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Dynamics of quasi-particles in graphene with impurities and sharp edges from the *kp*-method standpoint

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Dynamics of quasi-particles in graphene with an impurity and a sharp edge is considered with the *kp*-method that allows an unified approach without usage of any models. Dirac and Weyl equations are derived by the above-mentioned method. The wave function and its envelope function together with the scattering amplitude are found in the Born approximation. The wave functions are shown to be a superposition of virtual Bloch functions which exponential decay outward from the impurity and the edge. At distances much greater that the atomic spacing the wave functions are explicitly presented. Green's functions for Shrödinger and Dirac equations are derived as well. Boundary conditions for the Dirac equation for graphene with a sharp edge are also derived.

Keywords: scattering of quasiparticles in graphene, Weyl and Dirac equations, *kp*-approximation, Green's functions.

1. Introduction

Dynamic and kinetic properties of graphene have been attracting much attention during the last decades [1]. Fascinating dynamic and kinetic phenomena which arise in graphene can be described by the two dimensional differential Dirac equation [2, 3] supplemented by boundary conditions.

Details of the boundary conditions and scattering amplitudes depend on microscopic characteristics of the concrete structures of sample boundaries [4] and the scatterers. Theoretical derivations of the boundary conditions for Dirac equations and the scattering amplitudes are usually based on various models such as tight bound model (see, e.g., review papers [5, 6] and references there), the effective mass model [7], tight-binding model with a staggered potential at a zigzag boundary [8].

The object of this paper is to demonstrate that the *kp*-method [9] allows investigations of graphene (and Weyl semimetals) fundamental properties (including the above-mentioned) on the base a unified approach. This approach is justified by the fact that the cone points in graphene are on the Fermi level or close to it while the *kp*-approximation requires nothing but the series expansion in the quasi-particle momenta in their vicinity.

In this paper, on the basis of the *kp*-method and without usage of any models (1) the Dirac and Weyl equations for quasi-particles are derived; (2) Green's function, the wave function together with the scattering amplitude for graphene with an impurity are obtained in terms of Bloch functions; (3) Dirac equation, the envelope function together with the scattering amplitude, Dirac equation for Green function, Green's function are found; (4) boundary conditions for the Dirac equation for quasi-particles in graphene with an abrupt boundary are also presented (details of their derivation in the *kp*-approximation were earlier published in Ref. 10).

The outline of this paper is as follows. In Sec. 2 Dirac and Weyl equations are obtained on the base of the *kp*-approximation. In Sec. 3 elastic scattering of quasi-particles by an impurity in graphene is considered: the wave function, the envelope function and the scattering amplitude are found in the Born approximation; Green's functions for Schrödinger and Dirac equations are also obtained. In Sec. 4 dynamics of quasi-particles and boundary conditions at the sharp edge of graphene is shortly described. In Sec. 5 concluding remarks are presented.

2. Derivation of Dirac equation by *kp*-method

Here we shortly present derivation of the Dirac equation by the *kp*-method assuming that two quasi-particle energy bands are degenerated at a point $\mathbf{p}_0 = 0$ ("Dirac" point) in the quasi-momentum space (see Ref. 10 for details).

The Schrödinger equation for noninteracting quasi-particles is written as

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}^2} + U(\mathbf{r})\right]\varphi_{s,\mathbf{p}}(\mathbf{r}) = \varepsilon_s(\mathbf{p})\varphi_{s,\mathbf{p}}(\mathbf{r}), \qquad (1)$$

where $U(\mathbf{r}) = U(\mathbf{r}+\mathbf{a})$ is the lattice periodic potential ($\mathbf{a}$ is the lattice vector) and

$$\varphi_{s,\mathbf{p}}(\mathbf{r}) = \exp\left(i\frac{\mathbf{pr}}{\hbar}\right)u_{s,\mathbf{p}}(\mathbf{r}) \tag{2}$$

is the Bloch function and $u_{s,\mathbf{p}}(\mathbf{r})$ is its periodic factor, $\mathbf{p}$ is the electron quasi-momentum while $\varepsilon_s(\mathbf{p})$ is the dispersion law and s is the band number.

For further application of the kp-method it is convenient to re-write the Schrödinger equation, Eq. (1), as follows:

$$\left\{\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial\mathbf{r}}+\mathbf{p}\right)^2+U(\mathbf{r})\right\}u_{s,\mathbf{p}}(\mathbf{r}) = \varepsilon_s(\mathbf{p})u_{s,\mathbf{p}}(\mathbf{r}). \tag{3}$$

According to the kp-method one finds the quasi-particle dispersion law in the vicinity of the degeneration point presenting the proper wave functions as a superposition of Lattinger–Kohn functions [9]:

$$\chi_{\alpha,\mathbf{p}} = \exp\left(i\frac{\mathbf{pr}}{\hbar}\right)u_{s,0}(\mathbf{r}), \tag{4}$$

where the periodic Bloch factors are taken at the degeneration point $\mathbf{p}=0$.

In order to solve Eq. (3) by the perturbation theory with degeneration one takes the sought-for function as a superposition of the degenerated ones that is

$$u_{s,\mathbf{p}}(\mathbf{r}) = g_1(\mathbf{p})u_{1,0}(\mathbf{r})+g_2(\mathbf{p})u_{2,0}(\mathbf{r}). \tag{5}$$

Inserting the wave function, Eq. (5), in Eq. (3) and using the inequality $|\mathbf{p}| \ll \hbar/a$ one obtains the former equation in the following form:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\mathbf{r}^2}+U(\mathbf{r})+\mathbf{p}\hat{\mathbf{v}}-\varepsilon\right]\sum_{\alpha=1}^{2}g_\alpha u_{\alpha,0}(\mathbf{r}) = 0. \tag{6}$$

Here $\hat{\mathbf{v}} = (-i\hbar/m)\partial/\partial\mathbf{r}$ is the velocity operator $\alpha \equiv s = 1,2$ are the band numbers of the two degenerated bands.

Taking matrix elements of Eq. (6) one gets a set of algebraic equations for the expansion constants $g_{1,2}$:

$$\begin{aligned}(\mathbf{pv}_{11}-\varepsilon)g_1(\mathbf{p})+(\mathbf{pv}_{12})g_2(\mathbf{p}) = 0,\\ (\mathbf{pv}_{21})g_1(\mathbf{p})+(\mathbf{pv}_{22}-\varepsilon)g_2(\mathbf{p}) = 0,\end{aligned} \tag{7}$$

where the quasi-particle energy ε is measured from the degeneration energy, $\varepsilon_1(0)=\varepsilon_2(0)=0$, and the matrix elements of the velocity operator are

$$\mathbf{v}_{\alpha\alpha'} = \int u^*_{\alpha,0}(\mathbf{r})\hat{\mathbf{v}}u_{\alpha',0}(\mathbf{r})d\mathbf{r}. \tag{8}$$

Equating the determinant of Eq. (7) to zero one gets the conventional dispersion law of quasi-particles near the degeneration point:

$$\varepsilon_\pm(\mathbf{p}) = \frac{\mathbf{pv}_+ \pm\sqrt{(\mathbf{pv}_-)^2+4|\mathbf{pv}_{12}|^2}}{2}, \tag{9}$$

where $v_\pm = \mathbf{v}_{11}\pm\mathbf{v}_{22}$. From here it follows that the dispersion law of quasi-particles in the vicinity of the band intersection is of the graphene-type (see, e.g., review papers [5, 6])

$$\varepsilon_\pm(\mathbf{p}) = \pm v\sqrt{p_x^2+p_y^2} = \pm vp, \tag{10}$$

if the lattice symmetry imposes the following conditions on the velocity matrix elements at the degeneration point $p=0$:

$$\begin{aligned}\mathbf{v}_{11}(0) = \mathbf{v}_{22}(0) = 0, \quad |\mathbf{v}_{12}(0)| = v,\\ v_{12}^{(y)}(0) = \pm iv_{12}^{(x)}(0),\end{aligned} \tag{11}$$

where $v = v_F \approx 1\cdot10^6$ m/s for graphene.

Inserting the values of the velocity matrix elements Eq. (11) in Eq. (7), solving the latter equation and using Eq. (5) one finds the graphene Bloch functions;

$$\varphi^{(gr)}_{\alpha,\mathbf{p}}(r) = \mathrm{e}^{i\mathbf{pr}}\left[u_{1,0}(\mathbf{r})+\mathrm{e}^{-\alpha\theta}u_{2,0}(\mathbf{r}\right]/2\sqrt{v}, \tag{12}$$

where $\theta = \arctan(p_y/p_x)$ and the energy band number is $\alpha = \pm$.

Introducing the envelope functions

$$\Phi_{1,2}(\mathbf{r}) = \int g_{1,2}(\mathbf{p})\exp\left\{i\frac{p\mathbf{r}}{\hbar}\right\}\frac{d\mathbf{p}}{(2\pi\hbar)^2} \tag{13}$$

and using Eqs. (7) one finds the following equation:

$$\begin{aligned}\left(-i\hbar\mathbf{v}_{11}\partial_\mathbf{r}+V(\mathbf{r})-\varepsilon\right)\Phi_1(\mathbf{r})-i\hbar\mathbf{v}_{12}\partial_\mathbf{r}\Phi_2(\mathbf{r}) = 0,\\ -i\hbar\mathbf{v}_{21}\partial_\mathbf{r}\Phi_1(\mathbf{r})+\left(-i\hbar\mathbf{v}_{22}\partial_\mathbf{r}+V(\mathbf{r})-\varepsilon\right)\Phi_2(\mathbf{r}) = 0.\end{aligned} \tag{14}$$

Here we added an external potential $V(\mathbf{r})$ which smoothly changes at the atomic scale (it can be rigorously proved as it is shown in Ref. 10).

Equation (14) transforms into Weyl equation:

$$\sigma_0\varepsilon\Phi_W+\sigma_x\partial_x\Phi_W+\sigma_y\partial_y\Phi_W+\sigma_z\partial_z\Phi_W = 0, \tag{15}$$

where σ_0 is the unity matrix and $\sigma_x,\sigma_y,\sigma_z$ are the Pauli matrices if two energy bands of a 3D semi-metal are degenerated in the vicinity of the Fermi energy and the lattice symmetry imposes the following conditions on the velocity matrix elements:

$$\mathbf{v}_{11}(0) = \mathbf{v}_{22}(0) = 0, \quad |\mathbf{v}_{12}(0)| = v, \quad \mathbf{v}_{12} = v(1,-i,i). \tag{16}$$

Differential Eqs. (14) and (16) describe dynamics of various Weil semi-metals in accordance with their symmetry that determine the velocity matrix elements, Eq. (8).

Choosing the graphene symmetry (for which the matrix elements are given by Eq. (11) one obtains the conventional Dirac equation [5, 6]:

$$\begin{pmatrix}V(\mathbf{r})-\varepsilon & \hbar v(-i\partial_x+\partial_y)\\ \hbar v(-i\partial_x-\partial_y) & V(\mathbf{r})-\varepsilon\end{pmatrix}\begin{pmatrix}\Phi_1\\ \Phi_2\end{pmatrix} = 0. \tag{17}$$

3. Scattering of quasi-particles in graphene by impurity

Here we consider the elastic scattering of quasi-particles by an impurity in graphene. After solving the Schrödinger equation for a quasi-particle in the periodic crystal potential with an impurity by the *kp*-method, we derive the Dirac equation with an effective scattering potential for the envelope function. The scattering amplitude and Green's functions for the Schrödinger and Dirac equations are also found.

Elastic scattering of a free quasi-particle by an impurity in the periodic lattice is described by the following Schrödinger equation:

$$\left(\hat{H}_0 + V_i(\mathbf{r})\right)\Psi(\mathbf{r}) = \varepsilon\Psi(\mathbf{r}), \tag{18}$$

where $\hat{H}_0$ is the quasi-particle Hamiltonian for the pure crystal, Eq. (1), and $V_i(\mathbf{r})$ is the impurity potential.

Using the Green's function approach one presents the wave function of the scattered quasi-particle as follows:

$$\Psi(\mathbf{r}) = \varphi^{(\mathrm{in})}_{\alpha,\mathbf{p}}(\mathbf{r}) + \int G(\mathbf{r},\mathbf{r}')V_i(\mathbf{r}')\Psi(\mathbf{r}')d\mathbf{r}', \tag{19}$$

where $\varphi^{(in)}_{\alpha,\mathbf{p}}(\mathbf{r})$ is the incident "graphene" Bloch function, Eq. (12), and $G(\mathbf{r},\mathbf{r}')$ is Green's function satisfying the equation

$$\left(\hat{H}_0 - \varepsilon\right)G(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r} - r'). \tag{20}$$

Expanding $G(\mathbf{r},\mathbf{r}')$ in the series of Bloch functions $\varphi_{s,\mathbf{p}}(\mathbf{r})$ one finds Green's function as follows:

$$G(\mathbf{r},\mathbf{r}') = G_\alpha(\mathbf{r},\mathbf{r}') + G_{s\neq\alpha}(\mathbf{r},\mathbf{r}'), \tag{21}$$

where

$$G_\alpha(\mathbf{r},\mathbf{r}') = \sum_{\alpha=1}^{2}\int \frac{d\mathbf{p}}{(2\pi\hbar)^2}\frac{\varphi^*_{\alpha,\mathbf{p}}(\mathbf{r}')\varphi_{\alpha,\mathbf{p}}(\mathbf{r})}{\varepsilon - \varepsilon_\alpha(\mathbf{p}) + i0} \tag{22}$$

is the "graphene" Green's function in which the graphene dispersion law and the Bloch functions $\varphi_{\alpha,\mathbf{p}}(\mathbf{r})$ are defined in Eqs. (10) and (12), respectively, while

$$G_{s\neq\alpha} = \sum_{s\neq\alpha}\int \frac{d\mathbf{p}}{(2\pi\hbar)^2}\frac{\varphi^*_{s,\mathbf{p}}(\mathbf{r}')\varphi_{s,\mathbf{p}}(\mathbf{r})}{\varepsilon - \varepsilon_s(\mathbf{p}) + i0} \tag{23}$$

is the Green function of virtual states in which the Bloch functions, Eq. (2), are proper functions of quasi-particle energies $\varepsilon_s(\mathbf{p})$ belonging to other bands, $s \neq \alpha$.

Calculations of "graphene" Green's function

Using Eqs. (22), (12) one presents $G_\alpha(\mathbf{r},\mathbf{r}')$ as follows:

$$G_\alpha(\mathbf{r},\mathbf{r}') = \frac{1}{2}[u^*_{1,0}(\mathbf{r}')u_{1,0}(\mathbf{r}) + u^*_{2,0}(\mathbf{r}')u_{2,0}(\mathbf{r})]I_1 +$$

$$+\frac{(-1)^\alpha}{2}[u^*_{1,0}(\mathbf{r}')u_{2,0}(\mathbf{r})I_2^{(+)} + u^\star_{2,0}(\mathbf{r}')u_{1,0}(\mathbf{r})I_2^{(-)}], \tag{24}$$

where

$$I_1(\mathbf{r}-\mathbf{r}') = \int \frac{d\mathbf{p}}{(2\pi\hbar)^2}\frac{e^{i\mathbf{p}(\mathbf{r}-\mathbf{r}')/\hbar}}{\varepsilon - \varepsilon_\alpha(\mathbf{p}) + i0},$$

$$I_2^{(\pm)}(\mathbf{r}-\mathbf{r}') = \int \frac{d\mathbf{p}}{(2\pi\hbar)^2}\frac{e^{\mathbf{p}(\mathbf{r}-\mathbf{r}')/\hbar}e^{\pm i\theta_p}}{\varepsilon - \varepsilon_\alpha(\mathbf{p}) + i0}. \tag{25}$$

Performing integrations (see Appendix A) one finds

$$I_1 = I_2^{(\pm)} = -\frac{e^{i\pi/4}}{\hbar v}\sqrt{\frac{p_\varepsilon}{2\pi\hbar}}\frac{e^{ip_\varepsilon R/\hbar}}{\sqrt{R}} - \frac{\pi e^{i\pi/4}}{\varepsilon R^2}, \tag{26}$$

where $p_\varepsilon = \varepsilon / v$ is the quasi-particle momentum.

Calculations of Green's function for virtual states.

Here we calculate the part of Green's function determined by virtual states, Eq. (23):

$$G_{s\neq\alpha}(\mathbf{r}',\mathbf{r}) = \sum_{s\neq\alpha}\int \frac{u^*_{s;\mathbf{p}}(\mathbf{r}')u_{s;\mathbf{p}}(\mathbf{r})e^{i\mathbf{p}(\mathbf{r}-\mathbf{r}')}}{\varepsilon - \varepsilon_s(\mathbf{p})}\frac{d\mathbf{p}}{(2\pi\hbar)^2}. \tag{27}$$

In the polar coordinates the integral in Eq. (27) reads

$$G_{s\neq\alpha}(\mathbf{r}',\mathbf{r}) = \sum_{s\neq\alpha}\int_0^\infty \frac{dp\,p}{(2\pi\hbar)^2}\int_0^{2\pi} d\varphi \frac{U_s(p,\varphi)e^{ipR\cos\varphi}}{\varepsilon - \varepsilon_s(p,\varphi)}, \tag{28}$$

where

$$U_s(\mathbf{p}) = u^*_{s;\mathbf{p}}(\mathbf{r}')u_{s;\mathbf{p}}(\mathbf{r}); \quad R = |\,\mathbf{r}' - \mathbf{r}\,|$$

with the momenta taken in the polar coordinates.

At $Rp/\hbar \gg 1$ one may use the fastest descent method for calculations of the integral with respect to φ and find

$$G_{s\neq\alpha}(\mathbf{r}',\mathbf{r}) = \sqrt{\frac{2\pi\hbar}{R}}\sum_{s\neq\alpha}\int_0^\infty \frac{dp\sqrt{p}}{(2\pi\hbar)^2},$$

$$\left\{\frac{U_s(p,0)e^{-i\pi/4}}{\varepsilon - \varepsilon_s(p,0)}e^{ipR} + \frac{U_s(p,\pi)e^{i\pi/4}}{\varepsilon - \varepsilon_s(p,\pi)}e^{-ipR}\right\}. \tag{29}$$

For calculations of the above integrals it is convenient to choose the integration contours in the complex plane shown in Fig. 1.

In the general case, the dispersion equations $\varepsilon_s(p,\varphi)$ considered as functions of the complex variable $z = p + i\xi$ have branching points, their characteristic distances from the real axis being of the order of $\hbar/a$ (here a is the atomic spacing). In Fig. 1, they are schematically shown with small circles at the beginnings of branch cuts; as the energy ε is out of the energy band under consideration $s \neq \alpha$ the poles (which are shown with black dots) are in the complex planes with $|\,\xi\,| \gtrsim \Delta/v$ where Δ is the characteristic width of energy gaps.

Performing the contour integrations in the complex plane (see Appendix C) one finds Green's function for virtual states:

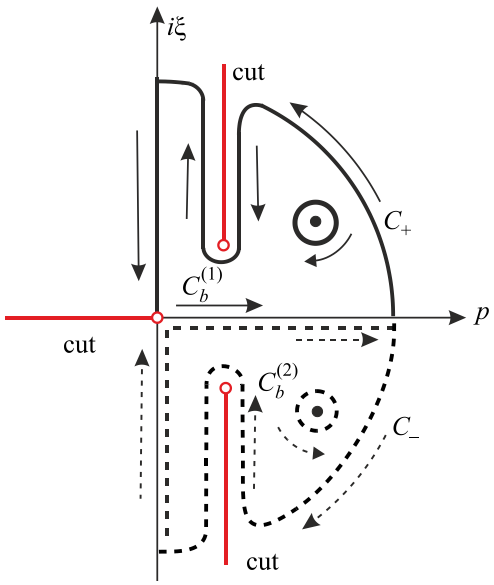

Fig. 1. Closed contours of integration C_+ and C_- for calculations of the first and second integrals in Eq.(28) are shown with solid and dotted lines, respectively; branching points are shown with small circles at the beginnings of branch cuts; poles of the integrands are shown with black dots.

$$G_{s\neq\alpha}(\mathbf{r}',\mathbf{r}) \sim \frac{\mathrm{e}^{-R/a}}{\hbar v\sqrt{2\pi aR}} + \frac{1}{R^2\Delta}. \qquad (30)$$

Finally, according to Eqs. (21), (24), (26), (30) the total Green function for the electron reads

$$G_e(\mathbf{r},\mathbf{r}') = -\frac{\mathrm{e}^{i\pi/4}}{2\hbar v}\sqrt{\frac{p_\varepsilon}{2\pi\hbar}}\frac{\mathrm{e}^{iRp_\varepsilon}}{\sqrt{R}}\times$$

$$\times\sum_{\alpha,\beta=1}^{2} u^*_{\alpha,0}(\mathbf{r}')u_{\beta,0}(\mathbf{r}') + \mathcal{O}\left(\frac{1}{\delta R^2}, \frac{\mathrm{e}^{-R/a}}{v\sqrt{aR}}\right). \qquad (31)$$

Inserting Eq. (31) into Eq. (19) one readily finds the integral equation for the wave function of the electron scattered by the impurity in graphene:

$$\Psi(\mathbf{r}) = \varphi^{(\mathrm{in})}_{\alpha,\mathbf{p}}(\mathbf{r}) - \frac{(2\pi)^{3/2}\sqrt{\hbar p_\varepsilon}}{v}\mathrm{e}^{i\pi/4}\times$$

$$\times\sum_{\alpha,\beta=1}^{2} u_{\alpha;0}(\mathbf{r})\int u_{\beta;0}(\mathbf{r}')V_i(\mathbf{r}')\Psi(\mathbf{r}')\frac{\mathrm{e}^{ip_\varepsilon|\mathbf{r}-\mathbf{r}'|}}{\sqrt{|\mathbf{r}-\mathbf{r}'|}}\frac{d\mathbf{r}'}{(2\pi\hbar)^2} +$$

$$+\mathcal{O}\left(\frac{a^2}{R^2}, \frac{\mathrm{e}^{-R/a}}{\sqrt{R/a}}\right). \qquad (32)$$

This equation can be easily solved in Born's or semiclassical approximations that gives the explicit expression for the wave function of the electron scattered by the impurity.

As one sees from Eq. (32), in the vicinity of the impurity the wave function of the quasi-particle scattered by the impurity is a superposition of the virtual states belonging to all available energy bands that fast decays as the distance from the impurity increases.

In the next section, using the *kp*-method we derive the Dirac equation for quasi-particles in graphene with an impurity. As is shown there solution of this equation in Born's approximation allows to present the envelope function and the scattering amplitude in an explicit form.

Envelope function and scattering amplitude for graphene with an impurity

First we derive the Dirac equation for quasi-particles in graphene with an impurity using the *kp*-method. For this purpose we write the Schrödinger equation considering the term with the impurity potential as a known function in the right-hand side of it:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\mathbf{r}^2} + U(\mathbf{r}) - \varepsilon\right]\Psi(\mathbf{r}) = -V_i(\mathbf{r})\Psi(\mathbf{r}). \qquad (33)$$

Expanding Ψ in the left-hand side of the above equation in the series of χ [see Eq. (4)]

$$\Psi = \sum_{\alpha=1}^{2}\int g_\alpha(\mathbf{p})\chi_{\alpha,\mathbf{p}}(\mathbf{r})\frac{d\mathbf{p}}{(2\pi\hbar)^2} \qquad (34)$$

and using Eq. (11) one finds the Schrödinger equation in the *p*-representation:

$$-\varepsilon g_\alpha(\mathbf{p}) + \sum_{\alpha'=1}^{2}(\mathbf{p}\cdot\mathbf{v}_{\alpha,\alpha'})g_{\alpha'}(\mathbf{p}) = -\int\chi^*_{\alpha,\mathbf{p}}(\mathbf{r})V_i(\mathbf{r})\Psi(\mathbf{r})d\mathbf{r}. \qquad (35)$$

In the above equation, contributions of the virtual states are neglected (see the previous section).

The envelope functions are given by Eq. (13) and hence, according to Eq. (34), they are related to the wave function of the Schrödinger equation, Eq. (18), by the following relation:

$$\Psi = \sum_{\alpha=1}^{2} u_{\alpha,0}(\mathbf{r})\Phi_\alpha(\mathbf{r}). \qquad (36)$$

After multiplying the both sides of Eq. (35) by $\exp\{i\mathbf{pr}/\hbar)\}$ and integrating with respect to $\mathbf{p}$ one finds the following equation for the envelope function:

$$\begin{cases}\varepsilon\Phi_1 + \hbar v(i\partial_x - \partial_y)\Phi_2 = u_{1,0}(\mathbf{r})V_i(\mathbf{r})\Psi(\mathbf{r}),\\ \hbar v(i\partial_x + \partial_y)\Phi_1 + \varepsilon\Phi_2 = u_{2,0}(\mathbf{r})V_i(\mathbf{r})\Psi(\mathbf{r}).\end{cases} \qquad (37)$$

Treating the right-hand side as a known function one finds the following solution of this Dirac equation:

$$\Phi_1(\mathbf{r}) = \Phi_1^{(\mathrm{in})} - \int V_i(\mathbf{r}')\Psi(\mathbf{r}')\sum_{\alpha=1}^{2} u^*_{\alpha,0}(\mathbf{r}')A_\alpha(\mathbf{r}',\mathbf{r})d\mathbf{r}',$$

$$\Phi_2(\mathbf{r}) = \Phi_2^{(\mathrm{in})} - \int V_i(\mathbf{r}')\Psi(\mathbf{r}')\sum_{\alpha=1}^{2} u^*_{\alpha,0}(\mathbf{r}')B_\alpha(\mathbf{r}',\mathbf{r})d\mathbf{r}'. \qquad (38)$$

where $\Phi_{1,2}^{(\mathrm{in})}$ are the envelope functions of the incoming quasi-particle (which are solutions of the above homogeneous Dirac equation) while functions A_α and B_α are integrals with respect to the momentum $\mathbf{p}$:

$$A_1 = B_1 = \varepsilon \int_{-\infty}^{\infty} \frac{e^{i\mathbf{p}(\mathbf{r}-\mathbf{r}')}}{(vp)^2 - \varepsilon} \frac{d\mathbf{p}}{(2\pi\hbar)^2},$$

$$A_2 = \int_{-\infty}^{\infty} \frac{v(p_x + ip_y)e^{i\mathbf{p}(\mathbf{r}-\mathbf{r}')}}{(vp)^2 - \varepsilon} \frac{d\mathbf{p}}{(2\pi\hbar)^2},$$

$$B_2 = \int_{-\infty}^{\infty} \frac{v(p_x - ip_y)e^{i\mathbf{p}(\mathbf{r}-\mathbf{r}')}}{(vp)^2 - \varepsilon} \frac{d\mathbf{p}}{(2\pi\hbar)^2}. \qquad (39)$$

Performing integrations analogous to those made in Appendix A one finds:

$$A_1 = A_2 = B_1 = B_2 = e^{i\pi/4} \frac{(2\pi)^{3/2}}{4(2\pi\hbar)^2} \frac{p_\varepsilon}{v} \frac{e^{ip_\varepsilon R/\hbar}}{\sqrt{p_\varepsilon R/\hbar}},$$

$$R = |\mathbf{r} - \mathbf{r}'|. \qquad (40)$$

Inserting Eq. (40) into Eq. (38) one finds the set of integral equations for the envelope functions of the graphene with an impurity as follows:

$$\begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} = \begin{pmatrix} 1 \\ e^{i\varepsilon} \end{pmatrix} e^{i\mathbf{r}\mathbf{k}_\varepsilon} - \begin{pmatrix} +1 \\ -1 \end{pmatrix} \int V_i(\mathbf{r}') \times$$

$$\times \sum_{\beta=1}^{2} u_{\beta,0}^{*}(\mathbf{r}')\Phi_\beta(\mathbf{r}') \sum_{\alpha=1}^{2} u_{\alpha,0}^{\star}(\mathbf{r}')A_1(\mathbf{r}',\mathbf{r})d\mathbf{r}, \qquad (41)$$

where $\varphi = \arctan p_y / p_x$ and for the sake of definiteness, the scattering of an electron is considered. While writing this equation Eq. (36) was used.

In the Born approximation the second term in the right-hand side of Eq. (41) is considered as a perturbation and at large distances from the impurity one finds the envelope function of the electron scattered by the impurity as follows:

$$\begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} = \begin{pmatrix} 1 \\ e^{i\varepsilon} \end{pmatrix} e^{i\mathbf{r}\mathbf{k}_\varepsilon} - \begin{pmatrix} +1 \\ -1 \end{pmatrix} f(\theta) \frac{e^{ik_\varepsilon R_0}}{\sqrt{R_0}}, \qquad (42)$$

where the scattering amplitude is

$$f(\theta) = -\frac{\pi^{3/2}}{\sqrt{2}} e^{i\pi/4} \sqrt{\frac{\hbar v}{\varepsilon}} \times$$

$$\times \frac{\varepsilon}{v^2} \int \frac{d\mathbf{r}'}{(2\pi\hbar)^2} e^{-i\mathbf{q}\mathbf{r}'} V_i(\mathbf{r}') \sum_{\alpha,\beta=1}^{2} u_{\alpha,0}^{*}(\mathbf{r}')u_{\beta,0}(\mathbf{r}')e^{i(\beta-1)\varphi}. \qquad (43)$$

While writing the above equation we chose the coordinate origin at the scattering center and introduced the radius vector $\mathbf{R}_0$ from the origin to the observation point, a unity vector along it being denoted by $\mathbf{n}'$. Therefore, in this coordinates vector $\mathbf{R}$ [see Eq. (40)] reads $\mathbf{R} = \mathbf{R}_0 - \mathbf{r}'$. At large distances from the center, $R_0 \gg |\mathbf{r}'|$, one has $R \approx R_0 - \mathbf{k}'\mathbf{n}'$. Vector $\mathbf{q} = \mathbf{k}' - \mathbf{k}$, where $\mathbf{k}' = k\mathbf{n}'$ is the wave vector of the quasi-particle after scattering;

$$q = 2k \sin\theta/2,$$

θ being the angle between $\mathbf{k}$ and $\mathbf{k}'$, i.e., the scattering angle.

As one sees the envelope function, Eq. (42), and Dirac equation for it, Eq. (17), are tightly coupled with the wave function, Eq. (32), and Schrödinger equation, Eq. (18) via the function-envelope function relation Eq. (36). Below we present a Green's function equation for the Dirac equation which is closely associated with Green's function of the Schrödinger equation.

Green's function for the Dirac equation

Green's functions are convenient tools for investigations of properties of various systems and it may be desirable to have an equation for Green's function for the Dirac equation, Eq. (17), closely related to the Schrödinger equation, Eq. (1), and the corresponding Green's function equation, Eq. (20).

Using Eq. (20) for Green's function $G(\mathbf{r},\mathbf{r}')$ of the Schrödinger equation, Eq. (1) and repeating the reasoning for derivation of Eq. (37) from Eq. (33) one finds the equation for Green's function of the Dirac equation as follows:

$$\begin{pmatrix} -\varepsilon & \hbar v(-i\partial_x + \partial_y) \\ \hbar v(-i\partial_x - \partial_y) & -\varepsilon \end{pmatrix} \begin{pmatrix} G_1^{(D)}(\mathbf{r},\mathbf{r}') \\ G_2^{(D)}(\mathbf{r},\mathbf{r}') \end{pmatrix} =$$

$$= -\begin{pmatrix} u_{1,0}(\mathbf{r}) \\ u_{2,0}(\mathbf{r}) \end{pmatrix} \delta(\mathbf{r} - \mathbf{r}'). \qquad (44)$$

In Eq. (44), expanding in the series of the proper function of the Dirac equation one finds that Green's function reads as follows:

$$\begin{pmatrix} G_1^{(D)}(\mathbf{r},\mathbf{r}') \\ G_2^{(D)}(\mathbf{r},\mathbf{r}') \end{pmatrix} = \sum_{\alpha=1}^{2} \int \frac{d\mathbf{p}}{(2\pi\hbar)^2} \times$$

$$\times \frac{u_{1,0}(\mathbf{r}) + (-1)^\alpha e^{i\theta} u_{2,0\mathbf{r}}}{\varepsilon - \varepsilon_\alpha(\mathbf{p})} \begin{pmatrix} 1 \\ (-1)^\alpha e^{-i\theta} \end{pmatrix} e^{\mathbf{p}(\mathbf{r}-\mathbf{r}')/\hbar}, \qquad (45)$$

where $\varepsilon_\alpha(\mathbf{p}) = (-1)^\alpha vp$ and $\theta = \arctan(p_x / p_y)$.

4. Derivation of boundary conditions for Dirac equation

Dynamics of quasiparticles in graphene that occupies the upper half plane $y \geq 0$ is described by Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} + U(\mathbf{r}) \right] \Psi(\mathbf{r}) = \varepsilon \Psi(\mathbf{r}) \qquad (46)$$

with the boundary condition

$$\Psi(\mathbf{r})|_{y=0} = 0, \qquad (47)$$

where $U(\mathbf{r}) = U(\mathbf{r} + \mathbf{a})$ is the lattice periodic potential.

To solve the problem of reflection by the sharp edge at $y = 0$, we use Green's function for Schrödinger equation Eq. (46):

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{r}^2} + U(\mathbf{r}) - \varepsilon\right) G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \qquad (48)$$

in which the lattice potential $U(\mathbf{r})$ covers the whole plane (x, y).

Using Eqs. (20), (46) and taking into account the boundary condition Eq. (47) one finds

$$\Psi(\mathbf{r}) = \frac{\chi^{(\mathrm{in})}_{\alpha,\mathbf{p}}(r)}{\sqrt{v_{y,\alpha}}} + \frac{\hbar^2}{2m}\int\limits_{-\infty}^{+\infty} (x',-0;\mathbf{r})\frac{\partial\Psi(\mathbf{r}')}{\partial y'}|_{y'=-0}\, dx. \quad (49)$$

Here $\chi^{(\mathrm{in})}_{\alpha,\mathbf{p}}(r)$ is the graphene Kohn–Lattinger function Eq. (4) incident to the graphene edge from the infinity $y \to \infty$ and $v_{y,\alpha} = \partial\varepsilon^{(\mathrm{gr})}_{\alpha}(\mathbf{p})/\partial y$ is the velocity y-projection that normalizes the incident function to the flux unity while $\varepsilon^{(\mathrm{gr})}_{\alpha}(\mathbf{p}) = \pm vp$ is the graphene dispersion; in order to define $\Psi(\mathbf{r})$ on the whole half-plane $y \ge 0$ the boundary contour is shifted to $y = -0 \equiv 0 - \delta'$, $\delta' \to 0$ (see Ref. 11).

Expanding $G(\mathbf{r},\mathbf{r}')$ in the series of Bloch wave functions and using Eq. (48) one finds

$$G(\mathbf{r},\mathbf{r}') = \sum_{\alpha=1,2}\int \frac{\chi^{*}_{\alpha,\mathbf{p}}(\mathbf{r})\chi_{\alpha,\mathbf{p}}(\mathbf{r}')}{\varepsilon - \varepsilon^{(gr)}_{\alpha}(\mathbf{p}) + i\delta} d\mathbf{p} +$$

$$+ \sum_{s\neq 1,2}\int \frac{\varphi^{*}_{s,\mathbf{p}}(\mathbf{r})\varphi_{s,\mathbf{p}}(\mathbf{r}')}{\varepsilon - \varepsilon_{s}(\mathbf{p}) + i\delta} d\mathbf{p}, \qquad (50)$$

where summation goes over all energy bands and $\delta \to +0$

Inserting Eq. (50) into Eq. (49) one finds the wave function on the right half-plane $x \ge 0$ as follows:

$$\Psi(\mathbf{r}) = \frac{\chi^{(\mathrm{in})}_{\alpha,\mathbf{p}_0}}{\sqrt{v_{y,\alpha}}} +$$

$$+\frac{\hbar^2}{2m}\int\limits_{-\infty}^{\infty} d\overline{x}\Psi'(\overline{x},0)\mathrm{e}^{ixp_x/\hbar}\left\{\sum_{\alpha=1,2} u^{*}_{\alpha,0}(\overline{x},0)u_{\alpha,0}(\mathbf{r})I^{(\mathrm{gr})}_{\alpha} + \right.$$

$$\left. + \sum_{s\neq 1,2} u^{*}_{s,\mathbf{p}}(\overline{x},0)u_{s,\mathbf{p}}(\mathbf{r})I^{(bnd)}_{s}\right\}, \qquad (51)$$

where $\Psi'_y(\overline{x},-0) = \partial\Psi(\mathbf{r})/\partial y$ at $y = -0$. While writing the above equation we assumed that along the edge line $y = 0$ the lattice is periodic with the period a_x that is $\Psi(x,0) = \Psi(x + a_x, 0)$ and hence the momentum projection p_x conserves; $I^{(\mathrm{gr})}_{\alpha}$ and $I^{(bnd)}_{s}$ are one-dimensional integrals defined below, Eqs. (52), (53)

Differentiating the both sides of Eq. (51) with respect to y one obtains the integral equation for $\Psi'_y(\overline{x},-0)$ the solution of which completes the definition of the sought wave function $\Psi(\mathbf{r})$. Despite this integral equation can not be solved in the general case important properties of the quasi-particle scattering by the sharp sample boundary may be derived from Eq. (51).

Indeed, let us consider one-dimensional integrals with respect to p_y in Eq. (51) re-writing them in the following forms:

$$I^{(\mathrm{gr})}_{\alpha} = \int\limits_{-b_y/2}^{b_y/2} \frac{\mathrm{e}^{iyp_y/\hbar}}{\varepsilon - \varepsilon_{\alpha}(p_x,p_y) + i\delta} dp_y \qquad (52)$$

and

$$I^{(bnd)}_{s} = \int\limits_{-b_y/2}^{b_y/2} \frac{u^{*}_{s,p_x,p_y}(\overline{x},0)u_{s,p_x,p_y}(\mathbf{r})\mathrm{e}^{iyp_y/\hbar}}{\varepsilon - \varepsilon_{s}(p_x,p_y) + i\delta} dp_y. \quad (53)$$

Here b_y is the period of the reciprocal lattice in the y-direction.

In the complex plane the dispersion law of the degenerated bands of graphene Eq. (10) considered as a function of the complex variable $z = p_y + i\xi$ (that is $\varepsilon(p_x,z) = +v\sqrt{z^2 + p_x^2}$) has branch points at $z = \pm ip_x$ and the two branches of this complex function are the two energy bands on the real axis $z = p_y$. The dispersion law functions of other energy bands are also multi-valued functions with branch points in the complex plane.

Therefore, integral Eq. (52) is a sum of the residues and the integral along the brunch cut in the upper complex half-plane $\xi \ge 0$ inside the contour schematically shown in Fig. 2. The left and right vertical lines of the contour are separated by the reciprocal period b_y and hence the integrals along them cancel each other because the integrands are periodic functions of the same period. The integral along its upper horizontal part exponentially goes to zero as this contour part goes to $i\infty$.

Below, for the sake of certainty we consider here one valley reflection of an electron, $\alpha = 1$. We also assume that

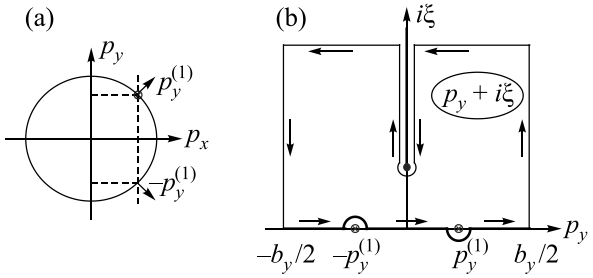

Fig. 2. (a) Equal energy contour $v\sqrt{p_x^2 + p_y^2} = \varepsilon$. The thick arrows show the velocity direction at fixed energy ε and p_x. The incident quasiparticle has conserving projection $p_y = -p_y^{(1)}$ while the outgoing quasiparticle has $p_y = +p_y^{(1)}$. (b) Contour of integration of Eq. (52). Dots on the real axis p_y show positions of the poles corresponding to points with positive and negative velocity v_y. Thick vertical line is the brunch line corresponding to the brunching point (thick dots), $p_y^{(\mathrm{gr})} = ip_x$, in the quasi-particle spectrum.

only one contour $\varepsilon_1(p_x,p_y)=\varepsilon$ exists at a fixed p_x as shown in Fig. 2.

In this case Eq. (52) reads

$$I_1^{(\mathrm{gr})}=\int\limits_{-b_y/2}^{b_y/2}\frac{\mathrm{e}^{iyp_y/\hbar}}{[\varepsilon-\sqrt{p_x^2+p_y^2}+i\delta]}dp_y. \qquad (54)$$

The pole of the integrand in Eq. 54 which contributes to the integral lies on the right upper side of the real axis (see Fig. 2).

$$p_y=p_1^{(1)}+i\frac{\delta}{v_x^{(\alpha)}},\ \delta\to 0,$$

where its real part is $p_y^{(1)}=\sqrt{(\varepsilon/v)^2-p_x^2}$. One easily sees from the denominator of the integrand that this pole is inside the integration contour because the velocity

$$v_y=\frac{\partial\varepsilon(p_x,p_y)}{\partial p_y}\Big|_{p_y=p_y^{(1)}}>0$$

and hence it corresponds to the quasiparticle state reflected back by the boundary.

Taking into account the above-mentioned pole and branch cut one easily carried out integration in Eq. (54) (calculations of the integral along the branch cut is presented in Appendix C) and finds $I_1^{(\mathrm{gr})}$ as follows:

$$I_1^{(\mathrm{gr})}=-\frac{2\pi i}{v_y(p_x,p_y^{(1)})}\mathrm{e}^{iyp_y^{(1)}/\hbar}+\frac{2\hbar i}{y\varepsilon}\mathrm{e}^{-yp_x\hbar}. \qquad (55)$$

For calculations of the integral in Eq. (53) one finds the poles from the equation $\varepsilon_s(p_x,p_y)=\varepsilon, s\neq\alpha$ where the energy bands $\varepsilon_s(p_x,p_y)$ do not overlap bands $\alpha=1,2$ in which the energy ε. In the general case the difference between those bands

$$\left|\varepsilon_\alpha(p_x,p_y)-\varepsilon_s(p_x,p_y')\right|\gtrsim\Delta_{\mathrm{gap}}^{(s)}\sim\hbar v/a,\ \ s\neq\alpha,$$

(where $\Delta_{\mathrm{gap}}^{(s)}$ is the characteristic value of the energy gap between the energy bands) and hence poles of the integrand in the upper imaginary plane have large imaginary parts $\xi\sim b_0^{(s)}=\Delta_{\mathrm{gap}}^{(s)}/v$. On the other hand the dispersion laws $\varepsilon_s(p_x,z)$ as functions of the complex variable $z=p_y+i\xi$ are also multi-brunched, the brunching points of which having also large imaginary parts $\xi\sim b_0^{(s)}$.

Performing integration in Eq. (53) in much the same manner as above one finds $I_s^{(bnd)}$ as follows (details of the calculations are presented in Ref. 10):

$$I_s^{(bnd)}\sim\frac{\mathrm{e}^{-yb_0/\hbar}}{v}. \qquad (56)$$

Using Eqs. (55), (56) together with Eq. (51) we found that at distances $y\gg a$ (here a is the characteristic period of the graphene lattice) the graphene wave fuction is the difference between the incident and outgoing Bloch functions of the infinite graphene:

$$\Psi_{p_x}(\mathbf{r})=\left(\varphi^{(\mathrm{gr})}_{\alpha;p_x,p_y^{(\mathrm{in})}}(\mathbf{r})-\varphi^{(\mathrm{gr})}_{\alpha;p_x,p_y(\mathrm{out})}(\mathbf{r})\right)+$$

$$+C\mathrm{e}\frac{ae^{-yp_x/\hbar}}{y}\mathrm{e}^{ixp_x/\hbar}u_{\alpha;0}(\mathbf{r}), \qquad (57)$$

where $p_y^{(\mathrm{in})}$ and $p_y^{(\mathrm{out})}=-p_y^{(\mathrm{in})}$ are the y-projections of the quasiparticle momentum while C is a constant ~ 1 (details of calculations are given in Ref. 10).

From Eq. (57) and Eq. (36) one easily finds that at the distances from the graphene sharp edge much greater than the atomic spacing, $l\gg a$, the graphene envelope function $\breve{\Phi}(\mathbf{r})$ is the difference between the incident and outgoing wave functions (which are two independent solutions of the Dirac equation Eq. (17)):

$$\breve{\Psi}(\mathbf{r})=\mathrm{e}^{ixp_x}\left[\mathrm{e}^{iyp_y^{(\mathrm{in})}}\begin{pmatrix}1\\ \mathrm{e}^{i\varphi}\end{pmatrix}-\mathrm{e}^{-i(yp_y^{(\mathrm{in})})}\begin{pmatrix}1\\ \mathrm{e}^{-i\varphi}\end{pmatrix}\right], \qquad (58)$$

where the phase $\varphi=\arctan(p_y^{(\mathrm{in})}/p_x)$.

5. Conclusion

In this paper dynamics of quasi-particles in graphene with an impurity and a sharp edge is considered with the *kp*-approach. Dirac equation for graphene and Weyl equation for semi-metals are derived in Sec. 2. For graphene with an impurity, the wave function and its evolution function together with the scattering amplitude are found in the Born approximation. As an auxiliary tool Green's functions for Schrödinger and Dirac equations are also derived. In the both cases of the impurity and the sharp edge, the wave functions of the scattered quasi-particles are shown to be superpositions of virtual states which exponentially decay outward from the scatterer. They are explicitly presented for distances much greater that the atomic spacing. In the case that the velocity direction of the incident quasiparticle is perpendicular to the edge the above-mentioned superposition of virtual states decays linear with the distance increase, Eq. (57). It is proved that at the distances much greater than the atomic spacing the graphene envelope function is the difference between the incident and outgoing wave functions which are two independent solutions of the Dirac equation for the infinite graphene, Eq. (58), the latter being the boundary condition for Dirac equation.

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Appendix A: Calculations of contour integrals for "graphene" Green's functions

Inserting the polar coordinates in the integrals in Eq. (25) one finds

$$I_1 = -\frac{2\pi}{v}\int_0^\infty \frac{p}{p - p_\varepsilon - i0} J_0(pR)\frac{d\,p}{(2\pi\hbar)^2},$$

$$I_2^{(\pm)} = -\frac{2\pi i}{v}\int_0^\infty \frac{p}{p - p_\varepsilon - i0} J_1(pR)\frac{d\,p}{(2\pi\hbar)^2}, \qquad \text{(A1)}$$

where $p_\varepsilon = \varepsilon / v$ and $R = |\mathbf{r} - \mathbf{r}'|$ while $J_{0,1}$ are the Bessel functions of the first kind. For the sake of certainty, here and below all calculations are done for electrons the dispersion law of which is $\varepsilon_+(p) = vp$ [see Eq. (10)].

Asymptotic of the Bessel functions for large arguments are

$$J_0(pR) = \sqrt{2/(\pi pR)}\cos(pR - \pi/4)$$

and

$$J_1(pR) = \sqrt{2/(\pi Rp)}\sin(pR - \pi/4)$$

and hence at $pR \gg 1$, Eq. (A1) reads

$$I_1(\mathbf{r} - \mathbf{r}') = -\frac{1}{v}\sqrt{\frac{2\pi}{R}}\int_0^\infty \frac{d\,p}{(2\pi\hbar)^2}\times$$

$$\times\frac{\sqrt{p}}{p - p_\varepsilon - i0}(\exp^{i(pR-\pi/4)} + \exp^{-i(pR-\pi/4)}),$$

$$I_2^{(\pm)}(\mathbf{r} - \mathbf{r}') = -\frac{1}{v}\sqrt{\frac{2\pi}{R}}\int_0^\infty \frac{d\,p}{(2\pi\hbar)^2}\times$$

$$\times\frac{\sqrt{p}}{p - p_\varepsilon - i0}(\exp^{i(pR-\pi/4)} - \exp^{-i(pR-\pi/4)}). \qquad \text{(A2)}$$

Using the contours of integration in the complex plane presented in Fig. 3 for calculations of the first and second integrals in the right-hand sides in Eq. (A1), respectively, one finds

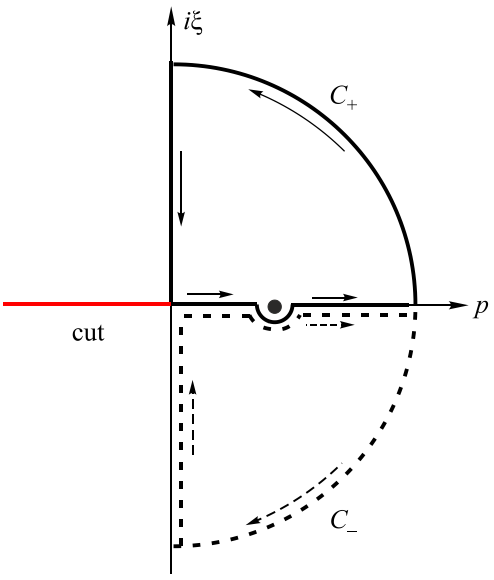

Fig. 3. Closed contour in the complex plane. The pole is shown with a dot.

$$I_1 = I_2^{(\pm)} = -\frac{1}{v}\sqrt{\frac{p_\varepsilon}{2\pi\hbar R}}\mathrm{e}^{i(p_\varepsilon R/\hbar + \pi/4)} +$$

$$+ i^{3/2}\sqrt{\frac{2\pi}{R}}\left[\mathrm{e}^{-i\pi/4}\int_0^\infty \frac{\sqrt{\xi}\mathrm{e}^{-R\xi}}{i\xi - p_\varepsilon}\frac{d\xi}{(2\pi\hbar)^2} + \right.$$

$$\left. + \mathrm{e}^{i\pi/4}\int_0^\infty \frac{\sqrt{\xi}\mathrm{e}^{-R\xi}}{i\xi + p_\varepsilon}\frac{d\xi}{(2\pi\hbar)^2}\right]. \qquad \text{(A3)}$$

As $Rp_\varepsilon \gg 1$ one may neglect $i\xi$ in the denominators of the integrals and readily finds Eq. (26) of the main text.

Calculations of the contour integrals for the "virtual" part of Green's function

In order to calculate integrals in Eq. (28) it is convenient to use contours in the upper and the lower complex planes for the first and second integrals respectively as it is shown in Eq. (28) with solid and dotted lines. As a result, Green's function is presented as follows:

$$G_{s\neq\alpha}(\mathbf{r}', \mathbf{r}) = \sum_{s\neq\alpha} I_s;$$

$$I_s = -\frac{1}{\hbar v}\frac{1}{\sqrt{2\pi\hbar R}}\times$$

$$\times\left\{\sqrt{z_1}U_s(z_1, 0)\mathrm{e}^{i(z_1-\pi/4)} + \sqrt{z_2}U_s(z_2, \pi)\mathrm{e}^{-i(z_2-\pi/4)}\right\} +$$

$$+\int_0^{i\infty}\frac{dz\sqrt{z}}{(2\pi\hbar)^2}\mathrm{e}^{izR}\left(\frac{U_s(z,0)\mathrm{e}^{-i\pi/4}}{\varepsilon - \varepsilon_s(z,0)} - \frac{U_s(-z,\pi)\mathrm{e}^{i\pi/4}}{\varepsilon - \varepsilon_s(-z,\pi)}\right) +$$

$$+\int_{C_b^1}\frac{dz\sqrt{z}}{(2\pi\hbar)^2}\frac{U_s(z,0)\mathrm{e}^{-i\pi/4}}{\varepsilon - \varepsilon_s(z,0)}\mathrm{e}^{izR} +$$

$$+\int_{C_b^2} d\frac{dz\sqrt{z}}{(2\pi\hbar)^2}\frac{U_s(z,\pi)\mathrm{e}^{i\pi/4}}{\varepsilon - \varepsilon_s(z,\pi)}\mathrm{e}^{-izR}, \qquad \text{(A4)}$$

where $z_1 = p_1 + i\xi_1$ and $z_2 = p_1 - i|\chi_2|$ (where $\xi_1 > 0$, $\xi_2 < 0$) are coordinates of the poles in the first and second integrals in Eq. (28), respectively, the residues of which contribute to the contour integration; the third term in the right-hand side is the integral along the imaginary axis while the last two terms are integrals along the pathes around the cuts (those pathes are marked as C_b^1 and C_b^2 in Fig. 1)

Using the inequality $R/a \gg 1$ one takes the integrals in Eq. (A4) and finds $G_{s\neq\alpha}(\mathbf{r}', \mathbf{r})$ written by the order of magnitude in Eq. (30) of the main text.

Appendix B: Matrix elements

Here calculations of matrix elements with Kohn–Lattinger functions are presented for the sake of convenience.

$$A \equiv \int_{\infty}^{\infty} \chi^{*}_{\alpha',\mathbf{p}'}(\mathbf{r})\chi_{\alpha,\mathbf{p}}(\mathbf{r}) =$$

$$= \sum_{\mathbf{n}=-\infty}^{+\infty} \int_{n_x a_x}^{(n_x+1)a_x} \int_{n_y a_y}^{(n_y+1)a_y} d\mathbf{r} e^{i(\mathbf{p}-\mathbf{p}')\mathbf{r}} u^{*}_{\alpha',0}(\mathbf{r}) u_{\alpha,0}(\mathbf{r}), \quad \text{(B1)}$$

where $\mathbf{n} = (n_x, n_y)$ while $n_{x,y} = 0, \pm 1, \pm 2, ...$

Changing integration variables $\mathbf{r} = \mathbf{r}' + \mathbf{a}$ one finds

$$A = \sum_{\mathbf{n}=-\infty}^{+\infty} e^{i(\mathbf{p}-\mathbf{p}')\mathbf{a}} \int_{0}^{(\mathbf{a})} d\mathbf{r} u^{*}_{\alpha',0}(\mathbf{r}) u_{\alpha,0}(\mathbf{r}). \quad \text{(B2)}$$

Here summation is over a unit cell.

Taking the sum one finally finds the normalization condition for the Kohn–Lattinger functions as follows:

$$\int_{\infty}^{\infty} \chi^{*}_{\alpha',\mathbf{p}'}(\mathbf{r})\chi_{\alpha,\mathbf{p}}(\mathbf{r}) \frac{d\mathbf{r}}{(2\pi\hbar)^2} = \delta_{\alpha,\alpha'}\delta(\mathbf{p}-\mathbf{p}'), \quad \text{(B3)}$$

where the the normalization condition for the periodic functions $u_{\alpha,0}(\mathbf{r}) = u_{\alpha,0}(\mathbf{r}+\mathbf{a}) = u_{\alpha,0}(\mathbf{r})$ was used:

$$\int_{0}^{(\mathbf{a})} u^{*}_{\alpha',0}(\mathbf{r}) u_{\alpha,0}(\mathbf{r}) \frac{d\mathbf{r}}{a^2} = \delta_{\alpha,\alpha'}. \quad \text{(B4)}$$

Performing analogous calculations one finds matrix elements of the velocity operator:

$$\int_{\infty}^{\infty} \chi^{*}_{\alpha,\mathbf{p}}(\mathbf{r}) \hat{\mathbf{v}} \chi_{\alpha',\mathbf{p}'}(\mathbf{r}) \frac{d\mathbf{r}}{(2\pi\hbar)^2} = \delta(\mathbf{p}-\mathbf{p}')\mathbf{v}_{\alpha,\alpha'}. \quad \text{(B5)}$$

Appendix C: Calculation of the integral along the cut for the edge scattering

Using Eq. (54) of the main text one writes the integral along the branch cut in Fig. 2 as follows:

$$I^{(\text{cont})} = 2\int_{ip_x}^{i\infty} \frac{e^{iy\xi/\hbar}}{[\varepsilon - v\sqrt{p_x^2+\xi^2}} d\xi =$$

$$= 2i\int_{p_x}^{\infty} \frac{e^{-y\zeta/\hbar}}{[\varepsilon - v\sqrt{p_x^2-\zeta^2}]} d\zeta. \quad \text{(C1)}$$

Changing the variables $\zeta - q \to \zeta$ one gets

$$I^{(\text{cont})} = 2ie^{-yp_x/\hbar}\int_{0}^{\infty} \frac{e^{-y\zeta/\hbar}}{\varepsilon - iv\sqrt{\zeta(\zeta+2p_x)}} d\zeta. \quad \text{(C2)}$$

As one sees from Eq. (C2) the main contribution of the integrand to the integral is at $\zeta \lesssim \hbar/y$. This inequality means that the square root in the integral denominator is much less than ε/v (note that $|p_x^{(\text{in})} \lesssim \varepsilon/v$). Therefore, neglecting the term with the square root one easily takes the integral and finds

$$I^{(\text{cont})} = \frac{2i\hbar e^{-p_x y/\hbar}}{y\varepsilon}. \quad \text{(C3)}$$

1. C. W. J. Beenakker, *Rev. Mod. Phys*. **80**, 1337 (2008).
2. P. R. Wallace, *Phys. Rev*. **71**, 622 (1947).
3. D. P. DiVincenzo and E. J. Mele, *Phys. Rev. B* **29**, 1685 (1984).
4. Y.-W. Son, M. L. Cohen, and S. G. Louie, *Phys. Rev. Lett*. **97**, 216803 (2006).
5. A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, *Rev. Mod. Phys*. **81**, 109 (2009).
6. S. Das Sarma, Shaffique Adam, E. H. Hwang, and Enrico Rossi, *Rev. Mod. Phys*. **83**, 109 (2011).
7. E. McCann and V. I. Fal'ko, *J. Phys.: Condens. Matter* **16**, 2371 (2004).
8. A. R. Akhmerov and C. W. J. Beenakker, *Phys. Rev. B* **77**, 085423 (2008).
9. J. M. Luttinger and W. Kohn, *Phys. Rev*. **97**, 869 (1955).
10. A. M. Kadigrobov, *Fiz. Nizk. Temp*. **44**, 1598 (2018) [*Low Temp. Phys*. **44**, 1245 (2018)].
11. P. M. Morse and H. Feshbach, *Methods of Rheoretical Physics*, McGraw-Hill Book Company, New York, Toronto, London (1953), Part I.

Дослідження динаміки квазічастинок в графені з домішками та гострими краями *kp*-методом

A. M. Kadigrobov

Динаміку квазічастинок у графені з домішками та гострими краями розглянуто за допомогою *kp*-методу, який допускає єдиний підхід без використання будь-якої моделі. Цим методом отримано рівняння Дірака та Вейля. Хвильову функцію та її обвідну, а також амплітуду розсіяння отримано в наближенні Борна. Показано, що хвильові функції є суперпозицією віртуальних блохівських функцій, які експоненціально загасають від домішки до краю. На відстанях, які набагато перевищують міжатомні, хвильові функції представлені в явному вигляді. Виведено функції Гріна для рівнянь Шредінгера та Дірака, а також граничні умови в рівнянні Дірака для графену з гострим краєм.

Ключові слова: розсіяння квазічастинок у графені, рівняння Вейля та Дірака, *kp*-метод, функції Гріна.