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Scattering of charge carriers by point defects in bilayer graphene

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Theory of scattering of massive chiral fermions in bilayer graphene by radial symmetric potential is developed. It is shown that in the case when the electron wavelength is much larger than the radius of the potential the scattering cross-section is proportional to the electron wavelength. This leads to the mobility independent on the electron concentration. In contrast with the case of single-layer, neutral and charged defects are, in general, equally relevant for the resistivity of the bilayer graphene.

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Bilayer graphene, that is a two-dimensional allotrope of carbon formed by two graphite atomic sheets [1], is a subject of hot interest now [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12] motivated by anomalous character of the quantum Hall effect [1, 2] and electron transmission through potential barriers [3] due to electron chirality and the Berry phase 2π , possible use of the bilayer graphene as a tunable-gap semiconductor [6] and its other unusual physical properties (for review, see Ref.10). At the same time, it is less studied than the single-layer graphene [13, 14]. In particular, almost nothing is known about mechanisms of scattering determining the electron transport in the bilayer graphene. Here we consider this problem theoretically. It will be shown that for any kind of point defects with small enough concentration their contribution in the resistivity is inversely proportional to the charge carrier concentration resulting in the concentration-independent electron mobility. In a framework of perturbation theory, this result has been obtained earlier in Ref.5 (see their Eq.(52)); we have generalized it on a case of a strong impurity potential. This situation is essentially different from the single-layer case when the scattering by Coulomb potential of charge impurities leads to the concentration-independent mobility whereas the short-range scattering centers are almost irrelevant [15, 16, 17, 18].

The bilayer graphene in a simplest approximation can be considered as a zero-gap semiconductor with parabolic touching of the electron and hole bands described by the single-particle Hamiltonian [1, 2, 10]

$$H = \begin{pmatrix} 0 & -(p_x - ip_y)^2/2m \\ -(p_x + ip_y)^2/2m & 0 \end{pmatrix} \quad (1)$$

where $p_i = -i\hbar\partial/\partial x_i$ are electron momenta operators and $m \simeq 0.054m_e$ is the effective mass, m_e being the free-electron mass. This description is accurate at the energy scale larger than few meV, otherwise a more complicated picture including trigonal warping takes place; we will restrict ourselves only by the case of not too small doping when the approximate Hamiltonian (1) works. Two components of the wave function are originated from crystallographic structure of graphite sheets with two carbon atoms in the sheet per elementary cell. There are

two touching points per Brillouin zone, K and K' . For smooth enough external potential, no Umklapp processes between these points are allowed and thus they can be considered independently.

The Fourier component of the impurity potential with dimensionless charge Z at small enough wave vector equals

$$V(q) = \frac{2\pi Ze^2}{\epsilon(q + \kappa)}, \quad (2)$$

where $\kappa = 2\pi e^2 N(E_F)/\epsilon$ is the inverse screening radius, $\epsilon \simeq 2.5$ is the dielectric constant due to quartz substrate, and $N(E_F)$ is the density of states at the Fermi energy E_F [15, 16]. In the model (1) $\kappa = 4me^2/\hbar^2\epsilon$ where we take into account contributions from two spin projections and two valleys. Due to the smallness of the effective mass the screening radius is 4.5 times larger than the nearest-neighbor interatomic distances which makes the single valley approximation accurate enough. At the same time, for any reasonable doping the Fermi wave vector $k_F \ll \kappa$ so one can assume that the electron wavelength is much larger than the scattering potential radius.

Let us consider the case of small concentration of point defects (to be specific, we will call them impurities) with the concentration n_{imp} and the angle-dependent scattering cross-section $\sigma(\phi)$. Then the defect contribution to the resistivity ρ reads [19, 20]

$$\rho = \frac{2}{\epsilon^2 v_F^2 N(E_F) \tau(k_F)}, \quad \frac{1}{\tau(k_F)} = n_{imp} v_F \int_0^{2\pi} d\phi \frac{d\sigma(\phi)}{d\phi} (1 - \cos \phi) \quad (3)$$

where $v_F = \hbar k_F/m$ is the Fermi velocity, τ is the mean-free-path time. Note that the product $v_F N(E_F)$ is proportional to $k_F = \sqrt{\pi n}$ (n is the electron concentration) for both single-layer and bilayer graphene, as well as for conventional two-dimensional electron gas and thus any essential difference in their transport properties can be related only to the behavior of the scattering cross-section.

The expression (3) is derived from the standard Boltzmann equation and does not take into account localization (or antilocalization) corrections which can change the results drastically in the regime of small doping when the resistivity is of order of h/e^2 [21, 22, 23, 24] (recently the problem of weak localization has been considered also for the bilayer graphene [12]). We will restrict ourselves only by the case $\rho \gg h/e^2$; formal derivation of the Boltzmann equation for graphene in this regime will be published elsewhere [25].

To determine the scattering cross section one has to solve the two-dimensional Schrödinger equation with the Hamiltonian (1) plus impurity potential $V(r)$ which, after simple manipulations (cf. Ref.9) can be written in the form

$$\begin{aligned} \left(\frac{d}{dr} - \frac{l+1}{r}\right) \left(\frac{d}{dr} - \frac{l}{r}\right) g_l &= \left(k^2 - \frac{2mV}{\hbar^2}\right) f_l, \\ \left(\frac{d}{dr} + \frac{l+1}{r}\right) \left(\frac{d}{dr} + \frac{l+2}{r}\right) f_l &= \left(k^2 - \frac{2mV}{\hbar^2}\right) g_l. \end{aligned} \quad (4)$$

where $l = 0, \pm 1, \dots$ is the angular-momentum quantum number, $g_l(r) e^{il\phi}$ and $f_l(r) e^{i(l+2)\phi}$ are components of the pseudospinor wave function, r and ϕ are polar coordinates; to be specific we will consider the case of electrons $E = \hbar^2 k^2 / 2m > 0$.

Modifying a standard scattering theory [26] for the two-dimensional case one should try the solutions of Eq.(4) outside the region of action of the potential in the form

$$\begin{aligned} g_l(r) &= A \left[J_l(kr) + t_l H_l^{(1)}(kr) + c_l K_l(kr) \right], \\ f_l(r) &= A \left[J_{l+2}(kr) + t_l H_{l+2}^{(1)}(kr) + c_l K_{l+2}(kr) \right], \end{aligned} \quad (5)$$

where the terms proportional to Bessel (Hankel) functions describe incident (scattering) waves; the terms proportional to the Macdonald functions are analogous to the exponentially decaying solutions in the case of potential barrier [3]. To calculate the scattering cross section one has to find the current operator $\mathbf{j} = \frac{1}{\hbar} \frac{\delta H}{\delta \mathbf{k}}$ and its normal component $j_n = j_x \cos \phi + j_y \sin \phi$. The result reads:

$$j_n = -\frac{\hbar k}{m} \begin{pmatrix} 0 & e^{-2i\phi} \\ e^{2i\phi} & 0 \end{pmatrix}. \quad (6)$$

The Bessel and Hankel functions in Eq.(5) correspond to the expansion of the incident plane wave and scattered radial wave, respectively. Calculating the average value of the current operator (6) over the scattered wave we find for the cross section

$$\frac{d\sigma(\phi)}{d\phi} = \frac{2}{\pi k} \left| \sum_{l=-\infty}^{\infty} t_l e^{il\phi} \right|^2, \quad (7)$$

which is formally the same expression as for the case of single-layer graphene [18].

The Schrödinger equation (4) has as important symmetry with respect to replacement $f \longleftrightarrow g, l \longleftrightarrow -l-2$ which means $t_l = t_{-l-2}$. This is the consequence of chiral properties of electrons with the Berry phase 2π ; a similar identity for the single-layer case with the Berry phase π reads [18] $t_l = t_{-l-1}$. Thus, Eq.(7) can be rewritten in the form

$$\frac{d\sigma(\phi)}{d\phi} = \frac{2}{\pi k} \left| t_{-1} + 2 \sum_{l=0}^{\infty} t_l \cos[(l+1)\phi] \right|^2. \quad (8)$$

To understand the behavior of the scattering parameters $t_l(k)$ in the interesting limit $k \rightarrow 0$ one can consider the simplest case of the potential $V(r) = V_0$ at $r < a$ and $V(r) = 0$ at $r > a$. Strictly speaking, a sharp jump of the potential with atomic scale is beyond applicability of our approach since it will induce Umklapp processes between the valleys. We assume that the boundary is smooth enough in comparison with the interatomic distance but much thinner than the electron wavelength (cf. Ref.3). The solution outside the potential well has the form (5), with $A = 1$ and the solution for $r < a$ regular at $r = 0$ can be tried as

$$\begin{aligned} g_l(r) &= \alpha_l J_l(qr) + \beta_l I_l(qr), \\ f_l(r) &= \sigma [\alpha_l J_{l+2}(qr) + \beta_l I_{l+2}(qr)], \end{aligned} \quad (9)$$

where $\sigma = \text{sign}(E - V_0)$ and $q = \sqrt{2m|E - V_0|}/\hbar$ is the wave vector inside the well. Using boundary conditions of continuity of the wave functions and their first derivatives at $r = a$ one can find the scattering parameters t_l as well as c_l, α_l and β_l (cf. the case of one-dimensional potential [3]).

For the case $l = -1$ taking into account identities $K_1(z) = K_{-1}(z), I_1(z) = I_{-1}(z), J_1(z) = -J_{-1}(z)$, and $H_1^{(1)}(z) = -H_{-1}^{(1)}(z)$ one can prove immediately that $c_{-1} = 0$ and $t_{-1} \propto (ka)^2$ at $ka \rightarrow 0$ so as we will see this contribution in the scattering cross section is negligible. Using asymptotic of the Macdonald and Hankel functions for $l > 2, z \rightarrow 0$

$$\begin{aligned} K_l(z) &\simeq \frac{1}{2} \left(\frac{2}{z}\right)^l (l-1)! - \frac{1}{2} \left(\frac{2}{z}\right)^{l-2} (l-2)!, \\ H_l^{(1)}(z) &\simeq -\frac{i}{\pi} \left(\frac{2}{z}\right)^l (l-1)! - \frac{i}{\pi} \left(\frac{2}{z}\right)^{l-2} (l-2)!, \end{aligned} \quad (10)$$

one can prove that for $l \geq 1$ and $ka \rightarrow 0$ both t_l and c_l are, at least, of order of $(ka)^{2l}$ or smaller and thus only s -channel ($l = 0$) contributes in the scattering cross section so that Eq.(8) can be rewritten as

$$\frac{d\sigma(\phi)}{d\phi} = \frac{8}{\pi k} |t_0(k)|^2 \cos^2 \phi. \quad (11)$$

For the single-layer graphene, $\sigma(\phi) \propto \cos^2 \phi/2$ and the back-scattering is forbidden. On the contrary, for the case of bilayer there is a strong suppression of the scattering at $\phi \simeq \pi/2$.

For the case $l = 0$ the wavefunctions outside the well (5) has the asymptotic form

$$\begin{aligned} g_l(r) &= 1 + t_0 + \tau_0 \left(\ln \frac{kr}{2} + \gamma \right) + \mathcal{O} \left((kr)^2 \ln kr \right), \\ f_l(r) &= -\frac{2i}{\pi} t_0 - \tau_0 \left(\frac{2}{(kr)^2} - \frac{1}{2} \right) + \mathcal{O} \left((kr)^2 \ln kr \right) \end{aligned} \quad (12)$$

where $\gamma \simeq 0.577\dots$ is the Euler constant, $\tau_0 = \frac{2i}{\pi} t_0 - c_0$. Using this we find that $t_0(k)$ tends to a finite complex number ($|t_0(k)|^2 \leq 1$) at $k \rightarrow 0$. Substituting this into Eqs.(11) and (3) one can find an estimation for the resistivity $\rho \simeq (h/4e^2) n_{imp}/n$. It seems to be in a qualitative agreement with the dependence of the resistance of bilayer graphene on the gate voltage measured in Ref.11. The same dependence of the resistivity on the charge carrier concentration takes place for the single-layer graphene with Coulomb scattering centers [15] whereas the point defects with short-range potential give much smaller resistivity [18] of order of $\rho \simeq (h/4e^2) n_{imp} a^2$. For the case of bilayer, on the contrary, there is, in general, no essential difference between charge impurities and neutral point defects such as, say, atomic-scale roughness of the substrate.

It is interesting to mention that the scattering by the short-range potential in the case of bilayer graphene is more efficient than not only in the case of the single-layer graphene but also for the conventional nonrelativistic two-dimensional electron gas where $t_0(k) \propto 1/\ln(ka)$ at $ka \rightarrow 0$ and thus [18, 27, 28]

$$\rho \simeq \frac{h}{4e^2} \frac{n_{imp}}{n \ln^2(k_F a)} \quad (13)$$

To summarize, we have proven that the scattering by point defects in bilayer graphene is more efficient than both in single-layer graphene and in conventional electron gas. The difference with the single-layer case is just due to vanishing density of states for the massless Dirac fermions whereas for the bilayer graphene (as well as for the conventional electron gas) it is constant. However, for the two-dimensional nonrelativistic electrons an arbitrary weak potential leads to formation of a bound state in the gap [29] which results in the logarithmic singularity of the scattering amplitude at small energies (see Eq.(13)). In the case of the bilayer, there is no gap and thus no localized states. As a result, the resistivity should be just inversely proportional to the Fermi energy, or, equivalently, to the charge carrier concentrations. This seems to be in agreement with the recent experimental data [11].

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