Electrons scattering in the monolayer graphene with a band-asymmetric annular potential well

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Electron scattering in the monolayer graphene with short-range impurities modelled by the annular well with a band-asymmetric potential has been considered. Band-asymmetry of the potential resulted in the mass (gap) perturbation in the Dirac equation. Exact explicit formulae for the scattering matrix have been derived. The results are presented in terms of the scattering phases and in the geometrical form of a relation between some 2-vectors. It has a form of the orthogonality condition. An approximate calculation of observables in terms the scattering theory results is outlined.

I. INTRODUCTION

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. Short-range potential impurities in graphene were considered in works [1], [2], [3]. In our work [4], 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. The diagonal matrix case corresponding to a presence of the potential and mass perturbation was considered. Annular geometry of the perturbation allows us to exclude a perturbation at small distances, which are unphysical in a crystal. Delta function model of the short-range diagonal matrix perturbation was considered in our works [4], [5]. We study here the potential and mass well model. We consider scattering of electrons by this potential and obtain exact explicit formulae for the scattering data. We also discuss application of these formulae for calculation of observables.

II. BASIC EQUATIONS

The Dirac equation for electronic states in graphene for our model of matrix annular well described above reads

\[
\left(-i\hbar v_F \sum_{\mu=1}^{2} \alpha_\mu \partial_\mu - \beta (m + \delta m (r)) v_F^2 \right) \psi = (E - V (r)) \psi, \tag{1}
\]

where \( v_F \) is the Fermi velocity of the band electrons, \( \alpha_\mu, \beta \) are the Dirac matrices \( \beta = \sigma_3, \alpha_1 = \sigma_1, \alpha_2 = i\sigma_2, \sigma_i \) are the Pauli matrices, \( 2m v_F^2 = E_g \) is the electronic bandgap, \( \psi (r) \) 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 configuration of graphene. \( \delta m (r) \) and \( V(r) \) are the local perturbations of the mass (gap) and the chemical potential:

\[
V (r) = -a \Delta (r), \quad \delta m (r) = -b \Delta (r), \tag{2}
\]

where \( \Delta (r) \) is determined as follows

\[
\Delta (r) = \begin{cases}
0, & 0 \leq r < r_1 \quad \text{(region I)}, \\
1, & r_1 \leq r < r_2 \quad \text{(region II)}, \\
0, & r \geq r_2 \quad \text{(region III)}. 
\end{cases} \tag{3}
\]
Let us present the two-component spinor in the form
\[
\psi_j(r, t) = \frac{\exp(-iEt)}{\sqrt{r}} \begin{pmatrix} f_j(r) \exp[i (j - 1/2) \varphi] \\ g_j(r) \exp[i (j + 1/2) \varphi] \end{pmatrix},
\]
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
\[
\frac{dg_j}{dr} + \frac{j}{r} g_j - (E - m) f_j = (a + b) \Delta (r) f_j,
\]
\[
-\frac{df_j}{dr} + \frac{j}{r} f_j - (E + m) g_j = (a - b) \Delta (r) g_j.
\]
These equations have a symmetry:
\[
f_j \leftrightarrow g_j, \quad E \to -E, \quad j \to -j, \quad a \to -a.
\]

III. SCATTERING MATRIX AND CHARACTERISTIC EQUATION

When \( r \in [r_1, r_2) \) (in regions I and III), we obtain from eq. (5) and eq. (6):
\[
\frac{d^2 f_j}{dr^2} + \left[ E^2 - m^2 - \frac{j (j - 1)}{r^2} \right] f_j = 0.
\]
This equation is related to the Bessel one. Its solution in the region I reads:
\[
f_j(r) = C_1 \sqrt{kr} J_{j-1/2}(kr),
\]
\[
g_j(r) = C_1 \sqrt{\frac{E - m}{E + m}} \sqrt{kr} J_{j+1/2}(kr),
\]
where \( \kappa = \sqrt{E^2 - m^2} \), \( J_n(x) \) is the Bessel function.

Let us introduce the function \( \varphi_j(r) \):
\[
\varphi_j(r) \equiv \frac{f_j}{g_j}.
\]
We obtain from (9) and eq. (10) for the region \( 0 \leq r < r_1 \):
\[
\varphi'_j(\kappa r) = \sqrt{\frac{E + m}{E - m}} \frac{J_{j-1/2}(\kappa r)}{J_{j+1/2}(\kappa r)}
\]
We have from (3), (5), and (6) within the region II:
\[
\frac{dg_j}{dr} + \frac{j}{r} g_j - (E - m) f_j = (a + b) f_j,
\]
\[
-\frac{df_j}{dr} + \frac{j}{r} f_j - (E + m) g_j = (a - b) g_j.
\]
These equations can be re-written in the form
\[
\frac{dg_j}{dr} + \frac{j}{r} g_j - \left( \bar{E} - \bar{m} \right) f_j = 0,
\]
\[
-\frac{df_j}{dr} + \frac{j}{r} f_j - \left( \bar{E} + \bar{m} \right) g_j = 0,
\]
where $\bar{E} = E + a$, $\bar{m} = m - b$. Thus we have the following second-order equation in the region $r_1 \leq r < r_2$:

$$\frac{d^2 f_j}{dr^2} + \left[ \frac{\bar{E}^2 - \bar{m}^2 - j(j-1)}{r^2} \right] f_j = 0. \quad (17)$$

Then the function $\varphi_j(r)$ can be written in the region II as follows:

$$\varphi_j^I(r) = \sqrt{\frac{E + \bar{m}}{E - \bar{m}}} \frac{J_{j-1/2}(\bar{\kappa}r) + C_j N_{j-1/2}(\bar{\kappa}r)}{J_{j+1/2}(\bar{\kappa}r) + C_j N_{j+1/2}(\bar{\kappa}r)}, \quad (18)$$

where $\bar{\kappa}^2 = \bar{E}^2 - \bar{m}$. Similarly we obtain for the region III:

$$\varphi_j^III(r) = \sqrt{\frac{E + \bar{m}}{E - \bar{m}}} \frac{H_{j-1/2}^{(2)}(\bar{\kappa}r) + S_j H_{j-1/2}^{(1)}(\bar{\kappa}r)}{H_{j+1/2}^{(2)}(\bar{\kappa}r) + S_j H_{j+1/2}^{(1)}(\bar{\kappa}r)} \quad (19)$$

Continuity of the spinor components leads to matching conditions for the functions $\varphi_j(r)$ at the boundaries between regions I, II and III. We obtain in result the following expressions for the coefficients $C_j$ and $S_j$:

$$C_j = -\frac{\sqrt{E + \bar{m}}}{\sqrt{E - \bar{m}}} \sqrt{\frac{J_{j-1/2}(\bar{\kappa}r_1) J_{j+1/2}(\bar{\kappa}r_1) - J_{j+1/2}(\bar{\kappa}r_1) J_{j-1/2}(\bar{\kappa}r_1)}{J_{j+1/2}(\bar{\kappa}r_1) J_{j+1/2}(\bar{\kappa}r_1) - J_{j-1/2}(\bar{\kappa}r_1) J_{j-1/2}(\bar{\kappa}r_1)}}, \quad (20)$$

$$S_j = -\frac{F_j^{(2)}}{F_j^{(1)}}, \quad (21)$$

where

$$F^{(\alpha)} = \sqrt{\frac{E + \bar{m}}{E - \bar{m}}} H_{j-1/2}^{(\alpha)}(\bar{\kappa}r_2) \left[ J_{j+1/2}(\bar{\kappa}r_2) + C_j N_{j+1/2}(\bar{\kappa}r_2) \right] - \sqrt{\frac{E + \bar{m}}{E - \bar{m}}} H_{j+1/2}^{(\alpha)}(\bar{\kappa}r_2) \left[ J_{j-1/2}(\bar{\kappa}r_2) + C_j N_{j-1/2}(\bar{\kappa}r_2) \right] \quad (22)$$

The constant $C_j$ is determined by the formula (20). Here $\alpha$ takes values 0, 1. The constant $S_j$ is a phase factor of the outgoing wave, i. e. the S-matrix element in the angular momentum representation. Since $H_{n}^{(2)}(z) = H_{n}^{(1)*}(z)$ for real $z$, the scattering matrix is unitary everywhere on the continuous spectrum. Equations (20), (21) and (22) solve the electron scattering problem for the given potential. The denominator of $S_j(E)$ is just the left-hand side of the characteristic equation for the bound and resonance electronic states:

$$F^{(1)} = 0 \quad (23)$$

or

$$\sqrt{\frac{E + \bar{m}}{E - \bar{m}}} H_{j-1/2}^{(1)}(\bar{\kappa}r_2) \left[ J_{j+1/2}(\bar{\kappa}r_2) + C_j N_{j+1/2}(\bar{\kappa}r_2) \right] - \sqrt{\frac{E + \bar{m}}{E - \bar{m}}} H_{j+1/2}^{(1)}(\bar{\kappa}r_2) \left[ J_{j-1/2}(\bar{\kappa}r_2) + C_j N_{j-1/2}(\bar{\kappa}r_2) \right] = 0. \quad (24)$$

Excluding the constant $C_j$ from eq. (21) and eq. (24), we obtain the explicit formula for $S_j$ and the characteristic equation:

$$\sqrt{\frac{E + \bar{m}}{E - \bar{m}}} \left[ J_{j+1/2}(\bar{\kappa}r_1) J_{j-1/2}(\bar{\kappa}r_1) - J_{j-1/2}(\bar{\kappa}r_1) J_{j+1/2}(\bar{\kappa}r_1) \right] \sqrt{\frac{E + \bar{m}}{E - \bar{m}}} \left[ J_{j+1/2}(\bar{\kappa}r_1) J_{j-1/2}(\bar{\kappa}r_1) - J_{j-1/2}(\bar{\kappa}r_1) J_{j+1/2}(\bar{\kappa}r_1) \right] = \sqrt{\frac{E + \bar{m}}{E - \bar{m}}} \left[ H_{j-1/2}^{(1)}(\bar{\kappa}r_2) - H_{j+1/2}^{(1)}(\bar{\kappa}r_2) \right]. \quad (25)$$
When \( r_1 = 0, r_2 = r_0 \), we have a case of the simple round well; the characteristic equation takes the form:

\[
\sqrt{\frac{E + m}{E - m}} J_{j-1/2} (\tilde{r} r_0) H^{(1)}_{j+1/2} (\kappa r_0) = \sqrt{\frac{E + m}{E - m}} J_{j+1/2} (\tilde{r} r_0) H^{(1)}_{j-1/2} (\kappa r_0)
\]  

(26)

A geometric interpretation of these expressions for the S-matrix and characteristic equation can be done here. Let us introduce the following column vectors:

\[
\mathbf{J}_j (r_1) = \begin{pmatrix} J_{j,1} \\ J_{j,2} \end{pmatrix} \equiv \begin{pmatrix} \sqrt{\frac{E + m}{E - m}} J_{j+1/2} (\kappa r_1) \\ - \sqrt{\frac{E + m}{E - m}} J_{j-1/2} (\kappa r_1) \end{pmatrix},
\]

(27)

\[
\mathbf{h}_j^{(\alpha)} (r_2) = \begin{pmatrix} h_{j,1} \\ h_{j,2} \end{pmatrix} \equiv \begin{pmatrix} \sqrt{\frac{E + m}{E - m}} H^{(\alpha)}_{j+1/2} (\kappa r_2) \\ - \sqrt{\frac{E + m}{E - m}} H^{(\alpha)}_{j-1/2} (\kappa r_2) \end{pmatrix}
\]

(28)

and the matrix

\[
\hat{D}_j (r) = \begin{pmatrix} J_{j-1/2} (\tilde{r} r) & J_{j+1/2} (\tilde{r} r) \\ N_{j-1/2} (\tilde{r} r) & N_{j+1/2} (\tilde{r} r) \end{pmatrix}
\]

(29)

Then eq. (20) can be written as follows

\[
C_j = \frac{\mathcal{J}_j,1}{\mathcal{J}_j,2},
\]

(30)

where the vector \( \mathcal{J}_j = \begin{pmatrix} \mathcal{J}_{j,1} \\ \mathcal{J}_{j,2} \end{pmatrix} \) is determined as follows

\[
\mathcal{J}_j (r_1) = \hat{D}_j (r_1) \mathbf{J}_j (r_1).
\]

(31)

Similarly, introducing the transformed vector \( \mathbf{H}_j^{(\alpha)} (r_2) = \hat{D} (r_2) \mathbf{h}_j^{(\alpha)} (r_2) \), we can write the S-matrix (21), (22) in a simpler form:

\[
S_j = - \frac{\mathbf{H}_j^{(2)} \mathcal{J}_j,1 \mathbf{J}_j,2 + \mathbf{H}_j^{(2)} \mathcal{J}_j,2 \mathbf{J}_j,1}{\mathbf{H}_j^{(1)} \mathcal{J}_j,2 \mathbf{J}_j,1 + \mathbf{H}_j^{(1)} \mathcal{J}_j,1 \mathbf{J}_j,2},
\]

(32)

This formula can be written in another form introducing the components transposition operator \( \hat{D} = \tilde{\sigma}_1 \):

\[
S_j = - \frac{\hat{D}_j (r_1) \mathbf{J}_j,1 (r_1) \cdot \tilde{\sigma}_1 \hat{D}_j (r_2) \mathbf{h}_j^{(2)} (r_2)}{\hat{D}_j (r_1) \mathbf{J}_j,1 (r_1) \cdot \tilde{\sigma}_1 \hat{D}_j (r_2) \mathbf{h}_j^{(1)} (r_2)},
\]

(33)

where \( (\mathbf{a}, \mathbf{b}) \) is a scalar product of the vectors \( \mathbf{a} \) and \( \mathbf{b} \). The formula (33) can be re-written in the form:

\[
S_j = - \frac{\hat{K}_j \mathbf{J}_j (r_1) \cdot \mathbf{h}_j^{(2)} (r_2)}{\hat{K}_j \mathbf{J}_j (r_1) \cdot \mathbf{h}_j^{(1)} (r_2)},
\]

(34)

where the matrix \( \hat{K}_j \) is determined as follows

\[
\hat{K}_j = \hat{D}_j^\dagger (r_2) \tilde{\sigma}_1 \hat{D}_j (r_1).
\]

(35)

The characteristic equation now reads

\[
\left( \hat{K}_j \mathbf{J}_j (r_1), \mathbf{h}_j^{(1)} (r_2) \right) = 0
\]

(36)
IV. S- AND T-MATRIX PROPERTIES. POSSIBLE APPLICATIONS

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

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

(37)

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

$$S_j(E) = \exp[i2\delta_j(E)],$$

(38)

where the scattering phase is given by the expression

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

(39)

Formulae (37), (38) show once more 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:

$$A = \sqrt{\frac{E + m}{E - m}} J_{j+1/2} (\kappa r_2) \left[ J_{j+1/2} (\kappa r_2) + C_j N_{j+1/2} (\kappa r_2) \right] = \sqrt{\frac{E + m}{E - m}} J_{j+1/2} (\kappa r_2) \left[ J_{j-1/2} (\kappa r_2) + C_j N_{j-1/2} (\kappa r_2) \right],$$

(40)

$$B = \sqrt{\frac{E + m}{E - m}} N_{j+1/2} (\kappa r_2) \left[ J_{j-1/2} (\kappa r_2) + C_j N_{j-1/2} (\kappa r_2) \right] - \sqrt{\frac{E + m}{E - m}} N_{j-1/2} (\kappa r_2) \left[ J_{j+1/2} (\kappa r_2) + C_j N_{j+1/2} (\kappa r_2) \right],$$

(41)

where the constant $C_j$ is given by eq. (20). It is seen from (20), (40), and (41) that all $\delta_j(E)$ ($j=\pm1/2, \pm3/2, \ldots$) vanish, when $a$ and $b$ tend to zero, i.e. in the absence of a perturbation.

It is easy to show that the phase is proportional to $\kappa r_0$ in the long-wave limit as it is necessary [10], [2] (here $r_0 \sim r_1, r_2$) (see also [3]). The scattering amplitude $f(\theta)$ and transport cross-section $\Sigma_{tr}$ can be expressed in terms of $S_j(E)$ as follow [2]:

$$f(\theta) = \frac{1}{i\sqrt{2\pi\kappa}} \sum_{j=\pm1/2, \pm3/2, \ldots} [S_j(E) - 1] \exp[i(j - 1/2)\theta],$$

(42)

$$\Sigma_{tr} = 2/\kappa \sum_{j=\pm1/2, \pm3/2, \ldots} \sin^2(\delta_{j+1} - \delta_j).$$

(43)

In the vicinity of the resonance state energy, the Breit-Wigner form of the phase is valid [10]:

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

(44)

where $E_j^{(0)}$ and $\Gamma_j$ are respectively the position and width of the resonance level, $\delta_j^{(0)}$ is the slowly-varying potential scattering phase. The presented above formulae can be used in order to calculate the Boltzmann conductivity [11]:

$$\sigma = \left( \frac{e^2}{2\pi h} \right) \frac{2E_F}{\hbar} \tau_{tr},$$

(45)

where the transport relaxation time equals

$$1/\tau_{tr} = N_i v_F \Sigma_{tr}.$$  

(46)

Here $N_i$ is the impurities areal density, $E_F = v_F \kappa_F$. The above equations transform the scattering data 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.
On the other hand, the derived here formulae for scattering data can be used to obtain an approximate density of states and other observables in lower order to the impurities density. The exact explicit formula for one-impurity S-matrix obtained here, which allows us to calculate the scattering amplitudes, bound and resonance states, determines also the on-shell one-impurity T-matrix \[^{13}\]:

\[
T^\text{on}_j (E) = (1/i) \left[ S_j (E) - 1 \right]
\]

(47)

Corresponding off-shell T-matrix \(\hat{T}^{\text{off}} (k, k', E)\) (here \(k\) generically does not lie on the mass shell, i.e. \(k^2 + m^2\) can be not equal to \(E^2\) can be written in the form \[^{12}\]:

\[
T^{\text{off}} (k, k', E) = \left( \Psi_0 (k) \hat{T}^{\text{off}} (E) \Psi_0 (k') \right).
\]

(48)

where the transition operator \(\hat{T}^{\text{off}} (E)\) is determined by the operator equation \[^{13}\]:

\[
\hat{T}^{\text{off}} = \hat{U} - \hat{G}_0 \hat{T}^{\text{off}}.
\]

(49)

Here \(\hat{G}_0 = \hat{H}_0^{-1}\) is the operator inverse to the free Hamiltonian. All components of the product in eq. \(^{18}\) are determined at different energies: \(E, E (k)\) and \(E (k')\). Let us write the Lippmann-Schwinger equation \(^{49}\) for off-shell one-impurity T-matrix in the matrix form:

\[
T^{\text{off}} (k, k', E) = U (k - k') - \int d^2 q U (k - q) \gamma_{\mu} q_{\mu} + m - \gamma_0 E \overline{q^2 + m^2 - E^2 + i0} T^{\text{off}} (q, k', E),
\]

(50)

where the Fourier transform of the potential is determined as follows

\[
U (k - k') = \int d^2 r \exp \left[ -i (k - k') \cdot r \right] U (r) = 2\pi \sum_m \epsilon_m \cos m\theta \int_0^\infty drr J_m (kr) U (r) J_m (k'r),
\]

(51)

\[
\epsilon_m = \begin{cases} 1 & \text{if } m = 0, \\ 2 & \text{if } m \neq 0. \end{cases}
\]

(52)

\(\gamma_{\mu} = \beta \alpha_{\mu}, \gamma_0 = \beta, \theta\) is the angle between the vectors \(k\) and \(k'\).

Now we consider a question: how the obtained above formalae for scattering data can be used for calculation of observables in the monolayer graphene. It is seen from \(^{31}\) that in the case of the short-range perturbation, \(U (q)\) is a slowly-varying function. Then equation \(^{50}\) shows that the off-shell T-matrix is a slowly-varying function of \(k\) and \(k'\) as well. At the same time, it can be a sharp function of energy \(E\) in the vicinity of a resonance. Therefore, in the case of a narrow resonance, the most important information on the off-shell transition matrix is given by the on-shell matrix, which is determined by the S-matrix (see \(^{47}\)).

\[
T^{\text{off}} (k, k', E) \approx T^{\text{on}} (k, k', E) = 2i \sum_j \epsilon_{j-1/2} \cos \left[ (j - 1/2) \theta \right] \left( S_j (E) - 1 \right).
\]

(53)

Using the derived above explicit formula for S-matrix \(^{31}\) (or \(^{21}\)), an approximate formula for the off-shell one-impurity T-matrix in the momentum representation can be obtained. Substituting the partial-wave projection of the S-matrix \(^{38}\) into equation \(^{53}\), we can obtain an expression for the T-matrix, which can be used for approximate calculation of such observables as the density of states, for instance. The scattering phases \(\delta_j (E)\) are completely determined by the formulae \(^{40},^{11}\) and \(^{89}\) obtained in this paper. The electronic density of states and other observables for systems with non-overlapping impurity potentials can be calculated on the base of Lloyd’s formula (see, for instance, \[^{13}\]). The simplest approximation can be obtained in the lower-order approximation to the mass operator \(M (k, E)\) in the impurities density \(n\) using the mean T-matrix method for a random distribution of impurities \[^{13}\]:

\[
M (k, E) = n \langle k | T^{\text{off}} (E) | k \rangle
\]

(54)

Thus, having the above formulae for the scattering data, we can calculate the averaged over impurities distribution Green functions, density of states and the optical absorption coefficient. Results of such calculations will be published elsewhere.
V. CONCLUSION

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 annular well. Exact explicit formulae for a single-impurity S-matrix and other scattering data have been obtained and analyzed for the short-range perturbation modelled with a use of the annular well with the band-asymmetric potential. The characteristic equation for bound and resonance states is derived for the case. This equation was shown to have a form of 2-vectors orthogonality condition. Possible application of these results to description of kinetical and optical properties of graphene is discussed. A procedure of approximate calculation of observables based on a substitution of the off-shell T-matrix by the one-impurity on-shell T-matrix, which can be expressed in terms of an exact S-matrix in the vicinity of a sharp resonance is suggested. The obtained in this paper explicit formulae for S-matrix can be used in this procedure. As an elementary example of this approach, we considered an approximate calculation of the mass operator in graphene with non-overlapping defects.

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