The Scattering of Massive Holes by Supercritical Impurity

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Abstract. The properties of charge carriers in doped graphene are considered. The closed set of explicit equations determining the spectrum and wavefunctions of charge carriers for total angular momentum \( J = M + \frac{1}{2} = 0, \pm \frac{1}{2}, \pm \frac{3}{2}, \ldots \) is obtained for the case of the Coulomb potential modified at small distances. The critical values \( Z_{cr} \) of the dopant charge at which the energy level with the given quantum numbers crosses the lower continuum boundary are determined. For \( Z < Z_{cr} \) for several values of the orbital angular momentum dependence of the position of the energy level as a function of charge \( Z \) is obtained. For \( Z > Z_{cr} \), the position \( \varepsilon_0 \) and width \( \gamma \) of the lowest quasidiscrete state, which may manifest itself as a resonance in hole-dopant scattering, are calculated. It’s shown that there is no electron-hole pairs creation because of unitarity of the partial scattering matrix.

1. Introduction

According to [1–3], the electronic properties of graphene doped by atomic nuclei or ions with charge \( Z \) can be described by the effective two-dimensional Dirac equation with the gap in electronic spectrum and with the Coulomb potential

\[
\hbar v_F \left( -i\sigma \frac{\partial}{\partial x} - \frac{q}{x} + \frac{m* v_F}{\hbar} \sigma_z \right) \Psi_E(x) = E \Psi_E(x) \tag{1}
\]

Here \( v_F \) is the velocity at the Fermi surface, \( x = (x_1, x_2) \), \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) are the Pauli matrices, \( q = Z \alpha_F \), \( \alpha_F = e^2/\hbar v_F \) is the effective fine structure constant for graphene, \( \Psi_E(x) \) - is the two-component wavefunction for an electron with the effective mass \( m* \) and energy \( E \).

In the case of doped graphene the energy spectrum of the two-dimensional heterostructure is absolutely similar to one for the three-dimensional Coulomb problem, including the case with the nuclear charge \( Z > 137 \), e.g. [4–6]. In [3] the authors discuss the screening by electrons created together with holes from the Dirac sea (by analogy with the three-dimensional case [8, 9]). In the present work, we demonstrate that such a mechanism of screening cannot be put into effect, see also [4–6], but resonances in the scattering of the holes by overcritical impurities occur.

Accounting for [3, 7] the gap width \( \Delta = 2m* v^2_F = 0.26 \text{ eV} \), the effective constant \( \alpha_F = 0.4 \) and the distance between carbon nuclei \( a_{cc} = 1.42 \text{ Å} \) for graphene deposited onto SiC substrate we have

\[
v_F = 5.5 \times 10^8 \text{ cm/s}, \quad m* = 7.6 \times 10^{-4} m_e, \quad a_{CC}/l_F = 5.5 \times 10^{-3}, \tag{2}
\]
where $m_e$ is the mass of the electron, $l_F = h/m_e v_F$ is the "Compton length" in graphene.

Owing to the axial symmetry, the conserving quantum number $|10]$ is the total angular momentum $J = M + 1/2$ (in $\hbar$ units), i.e., the eigenvalue of the generator for the two-dimensional rotations $-i\partial/\partial \varphi + 1/2\sigma_3$. The orbital angular momentum $M$ is the eigenvalue of the self-adjoint operator $-i\partial/\partial \varphi$ acting in the Hilbert space of square integrable functions on the circle $0 < \varphi < 2\pi$, which eigenfunctions are $[11, 12]$:

$$\Phi_M(\varphi) = \frac{1}{2\pi} e^{im\varphi}, \ M = \delta + m; \ \delta = 0, \frac{1}{2}, \ m = 0, \pm 1, \pm 2, \ldots$$

These functions realize irreducible single-valued ($\delta = 0$) or double-valued ($\delta = 1/2$) representations of $SO(2)$ group. In terms of

$$E = m_e v_F^2 \varepsilon, \ x = l_F \rho, \ \rho = (\rho \cos \varphi, \rho \sin \varphi),$$

the wavefunction with fixed total angular momentum is represented as:

$$\Psi_{\varepsilon, J}(\rho) = \frac{1}{\sqrt{2\pi \rho}} e^{iJ\varphi} \left( e^{-i\varphi/2} F(\rho) \right) \psi_{J, \rho}$$

2. Boundary conditions and short-range Coulomb problem

The functions $F(\rho)$ and $G(\rho)$ satisfy the two-dimensional Dirac equation:

$$H_D \Psi_{\varepsilon, J}(\rho) = \varepsilon \Psi_{\varepsilon, J}(\rho), \ H_D = \left( \begin{array}{cc} 1 - q \rho & j \rho + \frac{d}{d\rho} \\ j \rho - \frac{d}{d\rho} & -1 + q \rho \end{array} \right), \ \Psi_{\varepsilon, J} = \left( \begin{array}{c} F(\rho) \\ G(\rho) \end{array} \right), \ J = M + \frac{1}{2},$$

which up to the notation coincides with the set of equations for the radial functions for the three-dimensional problem [8]. In the two-dimensional case, however, half-integer values of $J = m + 1/2$, $m = 0, \pm 1, \pm 2, \ldots$ are possible.

The equation for the critical charge $q_{cr}^{(n)} = Z_n \alpha_F$, at which the $n$-th level with the given quantum number $J$ reaches the boundary of the lower continuum of the solutions of Eq. (5), was obtained in [4, 6]:

$$\arg \Gamma \left( 2i \sqrt{q_{cr}^{(n)}^2 - J^2} \right) = \sqrt{q_{cr}^{(n)^2} - J^2} \ln (2q_{cr}^{(n)}) - \theta_\tau(J) + \pi n, \ n = 0, 1, 2, \ldots$$

In these papers it was also shown that the parameters $\theta_\sigma(J)$ and $\theta_\tau(J)$ defining one-parameter families of self-adjoint radial Dirac hamiltonians, are defined by the following conditions:

$$\frac{u_\sigma}{u_{-\sigma}} = \left( \frac{u_\sigma}{u_{-\sigma}} \right)^* = \tan \theta_\sigma(J), \ -\frac{\pi}{2} \leq \theta_\sigma(J) \leq \frac{\pi}{2}, \ 0 < \sigma < 1/2$$

$$\frac{u_\tau}{u_{-\tau}} = \left( \frac{u_\tau}{u_{-\tau}} \right)^* = e^{2i\theta_\tau(J)}, \ Im \theta_\tau(J) = 0, \ \tau = \sqrt{q^2 - J^2} > 0, \ q > |J|,$$

$$u_{\pm \sigma} = \frac{\Gamma(\pm 2\sigma)(2\lambda)^{\pm \sigma}}{\Gamma(1 + \sigma - \frac{\pi}{4} \theta_\sigma(J))} \left[ q \sqrt{1 - \varepsilon} - (J \pm \sigma) \sqrt{1 + \varepsilon} \right]$$

1 The half-integer quantization of the orbital angular momentum comes into effect for two-dimensional quantum dots with an odd number of electrons [13]
Due to the Coulomb barrier in the lower continuum the width

\[ \varepsilon \]

The solutions of this equation determine both the position of a quasidiscrete level

\[ \text{stationary wavefunctions of (5) at any values of the charge} \]

\[ \varepsilon \]

dependence of the energy

states of holes corresponding to the poles of the scattering matrix

\[ S \]

\[ J \]

\[ J \]

\[ J \]

\[ J \]

\[ J \]

\[ J \]

Equation (5) with the replacement

\[ V_C(\rho) \rightarrow V_R(\rho) \]

at \( J \neq 0 \) has an analytical solution for

\[ f(\rho/R) \equiv 1. \]

Within the framework of this model we have

\[ \tan \theta_\sigma(J; R) = -\frac{(J + \sigma)q_{J+1/2\pm J}(q) \mp (J - \sigma)J_{\pm 1/2\pm J}(q)}{(J - \sigma)q_{J+1/2\pm J}(q) \mp (J + \sigma)J_{\pm 1/2\pm J}(q)}R^{\sigma}, \]

where \( J_\nu(q) \) is the Bessel functions with upper (lower) signs corresponding to \( J > 0 \) \( (J < 0) \)

respectively.

If \( q > |J| > 0 \), assuming in (9) \( \sigma = i\tau \), we obtain the equality

\[ \exp(2i\theta_\sigma(J; R)) = \tan \theta_\sigma(J; R), \quad \tau = \sqrt{q^2 - J^2} > 0, \quad J \neq 0 \]

The case of \( J = 0 \) may be solved analytically. This case was considered in [6], so we will consider cases with \( J \pm 1/2 \) and \( J = \pm 1 \).

Equation (6) determines the critical charge \( q_{cr}(J; R) \) as a function of the quantum number

\[ J \]

and the cutoff radius \( R \), see Table 1, whereas conditions (7) with (9) and (10) give the charge
dependence of the energy

\[ \varepsilon_J(q, R) \]

at the fixed cutoff radius (see Fig. 1).

The parameters \( \theta_\sigma(J; R) \) and \( \theta_\sigma(J; R) \)

completely determine the energy spectrum and

stationary wavefunctions of (5) at any values of the charge \( q = Z\alpha_F \).

In [4, 6] we obtained the equation for the spectrum of complex energies of quasistationary

states of holes corresponding to the poles of the scattering matrix \( S_J(k; q) = \exp(2i\delta_J(k; q)) \):

\[ \frac{(-2ik)^{i\tau}[q\sqrt{-\varepsilon - 1} + (iJ - \tau)\sqrt{-\varepsilon - 1}]\Gamma(-2i\tau)\Gamma(1 + i\tau - i\varepsilon q)}{(-2ik)^{-i\tau}[q\sqrt{-\varepsilon - 1} + (iJ + \tau)\sqrt{-\varepsilon - 1}]\Gamma(2i\tau)\Gamma(1 - i\tau - i\varepsilon q)} = e^{2i\theta_J(q; R)}, \]

The solutions of this equation determine both the position of a quasidiscrete level \( \varepsilon_0 \) and its

width \( \gamma \):

\[ \varepsilon_{qs} = -\varepsilon_p = \varepsilon_0 - \frac{i}{2} \gamma, \quad \varepsilon_0 > 0, \quad \gamma > 0, \]

Due to the Coulomb barrier in the lower continuum the width \( \gamma \ll 1 \)

\[ k = k_0' - ik_0'', \quad k_0' = \sqrt{\frac{2}{\varepsilon_0} - 1} > 0, \quad k_0'' = \frac{\gamma}{2k_0'} > 0, \]
Figure 1. Energy of the ground state $\varepsilon(q, J; R)$ versus the charge $q = Z\alpha_F$ for the Coulomb potential cutoff radius $R = 1/20$ for different values of quantum number $J$.

Figure 2. Positions of the quasidiscrete level $\varepsilon_0$ and its widths $\gamma$ versus the difference $q - q_{cr}$ at the cutoff radius $R = 1/20$ for $J = \pm 1/2$ and $J = \pm 1$. Values $\varepsilon^*$ and $\gamma^*$ are the position and width of the pole of $S$-matrix corresponding to the resonance, see Fig. 3:

a) for $J = 1/2$ at $q - q_{cr} = 0.3$ and for $J = -1/2$ at $q - q_{cr} = 0.16$;

b) for $J = 1$ at $q - q_{cr} = 0.34$ and for $J = -1$ at $q - q_{cr} = 0.29$.

and these poles are located on the second (unphysical) sheet [15], in accordance with the unitarity of the partial scattering matrix.

Figure 2 shows the position of the lowest quasidiscrete level $\varepsilon_0$ and its width $\gamma$ as a function of $q - q_{cr}$ for $J = \pm 1/2$ and $J = \pm 1$. If the hole energy $\overline{\varepsilon}$ is in the range of dramatic change of scattering phase, such states are evident as resonances in the hole-impurity scattering.

The scattering phases $\delta_J(\overline{\varepsilon}, q; R)$ for several $q = Z\alpha_F$ as functions of hole energy $\overline{\varepsilon} = -\varepsilon > 1$ for $J = \pm 1/2$ and $J = \pm 1$ when $q > q_{cr}$ are shown in Fig. 3. The values of $q$ are chosen so that the integer values of $Z$ were close to $Z_{cr}$ from Table 1 for SiC graphene with $\alpha_F = 0.4$. If the hole energy $\overline{\varepsilon}$ is in the range of dramatic change of scattering phase, such states are evident as resonances in the hole-impurity scattering and the partial cross-section $\sigma_J(\overline{\varepsilon}) = \sin^2 \delta_J$. 
Figure 3. Scattering phases $\delta_J(\varepsilon, q; R)$ as functions of hole energy for total momenta $J = 1/2, J = -1/2, J = 1, J = -1$. Resonances in the scattering of holes on impurity are marked with gears. Positions and widths of these resonances are given on Fig. 2. Dot-dashed line correspond to the asymptotic (13).

For controlling of numerical calculations asymptotic behaviour of scattering phases at small wavevectors $k = \sqrt{\varepsilon^2 - 1} \ll 1$ was used

$$\delta_J(k; q) \simeq \frac{q}{k} \left( \ln \frac{q}{k} - 1 \right) + \frac{\pi}{4} + O(k \ln k), \; k \ll 1. \quad (13)$$

3. Conclusions

Thus, the "cutoff" i.e., the regularization of the Coulomb potential at small distances, ensures that the Dirac Hamiltonian is self-adjoint both for two-dimensional and for three-dimensional problems. This implies that the one-particle approximation for the Dirac equation is consistent at any values of the Coulomb charge, including the overcritical range. It means that there is no spontaneous creation of electron-hole pairs. At the same time, owing to the presence of low permeable effective Coulomb barrier, the continuum states near the boundary of lower continuum form quasistationary states which may appear as resonances in the scattering of holes on supercritical impurity.

Since incident and diverging waves with total momentum $J$ are unitary equivalent, overcritical radial Coulomb problem differs markedly from "Klein paradox" [16]. Let’s consider the example with $J = 0$. 


Along with radial equation (1) with $J = 0$ with regularized potential determined in (8), we consider one-dimensional (along $z$ axis) Dirac equation

$$
\begin{pmatrix}
1 + V(\xi) & \frac{d}{d\xi} \\
-\frac{d}{d\xi} & -1 + V(\xi)
\end{pmatrix}
\begin{pmatrix}
F(\xi) \\
G(\xi)
\end{pmatrix} = \varepsilon
\begin{pmatrix}
F(\xi) \\
G(\xi)
\end{pmatrix},
$$

(14)

For the energy of the electron from upper (lower) continuum within the quasiclassical approximation we get $\varepsilon = \pm \sqrt{P^2(\xi) + 1 + V(\xi)}$. So, for the upper continuum bound $P(\xi) = 0$ we have $\varepsilon_+ = 1 + V(\xi)$, and for lower one $-\varepsilon_- = -1 + V(\xi)$, see Fig. 4a in the case of potential $V(\xi) = E \tanh \xi$, where $E > 1$ is the reduced electric field.

The electron-hole pair creation may be interpreted as tunneling of the electron from the Dirac sea to the upper continuum. The motion of the electron with $\varepsilon < -1$ should be considered as the "time-opposite" motion, see Fig. 4a. Such a tunneling is possible if the energetic spectra of these continua are overlapping. At the same time, in the radial problem electronic spectra does not overlap with hole one, see Fig. 4b.

This difference is related to the fact that in one-dimensional case the electron-hole pair is pulled apart by the electric field, whereas in the radial case both electron and hole are attracted to the impurity. So, spontaneous creation of electron-hole pairs do not realize in the relativistic Coulomb problem and it is an additional argument for the validity of one-particle approximation for the Dirac equation at $Z > Z_{cr}$.
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