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Electrons scattering and conductivity in monolayer graphene

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ARTICLE INFO

Article history:

Available online 24 October 2012

Keywords:

Dirac equation
Graphene
Scattering matrix

ABSTRACT

Resonance electronic states and scattering by point defects are studied for the monolayer graphene solving the 2+1-dimensional Dirac equation. Exact S- and T-matrices are calculated for the model potential. This effective potential takes into account possible band asymmetry of the point defect potential matrix elements. Regularization of the scattering problem for a singular potential has been carried out. Asymptotic analysis allowed us to obtain the conductivity dependence on the Fermi level position in the low-energy limit. Numerical calculations were carried out in the wide range of electronic energies. The transport relaxation time behaves as $1/E$ in the limit of E tending to zero and oscillates around a constant value due to the resonance scattering at higher energy magnitudes.

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The main novel element in our works is the band asymmetry of the defect potential in the Dirac equation. This asymmetry appears naturally if the defect violates the symmetry between the sublattices. Our goal in this work is to continue the study of the electron scattering in graphene with short range defects. We use the suggested in [1,2] shell delta function potential model taking into account a local band symmetry violation arising due to the defect presence. We analyze effect of the electron scattering on the electronic transport in the monolayer graphene and compare our theoretical results with the available experimental data.

The Dirac equation describing electronic states in zero-gap graphene reads [3]

$$\left(-iv_F \hbar \sum_{\mu=1}^2 \sigma_{\mu} \partial_{\mu} - \sigma_3 \delta m v_F^2 \right) \psi = (E - V) \psi, \quad (1)$$

where v_F is the Fermi velocity, σ_{μ} are the Pauli matrices, $\psi(\mathbf{r})$ is the two-component spinor. Here δm is the local mass (gap) perturbation related to a local sublattices symmetry violation. Let us comment the use of the terms “gap” and “mass” in the paper. Electronic spectrum of graphene in the vicinity of the Dirac points can be approximated by the “relativistic” formula $E = \pm \sqrt{m^2 v_F^4 + \hbar^2 k^2 v_F^2}$. Here m is the effective mass in the critical point. The gap equals $E_g = 2m v_F^2$. In pristine graphene $m=0$. Defects can locally make $m \neq 0$ and consequently, $E_g \neq 0$. So, the mass perturbation means a local gap perturbation according to the physicist’s jargon placing mass and gap on the same footing.

The spinor structure takes into account the two-sublattice structure of graphene. $V(\mathbf{r})$ is the local perturbations of the chemical potential. A local mass (gap) perturbation can be induced by defects in the graphene film or in the substrate [4]. The perturbation matrix elements

$$\text{diag}(V_1, V_2) r_0 \delta(r - r_0) \quad (2)$$

are related to the a, b parameters as follows

$$-V_1 = a + b, \quad -V_2 = a - b \quad (3)$$

Solving the Dirac equation in regions $0 < r < r_0$ and matching these solutions at the circumference of the circle of radius $r=r_0$, we obtain the scattering matrix and a characteristic equation for the resonance states. Calculating the ratio of the out-going and in-going waves, we obtain the S-matrix components in the angular momentum representation:

$$S_j(\epsilon) = -\frac{\mathcal{F}_j^{(2)}}{\mathcal{F}_j^{(1)}}, \quad (4)$$

where $\mathcal{F}_j^{(\alpha)}$ is given by the formula:

$$\begin{aligned} \mathcal{F}_j^{(\alpha)} = & \left(J_{j-1/2}(\epsilon) H_{j+1/2}^{(\alpha)}(\epsilon) - J_{j+1/2}(\epsilon) H_{j-1/2}^{(\alpha)}(\epsilon) \right) - \\ & \left[(a-b) J_{j+1/2}(\epsilon) H_{j+1/2}^{(\alpha)}(\epsilon) + (a+b) J_{j-1/2}(\epsilon) H_{j-1/2}^{(\alpha)}(\epsilon) \right], \quad (5) \\ \alpha = & 1, 2. \end{aligned}$$

Poles of the scattering matrix (4) are determined by the characteristic equation

$$\mathcal{F}_j^{(1)}(\epsilon) = 0, \quad (6)$$

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or

$$(a - b)J_{j+1/2}^2(\epsilon) + (a + b)J_{j-1/2}^2(\epsilon) = i \left[(a - b)J_{j+1/2}(\epsilon)N_{j+1/2}(\epsilon) + (a + b)J_{j-1/2}(\epsilon)N_{j-1/2}(\epsilon) \right] = -i \frac{2}{\pi\epsilon} \quad (7)$$

Using the relations $H_n^{(1)}(z) = J_n + iN_n$, $H_n^{(2)} = J_n - iN_n$, we can write S-matrix as follows

$$S_j(\epsilon) = -\frac{A_j(\epsilon) - iB_j(\epsilon)}{A_j(\epsilon) + iB_j(\epsilon)} = \frac{B_j(\epsilon) + iA_j(\epsilon)}{B_j(\epsilon) - iA_j(\epsilon)}, \quad (8)$$

and, therefore, it can be presented in the standard form:

$$S_j(\epsilon) = \exp[i2\delta_j(\epsilon)], \quad (9)$$

where the scattering phase is given by the expression

$$\delta_j(\epsilon) = \arctan \frac{A_j(\epsilon)}{B_j(\epsilon)}. \quad (10)$$

Formulae (8), (9) show that the scattering matrix $S_j(\epsilon)$ is unitary on the continuum spectrum. The functions $A_j(\epsilon)$ and $B_j(\epsilon)$ are determined as follows

$$A_j(\epsilon) = -\left[(a + b)J_{j-1/2}^2(\epsilon) + (a - b)J_{j+1/2}^2(\epsilon) \right], \quad (11)$$

$$B_j(\epsilon) = -\frac{2}{\pi\epsilon} \left[(a + b)J_{j-1/2}(\epsilon)N_{j-1/2}(\epsilon) + (a - b)J_{j+1/2}(\epsilon)N_{j+1/2}(\epsilon) \right] + \left[J_{j+1/2}(\epsilon)N_{j-1/2}(\epsilon) - J_{j-1/2}(\epsilon)N_{j+1/2}(\epsilon) \right] \quad (12)$$

Asymptotic behaviour of the scattering phases and other scattering data at $\epsilon \rightarrow 0$ can be obtained expanding the cylinder functions for small arguments:

$$J_n(z) \sim \frac{1}{n!} \left(\frac{z}{2} \right)^n, \quad N_n(z) = \begin{cases} -\frac{\Gamma(n)}{\pi} \left(\frac{2}{z} \right)^n & \text{for } n > 0, \\ (2/\pi) \log(\gamma_E z/2) & \text{for } n = 0, \quad z \rightarrow 0, \end{cases} \quad (13)$$

where $\gamma_E \approx 0, 577$ is the Euler–Mascheroni constant, $\Gamma(n)$ is the gamma-function. Then we have for the scattering phases in the lower order in ϵ :

$$\tan \delta_{\pm 1/2} \approx (b \pm a) \frac{\pi}{2} \epsilon, \quad \epsilon \rightarrow 0, \quad (14)$$

$$\tan \delta_{\pm(n+1/2)} \approx \pm \pi (\epsilon/2)^{2n+1} (b \pm a) \quad \epsilon \rightarrow 0. \quad (15)$$

The transport cross section can be written in terms of the scattering phases (we have returned to dimensional variables here)

$$\Xi_{tr} = \frac{2r_0}{\epsilon} \sum_{j=\pm\frac{1}{2}, \pm\frac{3}{2}, \dots} \sin^2(\delta_{j+1} - \delta_j). \quad (16)$$

The transport relaxation time can be calculated using the following relation:

$$1/\tau_{tr} = N_I v_F \Xi_{tr}. \quad (17)$$

Taking into account the approximate formulae for phases (14), (15), the series (16) can be written in the following asymptotic form for $\epsilon \rightarrow 0$:

$$\Xi_{tr} = \frac{2r_0}{\epsilon} \left[(\delta_{1/2} - \delta_{-1/2})^2 + (\delta_{3/2} - \delta_{1/2})^2 + (\delta_{-3/2} - \delta_{-1/2})^2 + \dots \right. \\ \left. + (\delta_{n+1/2} - \delta_{n-1/2})^2 + (\delta_{-n-1/2} - \delta_{-n+1/2})^2 + \dots \right] \approx \epsilon r_0 \pi^2 [2a^2 + O(\epsilon)]. \quad (18)$$

Then the asymptotic formula for the transport relaxation time reads:

$$1/\tau_{tr} = \epsilon N_I v_F \pi^2 2a^2 [1 + O(\epsilon)] \quad (19)$$

It is seen from (19) that asymptotic behaviour of the relaxation time at $\epsilon \rightarrow 0$ is determined by the parameter a , i.e. by the symmetric component of the perturbation.

Let us consider now the Born approximation for the scattering amplitude. A series of works was dedicated recently to this point with controversial conclusions. The partial wave series for the transport cross section converges rather slowly. That is why we consider a behaviour of the transport cross section without the partial wave expansion. In return we can use the Born approximation in this limit. The Born formula for the scattering amplitude reads:

$$f^{Born}(p, \theta) = -\frac{1}{\hbar v_F} \sqrt{\frac{p}{8\pi}} V(\mathbf{q}), \quad (20)$$

where $\hbar\mathbf{q} = \hbar\mathbf{p} - \hbar\mathbf{p}'$ is the transferred momentum, $q = 2p \sin \theta/2$, $V(\mathbf{q})$ is the perturbation Fourier transform:

$$V(\mathbf{q}) = \int d^2r e^{-i\mathbf{q}\mathbf{r}} V(\mathbf{r}) = \int_0^\infty dr r V(r) \int_0^{2\pi} d\phi \exp[-iqr \cos \phi] \\ = 2\pi \int_0^\infty dr r V(r) J_0(qr). \quad (21)$$

Inserting the potential (2) into (21) we obtain

$$V_i(\mathbf{q}) \equiv V(p, \theta) = 2\pi V_i^0 r_0^2 J_0(2pr_0 \sin \theta/2). \quad (22)$$

Substituting (22) into (20) we obtain the scattering amplitude:

$$f_i^{Born}(p, \theta) = -\frac{2\pi r_0^2 V_i^0}{\hbar v_F} \sqrt{\frac{p}{8\pi}} J_0(2pr_0 \sin \theta/2), \quad (23)$$

Now we can calculate the transport cross section:

$$\Xi_{tr}^{Born} = \int_0^\pi d\theta (1 - \cos \theta) |f^{Born}(p, \theta)|^2 \\ = (pr_0) r_0 \left(\frac{V_i^0}{\hbar v_F r_0} \right)^2 \pi/2 \int_0^\pi d\theta \\ \times (1 - \cos \theta) J_0^2(2pr_0 \sin \theta/2). \quad (24)$$

This integral can be expressed in terms of the hypergeometric functions [5]:

$$\int_0^\pi d\theta (1 - \cos \theta) J_0^2(2pr_0 \sin \theta/2) = \Gamma \left(\begin{matrix} 1/2, & 3/2 \\ 2, & 1, & 1 \end{matrix} \right) \\ {}_3F_4(3/2, 1/2, 1, 2, 1, 1, 1; -(2pr_0)^2), \quad (25)$$

where $\Gamma \left(\begin{matrix} \alpha_1, & \alpha_2 \\ \beta_1, & \beta_2, & \beta_3 \end{matrix} \right) \equiv \frac{\Gamma(\alpha_1)\Gamma(\alpha_2)}{\Gamma(\beta_1)\Gamma(\beta_2)\Gamma(\beta_3)}$, $\Gamma(\alpha)$ is the gamma function, ${}_3F_4(\alpha_1, \alpha_2, \alpha_3; \beta_1, \beta_2, \beta_3, \beta_4; x)$ is the generalized hypergeometric function. It is determined by the series:

$${}_3F_4(\alpha_1, \alpha_2, \alpha_3; \beta_1, \beta_2, \beta_3, \beta_4; x) = \sum_{k=0}^\infty \frac{(\alpha_1)_k (\alpha_2)_k (\alpha_3)_k}{(\beta_1)_k (\beta_2)_k (\beta_3)_k (\beta_4)_k} \frac{x^k}{k!}, \quad (26)$$

where $(\alpha)_k = \frac{\Gamma(\alpha+k)}{\Gamma(\alpha)}$ is the rising Pochhammer symbol. When $pr_0 < 1$, we can neglect all higher terms of this series and obtain in result the transport scattering cross section $\Xi_{tr}^{Born} pr_0$. The Born approximation is here asymptotically exact in the limit $pr_0 \rightarrow 0$. It must be noted here that the limit of pr_0 , E_F , $k_B T$, $\hbar\omega$ tending to zero is obviously nontrivial and many-particle effects must be taken into account in this case. Notice that while the Fermi energy of a 3d system is really completely determined by its chemical content (apart from the temperature factor), the Fermi level position of the 2d system (the only example is now graphene) can be controlled by the field effect. Therefore, the Fermi energy of graphene can be considered as an easily variable parameter. The opposite limit of $pr_0 > 1$ is not actual for scattering on rare point defects. It can be urgent for

the model of random potential with large correlation radius and for the quantum dot model, but they are outside of the scope of this work. However, there exist at least two other possibilities to obtain the cross section behaviour, different from the power law $\Xi_{tr}^{Born} p r_0$. First of them corresponds to a random potential with the correlation radius $r_0 \gg a$. In this case one can consider scattering of electrons with $p r_0 \sim 1$.

Let us consider the limit of large angular momentum $j \gg 1$ using the Bessel function asymptotics [5]:

$$J_\nu(z) \sim \frac{1}{\sqrt{2\pi\nu}} \left(\frac{ez}{2\nu}\right)^\nu (1 + O(1/\nu)), \quad \nu \rightarrow \infty, \quad (27)$$

$$N_\nu(z) \sim -\sqrt{\frac{2}{\pi\nu}} \left(\frac{ez}{2\nu}\right)^{-\nu} (1 + O(1/\nu)), \quad \nu \rightarrow \infty, \quad (28)$$

$$H_\nu^{(1)}(z) \sim \frac{1}{\sqrt{2\pi\nu}} \left[\left(\frac{ez}{2\nu}\right)^\nu - 2i \left(\frac{ez}{2\nu}\right)^{-\nu} \right] (1 + O(1/\nu)), \quad \nu \rightarrow \infty, \quad (29)$$

where e is the base of natural logarithms. The characteristic equation takes the following form in the limit of $j \gg 1$:

$$\frac{a-b}{(2j+1)(2j-1)^{2j+2}} (e\epsilon)^{2j+2} + \frac{a+b}{(2j-1)(2j-1)^{2j}} (e\epsilon)^{2j} = ie \left[\frac{\epsilon}{2j-1} \left(\frac{a-b}{j+1/2} + \frac{a+b}{j-1/2} \right) - \frac{2}{2j-1} \right], \quad (30)$$

Our numerical analysis shows that the energy dependence of the relaxation time crosses over to an approximate constant at high energy, and position of the crossing-over point depends on the ratio a/b . The Boltzmannian conductivity is determined by the formula:

$$\sigma = \frac{e^2}{h} (E_F \tau_{tr} / \hbar), \quad (31)$$

where τ_{tr} is determined as follows

$$\tau_{tr}^{-1} = N_I \Sigma_{tr} \nu_F. \quad (32)$$

The mobility can be determined as the ratio:

$$\mu = \frac{\sigma}{en}, \quad (33)$$

where the carrier density at low temperature is determined as follows

$$n \equiv N/S = \frac{1}{2\pi} \left(\frac{E_F}{\hbar v_F} \right)^2. \quad (34)$$

Substituting (31) and (34) into (33) and taking account of the obtained in our work result for the transport cross section Σ_{tr} and the transport relaxation time τ_{tr} (see (32)) we find:

$$\mu = \frac{e v_F \tau_{tr}}{E_F}. \quad (35)$$

Notice that the obtained formula (35) is in good agreement with the experimental results published by Bolotin et al. in paper [6].

Using (19), (31), and (32) we conclude that the conductivity tends to a constant value in the limit $E_F \rightarrow 0$.

We considered the electron scattering problem in the monolayer graphene with short-range impurities. Characteristic for the electronic two-band theory band asymmetry of the potential is equivalently described by the scalar potential and the mass (gap) local perturbation. The crystal perturbation by a single impurity is modelled by the shell delta function potential. Exact explicit formulae for a single-impurity S-matrix and other scattering data have been obtained and analyzed for the short-range perturbation with the band-asymmetric potential. The characteristic equation for bound and resonance states is derived for this case. The obtained results are in good agreement with the experimental data [6] and can be useful for understanding of the graphene electron properties.

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