Electrons scattering in the monolayer graphene with the short-range impurities

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\textbf{A B S T R A C T}

Scattering problem for electrons in monolayer graphene with short-range perturbations of the types “local chemical potential” and “local gap” has been solved. Zero gap and non-zero gap kinds of graphene are considered. The determined S-matrix can be used for calculation of such observables as conductance and optical absorption.

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During the last years much attention was payed to the problem of the electronic spectrum of graphene (see a review [1]). Two-dimensional structure of it and a presence of the cone points in the electronic spectrum make actual a comprehensive study of the external fields effect on the spectrum and other characteristics of the electronic states described by the Dirac equation in the 2 + 1 space–time. We consider in this work the electrons scattering in the 2 + 1 Dirac equation model of the monolayer graphene due to the short-range perturbations. We do not take into account the inter-valley transitions. Particular attention to this case stems from the effectiveness of short-range scatterers in contrast to the long-range ones: an effect of the latter is suppressed by the Klein paradox [2].

Short-range potential impurities in graphene were considered in works [3–5]. In our work [6], a new model of the short-range impurities in graphene was considered taking into account the obvious fact that the Kohn–Luttinger matrix elements of the short-range perturbation calculated on the upper and lower band wave functions are not equal in a general case. This means that the perturbation must be generically described by a Hermitian matrix. We considered the diagonal matrix case corresponding to a presence of the potential and mass perturbation. The bound states dependence on the perturbation parameters was studied in [6] within the framework of this model.

In the present Letter we study the electrons scattering by the short-range impurities within the framework of the model suggested in [6].

The Dirac equation describing electronic states in graphene reads

\begin{equation}
\left( -i\hbar v_F \sum_{\mu=1}^{2} \gamma_\mu \partial_\mu - \gamma_0 (m + \delta m) v_F^2 \right) \psi = (E - V) \psi,
\end{equation}

where $v_F$ is the Fermi velocity of the band electrons, $\gamma_\mu$ are the Dirac matrices

\[ \gamma_0 = \sigma_3, \quad \gamma_1 = \sigma_1, \quad \gamma_2 = i\sigma_2, \]

$\sigma_i$ are the Pauli matrices, $2mv_F^2 = E_F$ is the electronic bandgap, $\psi(\mathbf{r})$ is the two-component spinor. The electronic gap can appear in the graphene monatomic film lying on the substrate because of the sublattices mutual shift [7]. The spinor structure takes into account the two-sublattice structure of graphene. $\delta m(\mathbf{r})$ and $V(\mathbf{r})$ are the local perturbations of the mass (gap) and the chemical potential. A local mass perturbation can be induced by defects in a graphene film or in the substrate [7]. We consider here the delta function model of the perturbation:

\begin{equation}
\delta m(\mathbf{r}) = -b\delta(\mathbf{r} - \mathbf{r}_0), \quad V(\mathbf{r}) = -a\delta(\mathbf{r} - \mathbf{r}_0),
\end{equation}

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where \( r \) and \( r_0 \) are respectively the polar coordinate radius and the perturbation radius. Such short-range perturbation was used in the \((3+1)\)-Dirac problem for narrow-gap and zero-gap semiconductors in [8]. The perturbation matrix elements

\[
\text{diag}(V_1, V_2) \delta(r - r_0)
\]

are related to the \( a, b \) parameters as follows

\[
-V_1 = a + b, \quad -V_2 = a - b.
\]

The delta function perturbation is the simplest solvable short-range model. Finite radius \( r_0 \) plays a role of the regulator and is necessary in order to exclude deep states of the atomic energy scale. The finite perturbation radius \( r_0 \) leads to the quasi-momentum space form-factor proportional to the Bessel function that justifies our neglect of transitions between the Brillouin band points \( K \) and \( K' \) [8].

Let us present the two-component spinor in the form

\[
\psi_j(r, t) = \frac{\exp(-iEt)}{\sqrt{T}} \left( f_j(r) \exp[i(j - 1/2)\varphi] \right. \left. g_j(r) \exp[i(j + 1/2)\varphi] \right),
\]

where \( j \) is the pseudospin quantum number; \( j = \pm 1/2, \pm 3/2, \ldots \). In opposite to the relativistic theory, this quantum number has nothing to do with the real spin and indicates a degeneracy in the biconic Dirac point. The upper \( f_j(r) \) and lower \( g_j(r) \) components of the spinor satisfy the equations set

\[
\begin{align*}
&\frac{df_j}{dr} + \frac{j}{r} f_j - (E - m)f_j = (a + b)\delta(r - r_0)f_j, \\
&\frac{dg_j}{dr} + \frac{j}{r} g_j - (E + m)g_j = (a - b)\delta(r - r_0)g_j.
\end{align*}
\]

These equations have a symmetry:

\[
f_j \leftrightarrow g_j, \quad E \to -E, \quad j \to -j, \quad a \to -a.
\]

Let us introduce the function \( \tilde{\psi}_j(r, t) \equiv f_j/g_j \). It satisfies the equation:

\[
1/[{(a + b)\psi_j^2 + (a - b)}]\left( \frac{d\psi_j}{dr} - \frac{2j}{r} \psi_j - E(\psi_j^2 + 1) \right) + \delta(r - r_0) = 0.
\]

Integrating in the vicinity of \( r = r_0 \)

\[
\lim_{\delta \to 0} \int_{\psi_j(r_0 - \delta)}^{\psi_j(r_0 + \delta)} \frac{d\psi_j}{(a + b)\psi_j^2 + (a - b)} = -1,
\]

we obtain the matching condition

\[
\arctan(\psi_j^+/(a + b)/(a - b)) - \arctan(\psi_j^+/(a + b)/(a - b)) = \sqrt{a^2 - b^2}, \quad a^2 > b^2,
\]

where \( \psi_j^+ \equiv \psi_j(r_0 - \delta) \), \( \psi_j^- \equiv \psi_j(r_0 + \delta) \), \( \delta \to 0 \). Excluding the spinor component \( g_j \) from the equation set Eq. (6), Eq. (7) in the domains \( 0 \leq r < r_0 \) and \( r > r_0 \), we obtain the second-order equation:

\[
\frac{d^2f_j}{dr^2} + \left[ E^2 - m^2 - \frac{j(j - 1)}{r^2} \right]f_j = 0.
\]

This equation is related to the Bessel one. We assume \( E \) to be real and satisfying the inequality \( E^2 \geq m^2 \). Then the general solution of Eq. (12) in the region \( 0 \leq r < r_0 \) reads

\[
f_j = C_1\sqrt{\kappa r}J_{j - 1/2}(\kappa r) + C_2\sqrt{\kappa r}N_{j - 1/2}(\kappa r),
\]

where \( \kappa = \sqrt{E^2 - m^2} \) is the principal value of the root; \( J_j(z) \) and \( N_j(z) \) are respectively the Bessel and Neumann functions. The constant \( C_2 \) vanishes in the domain \( 0 \leq r < r_0 \) since the solution must be regular at the origin. Expressing the \( g_j \)-component from Eq. (7), we can write

\[
g_j = \frac{\sqrt{E - m}}{E + m}\kappa rC_1J_{j + 1/2}(\kappa r).
\]

Thus

\[
\psi_j^-(\kappa r_0) = \frac{\sqrt{E + m}J_{j - 1/2}(\kappa r_0)}{\sqrt{E - m}J_{j + 1/2}(\kappa r_0)}.
\]

Then we can obtain from Eq. (11):

\[
\arctan\left(\frac{a + b}{a - b}\psi_j^-(\kappa r_0)\right) = \arctan\left(\frac{a + b}{a - b}\sqrt{\frac{E + m}{E - m}J_{j - 1/2}(\kappa r_0)}\right) - \sqrt{a^2 - b^2}.
\]
and, therefore,

\[
\varphi_j^+(\kappa r_0) = \frac{\sqrt{E+m} J_{j-1/2}(\kappa r_0) - (a - b) T(a, b) J_{j+1/2}(\kappa r_0)}{J_{j+1/2}(\kappa r_0) + (a + b) \sqrt{E+m} T(a, b) J_{j-1/2}(\kappa r_0)},
\]

(16)

where \(T(a, b)\) is given by the formula:

\[
T(a, b) = \begin{cases} \frac{\tan(\sqrt{a^2-b^2})}{\sqrt{a^2-b^2}} & \text{if } a^2 > b^2, \\ \frac{\tan(\sqrt{b^2-a^2})}{\sqrt{b^2-a^2}} & \text{if } b^2 > a^2. \end{cases}
\]

(17)

On the other hand, an expression for \(\varphi_j^+(\kappa r_0)\) can be written similarly to (14):

\[
\varphi_j^+(\kappa r_0) = \frac{f_j^+}{g_j^+} = \sqrt{\frac{E+m}{E-m}} H_{j-1/2}^{(2)}(\kappa r_0) + S_j H_{j+1/2}^{(1)}(\kappa r_0),
\]

(18)

where \(S_j(\kappa)\) is a phase factor of the out-going wave, i.e. S-matrix element in the angular momentum representation. Substituting Eq. (18) into Eq. (16), we obtain an explicit expression for \(S_j(E)\):

\[
S_j(E) = -\frac{\mathcal{F}_{j+1}^{(2)}}{\mathcal{F}_{j+1}^{(1)}},
\]

(19)

where

\[
\mathcal{F}_{j+1}^{(a)} = \left( J_{j-1/2}(\kappa r_0) H_{j+1/2}^{(a)}(\kappa r_0) - J_{j+1/2}(\kappa r_0) H_{j-1/2}^{(a)}(\kappa r_0) \right)
- T(a, b) \left[ \frac{E-m}{E+m} (a - b) J_{j+1/2}(\kappa r_0) H_{j+1/2}^{(a)}(\kappa r_0) + \frac{E+m}{E-m} (a + b) J_{j-1/2}(\kappa r_0) H_{j-1/2}^{(a)}(\kappa r_0) \right].
\]

(20)

Here \(\alpha\) takes values 0, 1. Since \(H_{n+1}^{(2)}(z) = H_{n+1}^{(1)}(z)\) for real \(z\), the scattering matrix is unitary everywhere on the continuum spectrum. Eq. (19) solves the electron scattering problem for the given potential. The denominator of \(S_j(E)\) is just the left-hand side of the characteristic equation derived in [6]. Imaginary roots of it correspond to the real energy eigenstates (bound states) lying in the gap, which were studied in that paper. The characteristic equation reads

\[
\mathcal{F}_{j+1}^{(1)}(\kappa r_0) = 0,
\]

(21)

or

\[
\left( J_{j-1/2}(\kappa r_0) H_{j+1/2}^{(a)}(\kappa r_0) - J_{j+1/2}(\kappa r_0) H_{j-1/2}^{(a)}(\kappa r_0) \right)
= T(a, b) \left[ \frac{E-m}{E+m} (a - b) J_{j+1/2}(\kappa r_0) H_{j+1/2}^{(a)}(\kappa r_0) + \frac{E+m}{E-m} (a + b) J_{j-1/2}(\kappa r_0) H_{j-1/2}^{(a)}(\kappa r_0) \right].
\]

(22)

Using the relations \(H_{n+1}^{(2)}(z) = J_n + i N_n, H_{n+1}^{(1)}(z) = J_n - i N_n\), we can write S-matrix in the form:

\[
S_j(E) = \frac{A_j(E) + i B_j(E)}{A_j(E) - i B_j(E)} = \frac{B_j(E) + i A_j(E)}{B_j(E) - i A_j(E)},
\]

(23)

and, therefore, it can be presented in the standard form [10]

\[
S_j(E) = \exp[i 2 \delta_j(E)],
\]

(24)

where the scattering phase is given by the expression

\[
\delta_j(E) = \arctan \frac{A_j(E)}{B_j(E)}.
\]

(25)

Formulae (23), (24) show that the scattering matrix \(S_j(E)\) is unitary on the continuum spectrum. The functions \(A_j(E)\) and \(B_j(E)\) are determined as follows

\[
A_j(E) = -T(a, b) \left[ (a + b) \sqrt{\frac{E+m}{E-m}} J_{j+1/2}(\kappa r_0) + (a - b) \sqrt{\frac{E-m}{E+m}} J_{j-1/2}(\kappa r_0) \right],
\]

(26)

\[
B_j(E) = T(a, b) \left[ (a + b) \left( \frac{E+m}{E-m} J_{j-1/2}(\kappa r_0) N_{j-1/2}(\kappa r_0) + (a - b) \sqrt{\frac{E-m}{E+m}} J_{j-1/2}(\kappa r_0) N_{j+1/2}(\kappa r_0) \right) 
+ \left( J_{j+1/2}(\kappa r_0) N_{j-1/2}(\kappa r_0) - J_{j-1/2}(\kappa r_0) N_{j+1/2}(\kappa r_0) \right) \right].
\]

(27)
It is seen from (25), (27) that all $\delta_j(E)$ vanish, when $a$ and $b$ tend to zero, i.e. in the absence of a perturbation. Using the Bessel functions expansion [9]

$$J_n(x) \sim (1/n!(x/2)^n, \quad (2/\pi) \log(y_Nx/2)$$

for $n > 0$, \hspace{1cm} (28)

$$N_n(x) \sim \begin{cases} \frac{(-G(n)/\pi)}{2}x^n & \text{for } n > 0, \\ \frac{(2/\pi) \log(y_Nx/2)}{2} & \text{for } n = 0 \end{cases}$$

we conclude that for the low-energy scattering $\kappa r_0 \ll 1$, $\delta_j(E)$ is small as $(\kappa r_0)^{j+1/2}$ except of $j = \pm 1/2$. Here $\log y_N$ is the Eyler-Mascheroni constant. In the case of small radius $r_0$ and low energy $E$ we can neglect all higher angular momentum partial waves taking into account only phases $\delta_j$ for $j = \pm 1/2$:

$$\tan \delta_{1/2}(E) = - T(a, b) \sqrt{\kappa r_0/2} \log(y_N\kappa r_0/2) - \frac{1}{\pi} (2/\kappa r_0) + T(a, b) (a + b) \sqrt{\kappa r_0/2} + (a - b) \sqrt{\kappa r_0/2} \pi \right\}, \quad \kappa r_0 \to 0,$$

$$\approx T(a, b) \frac{E + m}{E - m} (a + b) \pi \left(\frac{\kappa r_0}{2}\right), \quad \kappa r_0 \to 0,$$

$$\tan \delta_{-1/2}(E) = - T(a, b) \sqrt{\kappa r_0/2} \log(y_N\kappa r_0/2) + T(a, b) (a - b) \sqrt{\kappa r_0/2} + (a + b) \sqrt{\kappa r_0/2} \pi \right\}, \quad \kappa r_0 \to 0,$$

$$\approx - T(a, b) \frac{E - m}{E + m} (a - b) \pi \left(\frac{\kappa r_0}{2}\right), \quad \kappa r_0 \to 0.$$ 

We see that the phase is proportional to $\kappa r_0$ in the long-wave limit as it is necessary [10,4]. The scattering amplitude $f(\theta)$ and transport cross-section $\Sigma_{tr}$ can be expressed in terms of $S_j(E)$ as follow [4]:

$$f(\theta) = \frac{1}{i\sqrt{2\pi} \kappa} \sum_{j=\pm 1/2, \pm 3/2, \ldots} \left[S_j(E) - 1\right] \exp[i(j - 1/2)\theta],$$

$$\Sigma_{tr} = 2/\kappa \sum_{j=\pm 1/2, \pm 3/2, \ldots} \sin^2(\delta_{j+1} - \delta_j).$$

Near the resonance states the Breit–Wigner form of the phase is valid [10]:

$$\delta_j \approx \delta^{(0)}_j + \arctan \frac{\Gamma_j}{2\kappa(E^{(0)}_j - E)},$$

where $E^{(0)}_j$ and $\Gamma_j$ are respectively the position and width of the resonance level, $\delta^{(0)}_j$ is the slowly-varying potential scattering phase.

The presented above formulas can be used in order to calculate the Boltzmann conductivity [11]:

$$\sigma = \left(\frac{e^2}{2\pi^2 \hbar}\right) \frac{2E_f}{T} \frac{1}{T_{tr}},$$

where the transport relaxation time equals

$$1/T_{tr} = N_i \nu_F \Sigma_{tr}.$$  

(35)

Here $N_i$ is the areal impurity density, $E_f = \nu_F k_F$. The above equations transform a dependence of the scattering data on the Fermi energy and impurity perturbation parameters $a$ and $b$ into the correspondent dependence of the Boltzmann conductivity. Thus characteristic features of the scattering data determine a behaviour of the electric conductivity. Proper numeric calculations will be presented elsewhere.

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