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 Schrödinger and Dirac equations are derived as well. Boundary conditions for the Dirac equation for graphene with a sharp edge are also derived.

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1 I. INTRODUCTION.

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

Details of the boundary conditions and scattering amplitudes depend on microscopic characteristics of the concrete structures of sample boundaries 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 and references there), the effective mass model, tight-binding model with a staggered potential at a zigzag boundary.

The object of this paper is to demonstrate that the kp-method allows investigations of graphene (and Weyl semi-metals) fundamental properties (including the particle dispersion law in the vicinity of the degeneration point) in the quasi-momentum space (see Ref. for details).

The Schrödinger equation for noninteracting quasi-particles is written as

\[
\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(r) \right] \phi_{s,p}(r) = \varepsilon_s(p)\phi_{s,p}(r) \tag{1}
\]

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

\[
\varphi_{s,p}(r) = e^{i\frac{p}{\hbar}r}u_{s,p}(r) \tag{2}
\]

is the Bloch function and \(u_{s,p}(r)\) is its periodic factor, \(p\) is the electron quasi-momentum while \(\varepsilon_s(p)\) 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:

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

According to the kp-method one finds the quasi-particle dispersion law in the vicinity of the degeneration

\[
\varepsilon_s(p) \approx \frac{1}{2m} \left| p \right|^2 + \frac{1}{2m} \left( \frac{\hbar}{e} \right)^2 \left( \frac{1}{2m} \right)^{-\frac{1}{2}} + \frac{1}{2m} \left( \frac{\hbar}{e} \right)^{\frac{3}{2}} \left( \frac{1}{2m} \right)^{-\frac{3}{2}} + \cdots
\]

II. 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 \(p_0 = 0\) ("Dirac" point) in the quasi-momentum space (see Ref. for details).

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\]
point presenting the proper wave functions as a superposition of Lattinger-Kohn functions:

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

where the periodic Bloch factors are taken at the degeneration point \( \mathbf{p} \).

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

\[ u_{s, \mathbf{p}}(r) = g_1(\mathbf{p}) u_{1,0}(r) + g_2(\mathbf{p}) u_{2,0}(r) \] (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:

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

Here \( \mathbf{p}_f = (-i\hbar/m) \partial / \partial r \) 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 \( g_{1,2} \):

\[ (\mathbf{p}v_{11} - \varepsilon) g_1(\mathbf{p}) + (\mathbf{p}v_{12}) g_2(\mathbf{p}) = 0; \]
\[ (\mathbf{p}v_{21}) g_1(\mathbf{p}) + (\mathbf{p}v_{22} - \varepsilon) g_2(\mathbf{p}) = 0; \] (7)

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

\[ \mathbf{v}_{\alpha \alpha'} = \int u^*_\alpha(r) \mathbf{p} u_{\alpha'}(r) \partial r \] (8)

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

\[ \varepsilon_{\pm}(\mathbf{p}) = \frac{\mathbf{p}v_{11} \pm \sqrt{(\mathbf{p}v_{12})^2 + 4|\mathbf{p}v_{12}|^2}}{2} \] (9)

where \( v_{\pm} = v_{11} \pm v_{22} \). 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\(^5^6\))

\[ \varepsilon_{\pm}(\mathbf{p}) = \pm v \sqrt{p_x^2 + p_y^2} = \pm vp \] (10)

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

\[ v_{11}(0) = v_{22}(0) = 0, \quad |v_{12}(0)| = v, \]
\[ \varepsilon_{\pm}(0) = \pm iv_{\pm}(0) \] (11)

where \( v = v_F \approx 1 \times 10^6 \text{ m/s} \) 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

\[ \varphi_{\alpha, \mathbf{p}}(r) = e^{i \mathbf{p} r} \left[ u_{1,0}(r) + e^{-\alpha} u_{2,0}(r) \right] / 2\sqrt{\alpha} \] (12)

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

Introducing the envelope functions

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

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

\[ (-i\hbar \mathbf{v}_{11} \partial_x + \mathbf{V}(r) - \varepsilon) \Phi_1(r) - i\hbar \mathbf{v}_{12} \partial_z \Phi_2(r) = 0; \]
\[ -i\hbar \mathbf{v}_{21} \partial_y \Phi_1(r) + (-i\hbar \mathbf{v}_{22} \partial_x + \mathbf{V}(r) - \varepsilon) \Phi_2(r) = 0 \] (14)

Here we added an external potential \( \mathbf{V}(r) \) which smoothly changes at the atomic scale (it can be rigorously proved as it is shown in Ref.\(^1^0\)).

Eq.(14) transforms into Weyl equation

\[ \sigma_0 \varepsilon \Phi_W + \sigma_x \partial_x \Phi_W + \sigma_y \partial_y \Phi_W + \sigma_z \partial_z \Phi_W = 0 \] (15)

where \( \sigma_0 \) 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:

\[ v_{11}(0) = v_{22}(0) = 0, \quad |v_{12}(0)| = v, \quad v_{12} = v(1 - i, i) \] (16)

Differential equations Eq.(14) and Eq.(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\(^5^6\):

\[ \left( \begin{array}{c} V(r) - \varepsilon \\ \hbar (-i \partial_x + \partial_y) \\ \hbar (-i \partial_x - \partial_y) \\ V(r) - \varepsilon \end{array} \right) \left( \begin{array}{c} \Phi_1 \\ \Phi_2 \end{array} \right) = 0 \] (17)

III. 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:

\[ \left( \hat{H}_0 + V_i(r) \right) \Psi(r) = \varepsilon \Psi(r) \] (18)
where $\hat{H}_0$ is the quasi-particle Hamiltonian for the pure crystal, Eq. (1), and $V_i(r)$ is the impurity potential.

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

$$ \Psi(r) = \varphi^{(in)}_{p}(r) + \int G(r,r')V_i(r')\Psi(r')dr' \quad (19) $$

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

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

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

$$ G(r,r') = G_0(r,r') + G_{s\neq\alpha}(r,r') \quad (21) $$

where

$$ G_0(r,r') = \sum_{\alpha=1}^{2} \int \frac{dp}{(2\pi\hbar)^2} \varphi^{*}_{p,p}(r')\varphi_{p,p}(r) \quad (22) $$

is the ”graphene” Green function in which the graphene dispersion law and the Bloch functions $\varphi_{p,p}(r)$ are defined in Eq.(10) and Eq.(12), respectively, while

$$ G_{s\neq\alpha} = \sum_{s\neq\alpha} \int \frac{dp}{(2\pi\hbar)^2} \varphi^{*}_{s,p}(r')\varphi_{s,p}(r) \quad (23) $$

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

a) Calculations of “graphene” Green’s function.

Using Eqs.(22,12) one presents $G_0(r,r')$ as follows:

$$ G_0(r,r') = \frac{1}{2} \left[ u_{1,0}(r')u_{1,0}(r) + u_{2,0}(r)u_{2,0}(r') \right] \quad (24) $$

where

$$ I_1(r-r') = \int \frac{dp}{(2\pi\hbar)^2} \frac{e^{ip(r-r')/\hbar}}{\varepsilon - \varepsilon_s(p) + i0} \quad (25) $$

$$ I_2^{(\pm)}(r-r') = \int \frac{dp}{(2\pi\hbar)^2} \frac{e^{ip(r-r')/\hbar}}{\varepsilon - \varepsilon_s(p) + i0} \quad (26) $$

Performing integrations (see Appendix A) one finds

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

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

b) Calculations of Green’s function for virtual states.

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

$$ G_{s\neq\alpha}(r',r) = \sum_{s\neq\alpha} \int \frac{u_{s,p,r'}^* u_{s,p}(r)}{\varepsilon - \varepsilon_s(p)} \frac{dp}{(2\pi\hbar)^2} \quad (27) $$

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

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

where

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

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 $\varphi$ and find

$$ G_{s\neq\alpha}(r',r) = \sqrt{\frac{2\pi\hbar}{R}} \sum_{s\neq\alpha} \int_0^\infty dp \sqrt{p} \left\{ \frac{U_s(p,0)e^{-i\pi/4} - e^{ipR}}{\epsilon - \varepsilon_s(p,0)} + \frac{U_s(p,\pi)e^{i\pi/4}}{\epsilon - \varepsilon_s(p,\pi)} e^{-ipR} \right\} \quad (29) $$

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 $h/a$ (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 $\varepsilon$ 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 $\Delta$ is the characteristic width of energy gaps.

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

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

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

$$ G_e(r,r') = -\frac{e^{i\pi/4}}{2hv} \sqrt{\frac{p_x}{2\pi\hbar}} e^{iR_{fp}} $$

$$ \times \sum_{\alpha,\beta=1}^2 \frac{u_{\alpha,0}(r')u_{\beta,0}(r')}{\varepsilon R^2} + O\left(\frac{1}{\Delta R^2},\frac{e^{-R/a}}{\varepsilon R^2} \right) \quad (31) $$

Inserting Eq.(31) into Eq.(19) one readily finds the integral equation for the wave function of the electron scat-
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 \( \mathbf{k}-\mathbf{p} \)-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 \( \mathbf{k}-\mathbf{p} \) 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:

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

Expanding \( \Psi \) in the left-hand side of the above equation in the series of \( \chi \) (see Eq.(4))

\[
\Psi = \sum_{\alpha=1}^{2} g_\alpha(\mathbf{p}) \chi_{\alpha,\mathbf{p}}(r) \frac{d\mathbf{p}}{(2\pi\hbar)^2} \quad (34)
\]

and using Eq.(11) one finds the Schrödinger equation in the \( \mathbf{p} \)-representation:

\[
-\varepsilon g_\alpha(\mathbf{p}) + \sum_{\alpha'=1}^{2} \langle \mathbf{p} \cdot \mathbf{v}_{\alpha,\alpha'} \rangle g_{\alpha'}(\mathbf{p})
= - \int \chi_{\alpha,\mathbf{p}}(r)V_i(r)\Psi(r)dr \quad (35)
\]

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

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

\[
\Psi = \sum_{\alpha=1}^{2} u_{\alpha,0}(r)\Phi_\alpha(r) \quad (36)
\]

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

\[
\begin{align*}
\varepsilon \Phi_1 + \hbar v(i\partial_\mathbf{r} - \partial_\mathbf{y})\Phi_2 &= u_{1,0}(r)V_i(r)\Psi(r) \\
\hbar v(i\partial_\mathbf{r} + \partial_\mathbf{y})\Phi_1 + \varepsilon \Phi_2 &= u_{2,0}(r)V_i(r)\Psi(r)
\end{align*}
\]

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

\[
\begin{align*}
\Phi_1(\mathbf{r}) &= \Phi_1^{(in)} - \int V_i(r')\Psi(r') \sum_{\alpha=1}^{2} u^*_{\alpha,0}(r')A_\alpha(r',r)dr' \\
\Phi_2(\mathbf{r}) &= \Phi_2^{(in)} - \int V_i(r')\Psi(r') \sum_{\alpha=1}^{2} u^*_{\alpha,0}(r')B_\alpha(r',r)dr'
\end{align*}
\]

where \( \Phi_1^{(in)}, \Phi_2^{(in)} \) are the envelope functions of the incoming quasi-particle (which are solutions of the above homogeneous Dirac equation) while functions \( A_\alpha \) and \( B_\alpha \) are integrals with respect to the momentum \( \mathbf{p} \):

\[
\begin{align*}
A_1 &= B_1 = \int_0^\infty \frac{e^{ip(r-r')}}{(vp)^2 - \varepsilon}(2\pi\hbar)^2dp \\
A_2 &= \int_{-\infty}^{\infty} \frac{v(p_x + ip_y)e^{ip(r-r')}}{(vp)^2 - \varepsilon}(2\pi\hbar)^2dp \\
B_2 &= \int_{-\infty}^{\infty} \frac{v(p_x - ip_y)e^{ip(r-r')}}{(vp)^2 - \varepsilon}(2\pi\hbar)^2dp
\end{align*}
\]
Performing integrations analogous to those made in Appendix A one finds:

\[ A_1 = A_2 = B_1 = B_2 = e^{i\pi/4} \left(\frac{(2\pi)^{3/2} p_x}{4(2\pi\hbar)^2} v \sqrt{\beta} R / \hbar\right); \]

\[ R = |r - r'|; \]

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:

\[ \left( \Phi_1 \Phi_2 \right) = \left( \begin{array}{c} 1 \\ e^{ikz} \end{array} \right) e^{ikz} + \left( \begin{array}{c} 1 \\ -1 \end{array} \right) \int V_i(r') \]

\[ \times \sum_{\beta=1}^{2} u_{\beta,0}(r') \Phi(r') \sum_{\alpha=1}^{2} u_{\alpha,0}(r') A_1(r', r) dr \]  \hspace{1cm} (41)

where \( \phi = \arctan p_y / p_x \) 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:

\[ \left( \Phi_1 \Phi_2 \right) = \left( \begin{array}{c} 1 \\ e^{ikz} \end{array} \right) e^{ikz} + \left( \begin{array}{c} 1 \\ -1 \end{array} \right) f(\theta) \frac{e^{ikz R_0}}{\sqrt{R_0}} \]  \hspace{1cm} (42)

where the scattering amplitude is

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

\[ \varepsilon \int \frac{d\varepsilon'}{(2\pi\hbar)^2} e^{-i\varepsilon' V_i(r')} \sum_{\alpha,\beta=1}^{2} u_{\alpha,0}(r') u_{\beta,0}(r') e^{i(\beta-1)\varepsilon'} \]  \hspace{1cm} (43)

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

\[ q = 2k \sin \theta / 2, \]

\( \theta \) being the angle between \( k \) and \( k' \), 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 function is a convenient tool 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 \( G(r, r') \) 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:

\[ \left( -\varepsilon - \hbar v(-i\partial_x + \partial_y) \right) \left( \begin{array}{c} G_1(r, r') \\ G_2(r, r') \end{array} \right) = -\left( \begin{array}{c} u_{1,0}(r) \\ u_{2,0}(r) \end{array} \right) \delta(r - r') \]  \hspace{1cm} (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:

\[ \left( \begin{array}{c} G_1^D(r, r') \\ G_2^D(r, r') \end{array} \right) = \sum_{\alpha=1}^{2} \frac{dp}{2(\pi\hbar)^2} \] \[ \times u_{1,0}(r) + (-1)^\alpha e^{\theta} u_{2,0}(r) \left( \begin{array}{c} 1 \\ (-1)^\alpha e^{-i\theta} \end{array} \right) e^{p(r - r') / \hbar} \]  \hspace{1cm} (45)

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

**IV. DERIVATION OF BOUNDARY CONDITIONS FOR DIRAC EQUATION.**

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

\[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + U(r) \Psi(r) = \varepsilon \Psi(r) \]  \hspace{1cm} (46)

with the boundary condition

\[ \Psi(r) \big|_{y=0} = 0 \]  \hspace{1cm} (47)

where \( U(r) = U(r + \mathbf{a}) \) 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):

\[ \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + U(r) - \varepsilon \right) G(r, r') = \delta(r - r') \]  \hspace{1cm} (48)

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

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

\[ \Psi(r) = \frac{\chi_{\alpha, p}(r)}{\sqrt{\Psi_{\alpha}}} \]

\[ + \frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} G(x', 0; r) \frac{\partial \Psi(r')}{\partial y'} \bigg|_{y'=0} dx' \]  \hspace{1cm} (49)
edge. Here $\chi_{\alpha,p}(r)$ is the graphene Kohn-Luttinger function Eq.(4) incident to the graphene edge from the infinity $y \to \infty$ and $v_{y,\alpha} = \partial \varepsilon_{\alpha}^{(gr)}(p)/\partial y$ is the velocity $y$-projection that normalizes the incident function to the flux unity while $\varepsilon_{\alpha}^{(gr)}(p) = \pm i p$ is the graphene dispersion; in order to define $\Psi(r)$ on the whole half-plane $y \geq 0$ the boundary contour is shifted to $y = -\infty \equiv 0 - \delta'$, $\delta' \to 0$ (see Ref.\textsuperscript{11}).

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

$$G(r,r') = \sum_{\alpha=1,2} \frac{\chi_{\alpha,0}(r)\chi_{\alpha,0}(r')}{\varepsilon - \varepsilon_{\alpha}^{(gr)}(p) + i\delta} dp + \sum_{s \neq 1,2} \int \frac{\varphi_{s,0}^*(r')\varphi_{s,p}(r')}{\varepsilon - \varepsilon_s(p) + i\delta} dp \quad \text{(50)}$$

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 $x \geq 0$ as follows:

$$\Psi(r) = \frac{\chi_{\alpha,0}^{(in)}}{\sqrt{v_{y,\alpha} p}} + \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} d\bar{y} \Psi_\gamma' (\bar{x}, 0) e^{i\bar{x}p_y} \left\{ \sum_{\alpha=1,2} u_{\alpha,0}^{(gr)}(\bar{x}, 0) u_{\alpha,0}(r) I_{\alpha}^{(gr)} + \sum_{s \neq 1,2} u_{s,p}^{*}(\bar{x}, 0) u_{s,p}(r) I_{s}^{(bnd)} \right\} \quad \text{(51)}$$

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

Differentiating the both sides of Eq.(51) with respect to $p_y$ in Eq.(51) re-writing them in the following forms:

$$I_{\alpha}^{(gr)} = \int_{-b_y/2}^{b_y/2} \frac{e^{i\bar{y}p_y} / h}{\varepsilon - \varepsilon_{\alpha}(p_x, p_y) + i\delta} dp_y \quad \text{(52)}$$

and

$$I_{s}^{(bnd)} = \int_{-b_y/2}^{b_y/2} \frac{u_{s,p_x,p_y}(\bar{x},0) u_{s,p_x,p_y}(r) e^{i\bar{y}p_y} / h}{\varepsilon - \varepsilon_s(p_x, p_y) + i\delta} dp_y \quad \text{(53)}$$

where $b_y$ 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 $\varepsilon(p_x,z) = +\sqrt{z^2 + p_y^2}$) 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 branch cut in the upper complex half-plane $\xi \geq 0$ 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 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

$$I_{1}^{(gr)} = \int_{-b_y/2}^{b_y/2} \frac{e^{i\bar{y}p_y} / h}{\varepsilon - \sqrt{p_x^2 + p_y^2} + i\delta} dp_y \quad \text{(54)}$$

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)

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

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

$$v_y = \left. \frac{\partial \varepsilon_1(p_x, p_y)}{\partial p_y} \right|_{p_y = p_y^{(1)}} > 0$$

![FIG. 2: (a) Equal energy contour $\sqrt{p_x^2 + p_y^2} = \varepsilon$. The thick arrows show the velocity direction at fixed energy $\varepsilon$ 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 branch line corresponding to the branching point (thick dots), $p_y^{(gr)} = 2p_x$, in the quasi-particle spectrum.](image-url)
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 \(I^{(\text{gr})}_1\) as follows:

\[
I^{(\text{gr})}_1 = - \frac{2\pi i}{v_y(p_x, p_y)} e^{yp_y(i)/\hbar} + \frac{2\hbar i}{y \varepsilon} e^{-yp_x\hbar} \tag{55}
\]

For calculations of the integral in Eq.\(53\) one finds the poles from the equation \(\varepsilon_x(p_x, p_y) = \varepsilon, s \neq \alpha\) where the energy bands \(\varepsilon_x(p_x, p_y)\) do not overlap bands \(\alpha = 1, 2\) in which the energy \(\varepsilon\). In the general case the difference between those bands \(|\varepsilon_x(p_x, p_y) - \varepsilon_s(p_x, p'_y)| \approx \Delta^{(s)}_{\text{gap}} \sim \hbar v/\alpha, s \neq \alpha\) (where \(\Delta^{(s)}_{\text{gap}}\) 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 \(\xi \sim \eta'_0\)).

Performing integration in Eq.\(53\) in much the same manner as above one finds \(I^{(\text{bnd})}_1\) as follows (details of the calculations are presented in Ref.\(^{10}\)):

\[
I^{(\text{bnd})}_1 \sim e^{-yp_y\hbar/v} \tag{56}
\]

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

\[
\Psi_{p_y}(r) = \left(\phi^{(\text{gr})}_{\alpha, p_x, p_y}(r) - \phi^{(\text{gr})}_{\alpha, p_x, p_y(\text{out})}(r)\right)
\]

\[
+C \frac{ae^{-yp_x\hbar}}{y} e^{yp_y\hbar} e^{yp_y i\varphi} \tag{57}
\]

where \(p_y^{(\text{in})}\) and \(p_y^{(\text{out})} = -p_y^{(\text{in})}\) are the \(y\)-projections of the quasiparticle momentum while \(C\) is a constant \(\sim 1\) (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, \(l >> a\), the graphene envelope function \(\Phi(r)\) is the difference between the incident and outgoing wave functions (which are two independent solutions of the Dirac equation Eq.\(17\)):

\[
\Phi(r) = e^{yp_x} \left[ e^{yp_y(i)} \left( \frac{1}{e^{iy\varphi}} - e^{-iyp_y^{(\text{in})}} \left( \frac{1}{e^{-iy\varphi}} \right) \right) \tag{58}\right]
\]

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

V. 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 section II. 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 quasi-particle is perpendicular to the edge the above-mentioned superposition of virtual states decays linear with the distance increase, Eq.\(57\). 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.\(58\), that is the boundary condition for Dirac equation.

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

\[ I_1 = -\frac{2\pi}{v} \int_0^\infty \frac{p}{p - p_\varepsilon - i0} J_0(pR) \frac{dp}{(2\pi\hbar)^2} \]
\[ I_2^{(\pm)} = -\frac{2\pi i}{v} \int_0^\infty \frac{p}{p - p_\varepsilon - i0} J_1(pR) \frac{dp}{(2\pi\hbar)^2} \]

(A1)

where \( p_\varepsilon = \varepsilon/v \) and \( R = |r-r'| \) while \( J_0, J_1 \) 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 \( J_1(pR) = \sqrt{2/(\pi pR)} \sin(pR - \pi/4) \) and hence at \( pR \gg 1 \), Eq.(A1) reads

\[ I_1(r-r') = -\frac{1}{v} \sqrt{\frac{2\pi}{R}} \int_0^\infty \frac{dp}{(2\pi\hbar)^2} \]
\[ \times \left( \exp(i(pR-\pi/4)) + \exp(-i(pR-\pi/4)) \right) \]
\[ I_2^{(\pm)}(r-r') = -\frac{1}{v} \sqrt{\frac{2\pi}{R}} \int_0^\infty \frac{dp}{(2\pi\hbar)^2} \]
\[ \times \left( \exp(i(pR-\pi/4)) - \exp(-i(pR-\pi/4)) \right) \]

(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

\[ I_1 = I_2^{(\pm)} = -\frac{1}{v} \sqrt{\frac{2\pi}{R}} e^{i(pR/R + \pi/4)} \]
\[ +i^{3/2} \sqrt{\frac{2\pi}{R}} \int_0^\infty \frac{d\xi}{\xi + p_\varepsilon} \frac{\exp(-R\xi)}{(2\pi\hbar)^2} \]
\[ +e^{i\pi/4} \int_0^\infty \frac{d\xi}{\xi + p_\varepsilon} \frac{\exp(-R\xi)}{(2\pi\hbar)^2} \]

(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:

\[ G_{s\neq\alpha}(r', r) = \sum_{s\neq\alpha} I_s; \]
\[ I_s = -\frac{1}{hv} \sqrt{\frac{2\pi}{\hbar R}} \]
\[ \times \left\{ \sqrt{\frac{R}{\sqrt{\pi}}} U_s(z_1, 0) e^{i(z_1 - \pi/4)} + \sqrt{\frac{R}{\sqrt{\pi}}} U_s(z_2, \pi) e^{-i(z_2 - \pi/4)} \right\} \]
\[ + \int_0^{\infty} \frac{dz}{\sqrt{2\pi \hbar R}} U_s(z, 0) e^{-iz/\hbar R} \left\{ e^{i\pi/4} \left[ e^{iz} - e^{-iz} \right] - e^{-iz} - e^{iz} \left[ e^{i\pi/4} \left[ e^{iz} - e^{-iz} \right] \right] \right\} \]
\[ + \int_{C_b^1} dz \sqrt{2\pi \hbar R} U_s(z, \pi) e^{iz/\hbar R} \left\{ e^{i\pi/4} \left[ e^{iz} - e^{-iz} \right] - e^{-iz} - e^{iz} \left[ e^{i\pi/4} \left[ e^{iz} - e^{-iz} \right] \right] \right\} \]

(A4)

where \( z_1 = p_1 + i\xi_1 \) and \( z_2 = p_1 - i\xi_2 \) (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 \( G_{s\neq\alpha}(r', r) \) written by the order of magnitude in Eq.(30) of the main text.

Appendix B: Matrix elements.

Here calculations of matrix elements with Kohn-Luttinger functions are presented for the sake of conve-
\[
A \equiv \int_{-\infty}^{\infty} \chi_{\alpha', p'}(r) \chi_{\alpha, p}(r) = \sum_{n=-\infty}^{+\infty} \int_{n_x a_x}^{(n_x+1) a_x} \int_{n_y a_y}^{(n_y+1) a_y} d\mathbf{r} e^{i(\mathbf{p}-\mathbf{p}') \cdot \mathbf{r}} u_{\alpha', 0}^*(\mathbf{r}) u_{\alpha, 0}(\mathbf{r}) \quad (B1)
\]

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

Changing integration variables \( \mathbf{r} = \mathbf{r}' + \mathbf{a} \) one finds
\[
A = \sum_{n=-\infty}^{+\infty} e^{i(\mathbf{p}-\mathbf{p}') \cdot \mathbf{a}} \int_{0}^{(a)} d\mathbf{r} u_{\alpha', 0}^*(\mathbf{r}) u_{\alpha, 0}(\mathbf{r}) \quad (B2)
\]

where summation is over a unit cell.

Taking the sum one finally finds the normalization condition for the Kohn-Luttinger functions as follows:
\[
\int_{-\infty}^{\infty} \chi_{\alpha', p'}(r) \chi_{\alpha, p}(r) \frac{dr}{(2\pi \hbar)^2} = \delta_{\alpha, \alpha'} \delta(\mathbf{p} - \mathbf{p}') \quad (B3)
\]

where 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:
\[
\int_{0}^{(a)} u_{\alpha', 0}^*(\mathbf{r}) u_{\alpha, 0}(\mathbf{r}) \frac{dr}{a^2} = \delta_{\alpha, \alpha'} \quad (B4)
\]

Performing analogous calculations one finds matrix elements of the velocity operator:
\[
\int_{-\infty}^{\infty} \chi_{\alpha', p'}(r) \tilde{v} \chi_{\alpha, p}(r) \frac{dr}{(2\pi \hbar)^2} = \delta(\mathbf{p} - \mathbf{p}') \mathbf{v}_{\alpha, \alpha'} \quad (B5)
\]

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:
\[
I^{(cont)} = 2 \int_{0}^{i\infty} \frac{e^{iy\xi/\hbar}}{\varepsilon - v \sqrt{p_x^2 + \xi^2}} d\xi = 2i \int_{-\infty}^{\infty} \frac{e^{-y\zeta/\hbar}}{\varepsilon - v \sqrt{\zeta^2 + 2p_x}} d\zeta \quad (C1)
\]

Changing the variables \( \zeta - q \to \zeta \) one gets
\[
I^{(cont)} = 2i e^{-yp_x/\hbar} \int_{0}^{\infty} \frac{e^{-y\zeta/\hbar}}{\varepsilon - iv \sqrt{\zeta + 2p_x}} d\zeta \quad (C2)
\]

As one sees from Eq. (C2) the main contribution of the integrand to the integral is at \( \zeta \ll h/y \). This inequality means that the square root in the integral denominator is much less than \( \varepsilon/v \) (note that \( |p_x^{(in)}| \ll \varepsilon/v \)). Therefore, neglecting the term with the square root one easily takes the integral and finds
\[
I^{(cont)} = \frac{2ihe^{-yp_y/\hbar}}{ye} \quad (C3)
\]