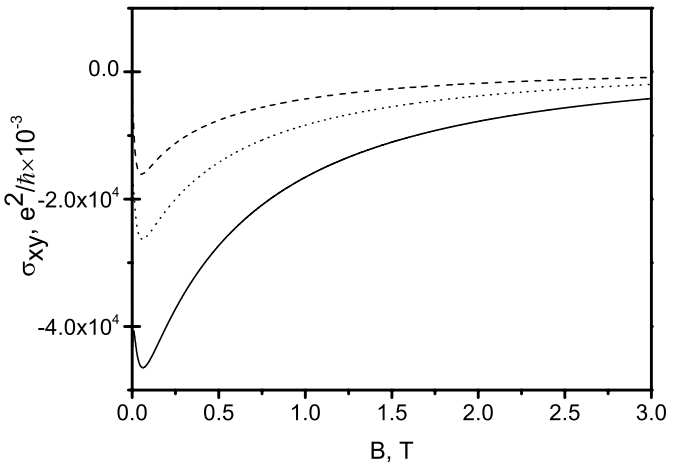

Fig. 2. The dependence of conductivity on the magnetic field for different values of the energy of the impurity atoms ($V = -0.5$ eV): (i) solid line, $\epsilon_a = -4$ eV; (ii) dotted line, $\epsilon_a = -5$ eV; (iii) dashed line, $\epsilon_a = -6$ eV.

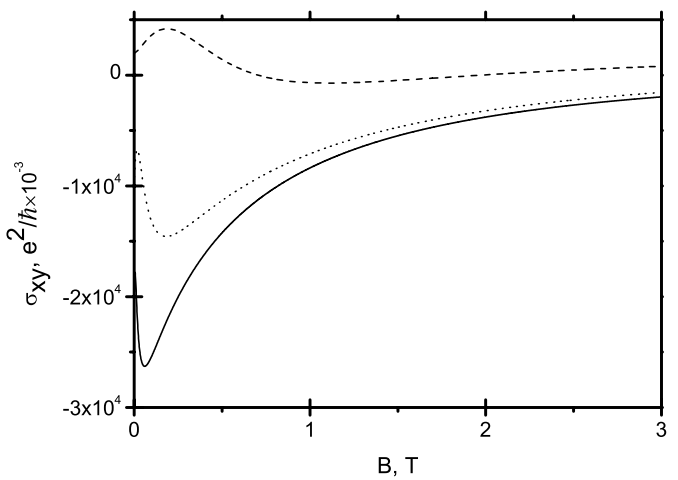

Fig. 3. The dependence of conductivity on the magnetic field for different values of the hybridization potential of the impurity atom and atom graphene lattice ($\epsilon_a = -5$ eV): (i) solid line, $V = -0.5$ eV; (ii) dotted line, $V = -0.7$ eV; (iii) dashed line, $V = -1.43$ eV.

to emphasize that we are working in the frame of long-wavelength approximation. More specifically, it is supposed that the levels should be nondegenerate and the strong inequality $E/B \ll \sqrt{\Delta/2m}$ (Δ is the bandgap) holds.[12] It means that our approach is quantitatively correct in the domain of strong enough magnetic field B and/or large hybridization potential V.

As can be seen from Fig. 1 that with an increase in absolute value of the adsorption energy, the magnitude of the peak corresponding to positive Hall conductivity

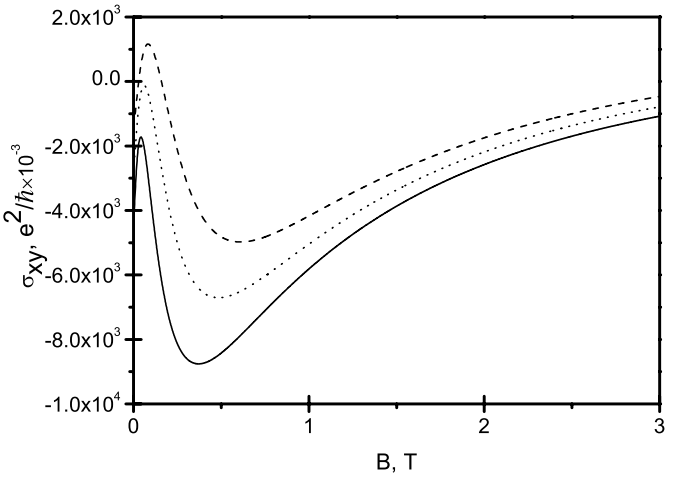

Fig. 4. The dependence of conductivity on the magnetic field for different values of the hybridization potential of the impurity atom and atom graphene lattice ($\epsilon_a = -5$ eV): (i) solid line, $V = -0.9$ eV; (ii) dotted line, $V = -1$ eV; (iii) dashed line, $V = -1.1$ eV.

increases, and the peak shifts toward lower values of the magnetic field. At the same time, the magnitude of the peak corresponding to negative Hall conductivity decreases. This behavior can be associated with hops of the Larmor orbit centers,[13] which are responsible for the appearance of absolute negative conductivity.

Figure 4 demonstrates the dependence of the Hall conductivity on the magnetic field for three different values of the hybridization potential in the vicinity of $V = -1$ eV. With the increase in the absolute value of the hybridization potential, the peak of the positive conductivity increases and shifts toward higher values of the magnetic field, while the peak of negative conductivity decreases in absolute value. This behavior is also related to the hops of the Larmor orbit centers.[13] Thus, with an increase in the absolute value of the hybridization energy V, the electrons become more strongly associated with the adsorption centers and, accordingly, the Larmor orbits hops are less likely, therefore leading to a decrease in the effect of absolute negative conductivity.

Note that a state with absolute negative conductivity is unstable and would not be observed experimentally. As already noted in Ref. 11, the experimental observations indicate a splitting into domains, in which the current flows in different directions, which in turn will lead to a state with zero conductivity. With increasing magnetic field the domains will merge, and eventually the formation of a single domain will again lead to nonzero conductivity.

Based on Eq. (6), one can say that a stronger influence of hybridization on the conductivity can be attributed to the change of the electron mobility and the structure of the Landau levels. Note that similar effects have been observed in other systems with intricate electronic spectra.[14,15]

4. Conclusions

In conclusion, the main results of this work can be summarized as follows:

(i) Landau levels in doped graphene subjected to a constant external magnetic field applied in the direction perpendicular to its plane were calculated
(ii) The dependence of of electrical conductivity on the magnetic field has been studied taking into account the Landau levels. The presence of impurities has a significant influence on this quantity.
(iii) When increasing the potential of hybridization of the electron clouds of graphene and impurity atoms, the extent of the negative conductance region decreases, which is assumed to be due to the influence of the magnetic field on the impurity levels of the system.

Acknowledgments

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