6

Complex WKB Approximations in Graphene Electron-Hole Waveguides in Magnetic Field

V.V. Zalipaev
School of Mathematical Sciences, University of Loughborough, Loughborough UK

1. Introduction

Application of semiclassical analysis in studying quantum mechanical behaviour of electron has been demonstrated in various fields of modern physics such as nano-structures, electronic transport in mesoscopic systems, quantum chaotic dynamics of electronic resonators (1), (2), (3), (4) and many others. One of the examples of the application of semiclassical analysis are quantum electronic transport in waveguides and resonators in semiconductors, and in particularly in graphene structures (see, for example, (5), (6), (7)), (8), (9)).
Here we review some theoretical aspects of semiclassical description of the Dirac electron motion inside graphene, a one-atom-thick allotrope of carbon (5). A general introduction of ray asymptotic method and boundary layer techniques of complex Gaussian beams (Gaussian wave packages) is given to construct semiclassical approximations of Green's function inside electron-holes waveguide in graphene structures. The Dirac electrons motion can be controlled by application of electric and magnetic fields. This application could lead in some cases to a generation of a waveguide (drift) motion inside infinite graphene sheets. Constructions of semiclassical approximations of Green's function inside electronic waveguides or resonators has been a key problem in the analysis of electronic transport problems both different types semiconductors ((10), (11), (12), (13)) and graphene structures such as graphene nano-ribbons (5), (6), (7)), (8), (9)). It is deserved mention that a semiclassical approximation for the Green's function in graphene as well as a relationship between the semiclassical phase and the adiabatic Berry phase was discussed in the paper (14).
An application of semiclassical analysis to graphene quantum electron dynamics is demonstrated for one important problem of constructions of semiclassical approximation of Green's function in electronic waveguide inside graphene structure with linear potential and homogeneous magnetic field. The problem can be described by the following 2D Dirac system with magnetic and electrostatic potentials in axial gauge $\mathbf{A} = 1/2B(-x_2, x_1, 0)$ (see (5))

$$v_F < -i\hbar\nabla + \frac{e}{c}\mathbf{A}, \bar{\sigma} > \psi(\mathbf{x}) + U(\mathbf{x})\psi(\mathbf{x}) = E\psi(\mathbf{x}), \quad \psi(\mathbf{x}) = \begin{pmatrix} u \\ v \end{pmatrix}, \tag{1}$$

where $\mathbf{x} = (x_1, x_2)$, u, v are the components of spinor wave function describing electron localisation on sites of sublattice A or B of honeycomb graphene structure, e is the electron charge, c is the speed of light, and v_F is the Fermi velocity, the symbol $<,>$ means a scalar product, and $\bar{\sigma} = (\sigma_1, \sigma_2)$ with Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

However, classical trajectories structure for waveguides and resonators with rather strong magnetic fields is getting very complicated, and, owing to the presence of multiple caustics and focal points, the semiclassical approximation, well-known as ray asymptotic method, is not valid. In this case one of the possibilities to tackle the problem of computing Green's function is Maslov's canonical operator method (15). The method gives a cumbersome universal asymptotic construction depending on geometrical and topological properties of families of classical trajectories of electronic motion. Fortunately, an alternative method of summation of Gaussian beams (integral over Gaussian beams) which was developed for acoustic, and later electromagnetic and elastic wave propagation may be found much more suitable especially in practical applications and especially numerical analysis of electronic motion in graphene structures (16), (17).

The theoretical foundations of the method are rather simple in comparison with the Maslov's canonical operator method. Gaussian beam as a localised asymptotic solution is always regular near caustics or focal point. Realization of the method does not require any knowledge about geometrical properties of caustics, and numerous numerical tests demonstrated this effect (16), (17). This is due to the fact that the structure of the asymptotic Gaussian beam solution does not depend on geometrical properties of caustics, and the final asymptotic approximation is just a superposition of Gaussian beams. Thus, in a general case, the method of summation of Gaussian beams gives universal semiclassical uniform approximation for solutions to various problems of wave propagation and quantum mechanics. This approximation is valid near caustics or focal points of arbitrary geometric structure. Application of the method to computations of high-frequency acoustic and elastic wave fields was proved to be very efficient and robust.

This method is convenient to construct a semiclassical uniform approximation for Green's function for interior of waveguides and resonators quantum problems. Application of this method to problems of electron motion in magnetic field in graphene required a generalization of the approach originally developed for acoustic wave propagation problems. The first step in this direction has been done in ((18), (19)).

The chapter is organized as follows. First, in section 2, we give a description of the ray asymptotic solution and the boundary layer semiclassical method used to construct the asymptotic solution of the Gaussian beam in the presence of a magnetic field and any scalar potential. Subsecuently, in section 3, the techniques of the Gaussian beams summation method is presented. Finally, in section 4, some numerical results of computation of semiclassical uniform approximation for Green's function for interior of graphene waveguide with magnetic field and linear electrostatic potential is described.

2. Electronic Gaussian beams

First, the basic steps of the ray method recurrence relations (see (20), (21)) are presented for the stationary problem for the Green's tensor for the Dirac system describing an electron-hole quantum dynamics in the presence of a homogeneous magnetic field and arbitrary scalar potential

$$v_F < -i\hbar\nabla + \frac{e}{c}\mathbf{A}, \bar{\sigma} > G(\mathbf{x}) + (U(\mathbf{x}) - E)G(\mathbf{x}) = \begin{pmatrix} \delta(x) & 0 \\ 0 & \delta(x) \end{pmatrix}, \tag{2}$$

$$G(\mathbf{x}) = \begin{pmatrix} G_{11}(\mathbf{x}) & G_{12}(\mathbf{x}) \\ G_{21}(\mathbf{x}) & G_{22}(\mathbf{x}) \end{pmatrix}.$$

These are to be used in derivation of electronic Gaussian beam asymptotic expansion. Ray asymptotic solution is the principal part of the method summation of Gaussian beams.

2.1 Ray asymptotic solutions

Consider the axial gauge of the magnetic field $\mathbf{A} = B/2(-x_2, x_1, 0)$. The WKB ray asymptotic solution to the Dirac system

$$\begin{pmatrix} U(\mathbf{x}) - E & v_F[\hbar(-i\partial_{x_1} - \partial_{x_2}) - i\frac{\alpha x_1}{2} - \frac{\alpha x_2}{2}] \\ v_F[\hbar(-i\partial_{x_1} + \partial_{x_2}) + i\frac{\alpha x_1}{2} - \frac{\alpha x_2}{2}] & U(\mathbf{x}) - E \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{3}$$

is to be sought in the form

$$\psi = \begin{pmatrix} u \\ v \end{pmatrix} = e^{\frac{i}{\hbar}S(\mathbf{x})} \sum_{j=0}^{+\infty} (\frac{\hbar}{i})^j \begin{pmatrix} u_j \\ v_j \end{pmatrix} = e^{\frac{i}{\hbar}S(\mathbf{x})} \sum_{j=0}^{+\infty} (\frac{\hbar}{i})^j \psi_j(\mathbf{x}), \tag{4}$$

where $\alpha = B\frac{e}{c}$. Substituting this series into the Dirac system, and equating to zero corresponding coefficients of successive degrees of the small parameter $\hbar$, we obtain recurrent system of equations which determines the unknown $S(\mathbf{x})$ and $\psi_j(\mathbf{x})$, namely,

$$(H - EI)\psi_0 = 0, \quad (H - EI)\psi_j = -R\psi_{j-1},$$

$$H = \begin{pmatrix} U(\mathbf{x}) & v_F(S_{x_1} - \frac{\alpha x_2}{2} - i(S_{x_2} + \frac{\alpha x_1}{2})) \\ v_F(S_{x_1} - \frac{\alpha x_2}{2} + i(S_{x_2} + \frac{\alpha x_1}{2})) & U(\mathbf{x}) \end{pmatrix}, \quad R = v_F \begin{pmatrix} 0 & \partial_{x_1} - i\partial_{x_2} \\ \partial_{x_1} + i\partial_{x_2} & 0 \end{pmatrix},$$

where I is the identity matrix. The hamiltonian H has two eigenvalues and eigenvectors

$$He_\alpha = h_\alpha v_\alpha, \ \ \alpha = 1, 2,$$

where

$$h_\alpha = U(\mathbf{x}) \pm v_F \sqrt{(p_1 - \frac{\alpha x_2}{2})^2 + (p_2 + \frac{\alpha x_1}{2})^2} = U(\mathbf{x}) \pm v_F p,$$

and

$$v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \frac{p_1 - \frac{\alpha x_2}{2} + i(p_2 + \frac{\alpha x_1}{2})}{p} \end{pmatrix}, \quad v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\frac{p_1 - \frac{\alpha x_2}{2} + i(p_2 + \frac{\alpha x_1}{2})}{p} \end{pmatrix},$$

where $S_{x_1} = p_1$ and $S_{x_2} = p_2$. However, for the sake of simplicity instead of v_α, below we shall use

$$\mathbf{e}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix}, \quad \mathbf{e}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{i\theta} \end{pmatrix}, \quad e^{i\theta} = v_F \frac{p_1 - \frac{\alpha x_2}{2} + i(p_2 + \frac{\alpha x_1}{2})}{E - U(\mathbf{x})},$$

If $E > U(\mathbf{x})$, then

$$E = h_1, \quad e^{i\theta} = \frac{p_1 - \frac{\alpha x_2}{2} + i(p_2 + \frac{\alpha x_1}{2})}{p}, \quad e_1 = v_1, \quad e_2 = v_2,$$

if $E < U(\mathbf{x})$, then

$$E = h_2, \quad e^{i\theta} = -\frac{p_1 - \frac{\alpha x_2}{2} + i(p_2 + \frac{\alpha x_1}{2})}{p}, \quad e_1 = v_2, \quad e_2 = v_1.$$

In a domain $\Omega_e = \{\mathbf{x} : E > U(\mathbf{x})\}$, the hamiltonian

$$h_1 = U(\mathbf{x}) + v_F\sqrt{(p_1 - \frac{\alpha x_2}{2})^2 + (p_2 + \frac{\alpha x_1}{2})^2}$$

on the level set $h_1 = E$ describes dynamic of electrons (a quasi-particle described by the initial Dirac system behaves like electron, negatively charged). The corresponding classical trajectories can be obtained from the hamiltonian system

$$\dot{x} = H^e_p, \quad \dot{p} = -H^e_x, \quad x = (x_1, x_2), \;\; p = (p_1, p_2),$$

with hamiltonian (see (15))

$$H^e = \frac{1}{2}((p_1 - \frac{\alpha x_2}{2})^2 + (p_2 + \frac{\alpha x_1}{2})^2 - (\frac{E - U(\mathbf{x})}{v_F})^2)$$

on the level set $H^e = 0$.
Opposite to this case, in a domain $\Omega_h = \{\mathbf{x} : E < U(\mathbf{x})\}$, the hamiltonian

$$h_2 = U(\mathbf{x}) - v_F\sqrt{(p_1 - \frac{\alpha x_2}{2})^2 + (p_2 + \frac{\alpha x_1}{2})^2}$$

on the level set $h_2 = E$ describes dynamic of holes (a quasi-particle described by the initial Dirac system behaves like hole, positively charged). The corresponding classical trajectories can be obtained from the hamiltonian system with hamiltonian

$$H^h = \frac{1}{2}\big(-(p_1 - \frac{\alpha x_2}{2})^2 - (p_2 + \frac{\alpha x_1}{2})^2 + (\frac{E - U(\mathbf{x})}{v_F})^2\big)$$

on the level set $H^h = 0$.
Thus, for electrons and holes, two different families of classical trajectories $x_{1,2} = x_{1,2}(t, \gamma)$, $p_{1,2} = p_{1,2}(t, \gamma)$ should be taken into account, where t is the time with respect to the hamiltonian system with h_α, and the parameter γ gives the parametrisation of the initial manifold in a phase space $R^4_{x,p}$. For the Green's tensor point source problem, γ is a polar angle at which a trajectory issues from the source. Thus, taking the initial conditions for $x_{1,2} = x_{1,2}(t, \gamma)$, $p_{1,2} = p_{1,2}(t, \gamma)$

$$x|_{t=0} = x^{(0)}, \quad p|_{t=0} = \frac{|E - U(x^{(0)})|}{v_F}\Big(\cos\gamma, \sin\gamma\Big)^T,$$

we obtain the classical trajectories connecting $\mathbf{x}^{(0)}$ and $\mathbf{x}$.
For electrons and holes one should seek solution to the Dirac system zero-order problem in the form

$$\psi_0 = \sigma^{(0)}(\mathbf{x})\mathbf{e}_1 \tag{5}$$

with unknown amplitude $\sigma^{(0)}(\mathbf{x})$. Solvability of the problem

$$(H - EI)\psi_1 = -R\psi_0, \quad E = h_{1,2},$$

requires that the orthogonality condition with complex conjugation must hold

$$< \mathbf{e}_1, R(\sigma^{(0)}(\mathbf{x})\mathbf{e}_1) >= 0,$$

Using the basic elements of the techniques in (15), from the orthogonality condition one should obtain the transport equation for $\sigma^{(0)}(\mathbf{x})$

$$\frac{d\sigma^{(0)}}{dt} + \frac{1}{2}\sigma^{(0)} \log J + \sigma^{(0)} < \mathbf{e}_1, \frac{d\mathbf{e}_1}{dt} >= 0, \tag{6}$$

where

$$J(t,\gamma) = \left| \frac{\partial(x_1, x_2)}{\partial(t,\gamma)} \right|$$

is the geometrical spreading with respect to the hamiltonian system with $h_{1,2} = U \pm v_F p$. It has a solution

$$\sigma^{(0)} = \frac{c_0}{\sqrt{J}} e^{-i\theta/2}, \quad c_0 = const.$$

For upper order terms,

$$(H - EI)\psi_j = -R\psi_{j-1},$$

one should seek solution in the form

$$\psi_j = \sigma_1^{(j)}\mathbf{e}_1 + \sigma_2^{(j)}\mathbf{e}_2, \tag{7}$$

where $\sigma_2^{(j)}$ may be found straight forward

$$\sigma_2^{(j)} = \frac{< \mathbf{e}_2, R(\psi_{j-1}) >}{2(E - U(\mathbf{x}))}.$$

Then, from the orthogonality condition,

$$< \mathbf{e}_1, R(\sigma_1^{(j)}\mathbf{e}_1 + \sigma_2^{(j)}\mathbf{e}_2) >= 0,$$

one should obtain

$$\sigma_1^{(j)} = \frac{1}{\sqrt{J}} e^{-i\theta/2}\left(c_j - \int_0^t e^{i\theta/2}\sqrt{J} < \mathbf{e}_1, R(\sigma_2^{(j)}\mathbf{e}_2) > dt\right), \quad c_j = const.$$

Classical action $S(x)$ satisfies the Hamilton-Jacobi equation

$$S_{x_1}^2 + S_{x_2}^2 - \alpha x_2 S_{x_1} + \alpha x_1 S_{x_2} + \frac{\alpha^2}{4}(x_1^2 + x_2^2) - (\frac{E - U(\mathbf{x})}{v_F})^2 = 0. \tag{8}$$

Its solution for electrons and holes is given by the following curvilinear integral over a classical trajectory

$$S = \int_{x^{(0)}}^{x} \frac{E - U(\mathbf{x})}{v_F} ds - \frac{e}{c}\int_{x^{(0)}}^{x} \mathbf{A} d\mathbf{x} = \tag{9}$$

$$\int_{x^{(0)}}^{x} \left(\frac{E - U(\mathbf{x})}{v_F}\sqrt{\dot{x}_1^2 + \dot{x}_2^2} - \frac{\alpha}{2}(-x_2\dot{x}_1 + x_1\dot{x}_2) \right) dt,$$

where s is the arck length.
Finally, taking into account finite number of trajectories connecting $\mathbf{x}^{(0)}$ and $\mathbf{x}$ up to the leading order ray asymptotic solution to the Green's tensor for electrons and holes is given by

$$G(\mathbf{x}, \mathbf{x}^{(0)}) = \frac{1}{2\hbar}\sqrt{\frac{k}{2\pi}} \sum_n \frac{e^{\frac{i}{\hbar}S(t^{(n)},\gamma^{(n)}) - i\frac{\pi}{2}\mu_n + i\pi/4}}{\sqrt{|J(t^{(n)},\gamma^{(n)})|}} \begin{pmatrix} e^{-i\frac{\theta-\gamma}{2}} & e^{-i\frac{\theta+\gamma}{2}} \\ e^{i\frac{\theta+\gamma}{2}} & e^{i\frac{\theta-\gamma}{2}} \end{pmatrix} (1 + O(\hbar)), \tag{10}$$

where

$$k = \frac{E - U(\mathbf{x}^{(0)})}{\hbar v_F},$$

μ_n is the Maslov index of the n-th trajectory ((15)).
This solution is singular near caustics or focal points where

$$J(t, \gamma) = 0.$$

Here is an example of ray asymptotic expansion of the Green's tensor of electron or hole in magnetic field with $U(\mathbf{x}) = 0$

$$G(\mathbf{x}, \mathbf{x}^{(0)}) = \frac{1}{1 - \exp\left[i\pi(\frac{R^2\alpha}{\hbar} - 1)\right]} \frac{1}{2\hbar}\sqrt{\frac{k}{2\pi}}$$

$$\sum_{n=1,2} \frac{e^{\frac{i}{\hbar}S_n - i\frac{\pi}{2}\mu_n + i\pi/4}}{\sqrt{|J(s^{(n)},\gamma^{(n)})|}} \begin{pmatrix} e^{-i\frac{\theta-\gamma}{2}} & e^{-i\frac{\theta+\gamma}{2}} \\ e^{i\frac{\theta+\gamma}{2}} & e^{i\frac{\theta-\gamma}{2}} \end{pmatrix} (1 + O(\hbar)), \tag{11}$$

where cyclotronic radius $R = |E|/\alpha$,

$$S = \frac{RE}{2}(\frac{s}{R} + \sin\frac{s}{R}),$$
$$J = R\sin\frac{s}{R},$$

where s being the arc length instead of t and measured along trajectory from $\mathbf{x}^{(0)}$. This ray asymptotic solution was constructed with the help of the ray coordinates s, γ. For electrons the corresponding family of trajectories is given by

$$x_1 = R[\sin(\frac{s}{R} + \gamma) - \sin\gamma] + x_1^{(0)},$$

$$x_2 = R[-\cos(\frac{s}{R} + \gamma) + \cos\gamma] + x_2^{(0)},$$

and $\theta = \frac{s}{R} + \gamma$ (see Fig. 1). For holes, we have

$$x_1 = R[\sin(\gamma - \frac{s}{R}) - \sin\gamma] + x_1^{(0)},$$

$$x_2 = R[-\cos(\gamma - \frac{s}{R}) - \cos\gamma] + x_2^{(0)},$$

and $\theta = \gamma + \pi - \frac{s}{R}$. The asymptotic solution is valid if $kR >> 1$. This solution is in full agreement with the Green's tensor for the problem in a sense of matching as $\alpha \to 0$

$$v_F < -i\hbar\nabla, \bar{\sigma} > G(\mathbf{x}) - EG(\mathbf{x}) = \begin{pmatrix} \delta(x) & 0 \\ 0 & \delta(x) \end{pmatrix}, \tag{12}$$

which exact representation can be found by Fourier transform

$$G(\mathbf{x}, (0,0)) = \frac{-i}{4\hbar} \begin{pmatrix} -kH_0^{(1)}(kr) & (i\partial_{x_1} + \partial_{x_2})H_0^{(1)}(kr) \\ (i\partial_{x_1} - \partial_{x_2})H_0^{(1)}(kr) & -kH_0^{(1)}(kr) \end{pmatrix} = \tag{13}$$

$$\frac{\sqrt{k}}{\hbar} \frac{e^{ikr + i\pi/4}}{2\sqrt{2\pi r}} \begin{pmatrix} 1 & e^{-i\gamma} \\ e^{i\gamma} & 1 \end{pmatrix} (1 + O(k^{-1})),$$

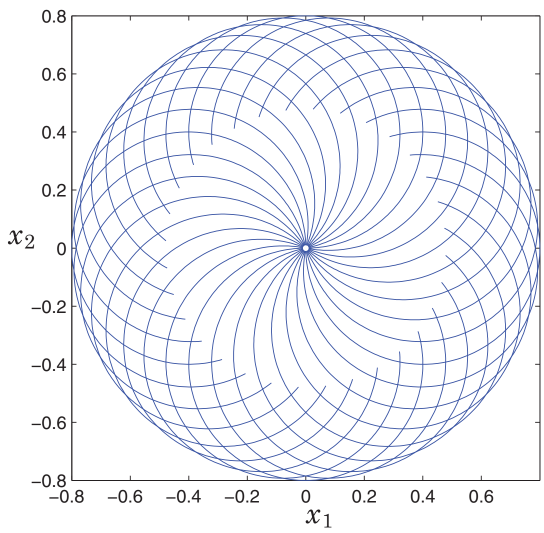
where $r = |\mathbf{x}|$, $x_1 = r\cos(\gamma)$, $x_2 = r\sin(\gamma)$, $k = E/(\hbar v_F)$, and $H_0^{(1)}(x)$ is the Hankel function. The property of the solution being singular at

$$E = E_l = \pm v_F \sqrt{\hbar\alpha(2l+1)}, l = 0, 1, 2, \dots,$$

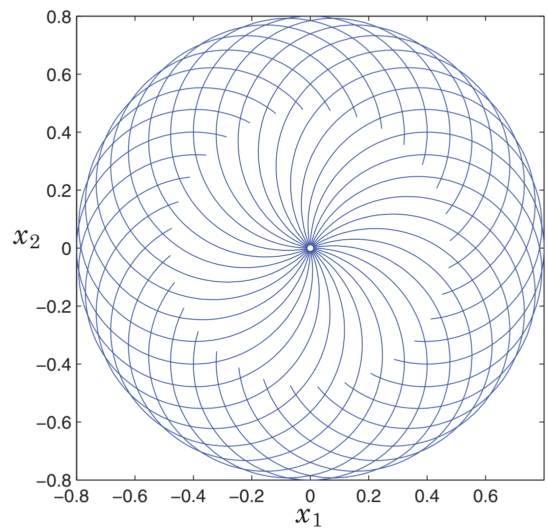
gives the quantization of the energy spectrum already well-known in graphere electron-hole motion in magnetic field ((5)). This solution is singular at $s = \nu\pi R$, $\nu \in \mathbf{N}$ (see (19)). The set of singular points are the circle with $\nu = 2n + 1$ (see Fig. 1), which is a smooth caustic, and the focal point $\mathbf{x}^{(0)}$, where $\nu = 2n$ ($n \in \mathbf{N}$).

Frequently in practice, the structure of classical trajectories looks very complicated due to the presence of multiple caustics and focal points. This situation takes place for a charged particle moving in strong magnetic fields. Thus, the ray method asymptotic expansion is not effective. Alternative approach is well-known - the method of Maslov canonical operator (15) which gives a cumbersome asymptotic construction depending on geometrical and topological properties of lagrangian manifolds represented by families of by-characteristics in the phase space. In some simple cases it reduces the answer to local asymptotic expansions for wave fields expressed via special functions of wave catastrophes, for example Airy function for smooth caustic

$$v(z) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp\left(i(t^3/3 + tz)\right) dt,$$



(a)



(b)

Fig. 1. Family of classical trajectories (circles) for the problem of the Green's tensor for electrons (1a) and holes (1b) in magnetic field with $U(\mathbf{x}) = 0$ and $\mathbf{x}^{(0)} = (0,0)$.

and Piercy integral - in case of casp

$$I(x,y) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp\left(i(t^4 + xt^2 + yt)\right) dt.$$

However, there exist alternative approach known as the method of Gaussian beams summation method which is universal, simple, effective and robust in developing numerical algorithms. It was shown for acoustic, electromagnetic and elastic waves (17). In the next section a generalization of the method is described for the wave function of graphene electron-hole motion in magnetic field and potential. It gives analytical representation of Green's tensor of Dirac system as an integral over Gaussian beams.

2.2 Localized asymptotic solution - electronic Gaussian beam in graphene

Let $\mathbf{x}_0 = (x_1(s), x_2(s))$ be a particle (electron or hole) classical trajectory, where s is the arc length measured along a trajectory. Consider the neighborhood of the trajectory in terms of local coordinates s, n, where n is the distance along the vector normal to the trajectory such that

$$\mathbf{x} = \mathbf{x}^{(0)}(s) + \mathbf{e_n}(s)n, \tag{14}$$

where $\mathbf{e_n}(s)$ is the unit vector normal to the trajectory.
Following (21), we apply the asymptotic boundary-layer method to the homogeneous Dirac system (1). We assume that the width of the boundary layer is determined by $|n, \dot{n}| = O(\sqrt{\hbar})$ as $\hbar \to 0$. Introducing $\nu = n/\sqrt{\hbar} = O(1)$, we seek an asymptotic solution to (3) in the form

$$\psi = \begin{pmatrix} u \\ v \end{pmatrix} = e^{\frac{i}{\hbar}(S_0(s)+S_1(s)n)} \sum_{j=0}^{+\infty} \hbar^{j/2} \begin{pmatrix} u_j(s,\nu) \\ v_j(s,\nu) \end{pmatrix} \tag{15}$$

$$= e^{\frac{i}{\hbar}(S_0(s)+S_1(s)n)} \sum_{j=0}^{+\infty} \hbar^{j/2} \psi_j(s,\nu),$$

where $S_0(s)$ and $S_1(s)$ were chosen as in (18), (19)

$$S_0(s) = \int \left(a(s) + \frac{\alpha}{2}(x_1^{(0)}\gamma_1 + x_2^{(0)}\gamma_2) \right) ds,$$

$$S_1(s) = \frac{\alpha}{2}(x_2^{(0)}\gamma_1 - x_1^{(0)}\gamma_2),$$

$$a(s) = \frac{E - U_0(s)}{v_F},$$

where

$$U(\mathbf{x}) = U_0(s) + U_1(s)n + U_2(s)n^2 + ...,$$

$\gamma_i(s),\ i = 1,2$ are the cartesian components of $\mathbf{e_n}(s)$. Thus, for unknown $\psi_j(s,\nu)$ we obtain a recurrent system

$$(H_0 - EI)\psi_0 = 0, \quad (H_0 - EI)\psi_1 = -v_F H_1 \psi_0, \quad (H_0 - EI)\psi_2 = -v_F H_1 \psi_1 - v_F H_2 \psi_0, ...$$

with operators $H_0, H_1, H_2, ...$

$$H_0 = \begin{pmatrix} U_0 & v_F((\gamma_2 + i\gamma_1)\dot{S}_0 + (\gamma_1 - i\gamma_2)\dot{S}_1 - \frac{\alpha x_2^{(0))}}{2} - i\frac{\alpha x_1^{(0))}}{2}) \\ v_F((\gamma_2 - i\gamma_1)\dot{S}_0 + (\gamma_1 + i\gamma_2)\dot{S}_1 - \frac{\alpha x_2^{(0))}}{2} + i\frac{\alpha x_1^{(0))}}{2}) & U_0 \end{pmatrix}$$

$$= \begin{pmatrix} U_0 & (\gamma_2 + i\gamma_1)(E - U_0) \\ (\gamma_2 - i\gamma_1)(E - U_0) & U_0 \end{pmatrix},$$

$$H_1 = v_F \begin{pmatrix} (U_1 - \frac{U_0 - E}{\rho})\nu & -e^{-i\theta}(\partial_\nu + \alpha\nu) \\ e^{i\theta}(\partial_\nu - \alpha\nu) & (U_1 - \frac{U_0 - E}{\rho})\nu \end{pmatrix},$$

$$H_2 = v_F \begin{pmatrix} (U_2 - \frac{U_1}{\rho})\nu^2 & e^{-i\theta}(\frac{\nu}{\rho}\partial_\nu + \frac{\alpha\nu^2}{2\rho} - i\partial_s) \\ e^{i\theta}(-\frac{\nu}{\rho}\partial_\nu + \frac{\alpha\nu^2}{2\rho} - i\partial_s) & (U_2 - \frac{U_1}{\rho})\nu^2 \end{pmatrix},$$

$$H_j = \begin{pmatrix} (U_j - \frac{U_{j-1}}{\rho})\nu^j & 0 \\ 0 & (U_j - \frac{U_{j-1}}{\rho})\nu^j \end{pmatrix}, \quad j > 2,$$

where $e^{i\theta} = \gamma_2 - i\gamma_1$, $\rho(s)$ is the radius of curvature of the classical trajectory, and $\dot{S}_0$ means a derivative with respect to s.
Solving the zero-order problem $(H_0 - EI)\psi_0 = 0$, we come to the eigen-vector problem

$$H_0 \mathbf{e}_\alpha = h_\alpha \mathbf{e}_\alpha, \ \ \alpha = 1,2,$$

$$h_\alpha = U_0 \pm v_F |a(s)|,$$

$$\mathbf{e}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix}, \quad \mathbf{e}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{i\theta} \end{pmatrix}.$$

If $E > U_0$, then $E = h_1$, if $E < U_0$, then $E = h_2$.

Thus, one should seek solution in the form

$$\psi_0 = \sigma^{(0)}(s,\nu)\mathbf{e}_1. \tag{16}$$

Solvability of the problem $(H_0 - EI)\psi_1 = -v_F H_1 \psi_0$ leads to the orthogonality condition

$$< \mathbf{e}_1, H_1\psi_0 >= 0,$$

which can be simplified as follows

$$U_1 - \frac{U_0 - E}{\rho} = \alpha. \tag{17}$$

This relation is well-known in the asymptotic theory of Gaussian beams (see (20), (21), (17),(18) (19)). It is equivalent to the requirement that everything is being constructed in a asymptotically small neighbourhood of the fixed curve which is a classical trajectory - solution to hamiltonian system.
Solvability of the problem requires the orthogonality condition

$$(H_0 - EI)\psi_2 = -v_F H_1\psi_1 - v_F H_2\psi_0$$

which leads to transport equation for the unknown $\sigma^{(0)}(s,\nu)$

$$2ia(s)\sigma_s^{(0)} + \sigma_{\nu\nu}^{(0)} - a(s)(\nu^2 a(s)d(s) + \dot{\theta})\sigma^{(0)} = 0, \tag{18}$$

$$d(s) = \frac{1}{a(s)}\big(2(U_2 - \frac{U_1}{\rho}) + \frac{\alpha}{\rho}\big).$$

This is so-called parabolic equation of Gaussian beam boundary layer (see (20), (21), (17),(18) (19)). It has a solution

$$\sigma^{(0)} = \frac{e^{i\Gamma\nu^2/2}}{\sqrt{z}}e^{-i\theta/2}, \quad \Gamma = a\frac{\dot{z}}{z}, \tag{19}$$

(see (20), (21), (18) (19)). Here Γ satisfies the Ricatti equation ,

$$\dot{\Gamma} + \frac{1}{a}\Gamma^2 + ad = 0. \tag{20}$$

The expression

$$S = S_0(s) + S_1(s)n + \frac{1}{2}\Gamma(s)n^2 + ...$$

gives the approximate solution to the Hamilton-Jacobi equation (8).
The function $z(s)$ satisfies the system of equations in the hamiltonian form

$$\begin{aligned} \dot{z} &= p/a(s), \\ \dot{p} &= -a(s)d(s)z \end{aligned} \tag{21}$$

with the hamiltonian

$$H(z,p) = \frac{p^2}{2a(s)} + \frac{a(s)d(s)z^2}{2}.$$

It is worth remarking that this is so-called system of equations in variations which describes a family of trajectories close to $\mathbf{x}_0(s)$, that is, $z(s) = n(s)$, and these trajectories are given by

$$\mathbf{x}(s) = \mathbf{x}_0(s) + n(s)\mathbf{e}_\mathbf{n}(s),$$

(see (20), (21), (17),(18) (19)).
The crucial point of the analysis is that it is possible to choose a solution of (21) in such a way that $Im\Gamma > 0$, thus, providing asymptotic localization of ψ. Namely, if $z(s)$ is a complex solution to (21), wronskian of $Re(z(s))$ and $Im(z(s))$ may be chosen in such a way that

$$a(s)W(Re(z), Im(z)) = 1.$$

Then, the following inequality holds true

$$Im(\Gamma(s)) = \frac{a(s)W(Re(z), Im(z))}{Re(z)^2 + Im(z)^2} = \frac{1}{|z(s)|^2} > 0$$

along the trajectory. This leads to the localisation.
Thus, we obtain that to the leading order the Gaussian beam asymptotic solution for electron or hole is given by

$$\psi = e^{\frac{i}{\hbar}\left(S_0(s)+S_1(s)n+\frac{p(s)}{2z(s)}n^2\right)} \frac{e^{-i\theta/2}}{\sqrt{z(s)}}\mathbf{e}_1(1 + O(\hbar^{1/2})). \tag{22}$$

It is always regular near caustics and focal points regardless its complicated geometrical structure.

3. Asymptotic expansion of the Green's tensor for electron-hole in magnetic field in the form of integral of Gaussian beams

The theoretical background of the method of Gaussian beams summation originally was developed for acoustic wave fields ((16)), and later, for electromagnetic and elastic fields ((17)). The generalisation of the method of Gaussian beams summation for electron motion in magnetic field was done in (18), (19). In this section, the approximation of electron-hole Green's tensor near to caustics and focal points as an integral over Gaussian beams is described briefly.
According to (17), (18), (19), and taking into account ray asymptotics of electron-hole Green's tensor (see (10)), the integral over all Gaussian beams irradiated from the point source $\mathbf{x}^{(0)}$ is represented as follows

$$G(\mathbf{x}, \mathbf{x}^{(0)}, E) = \int_0^{2\pi} e^{\frac{i}{\hbar}\left(S_0(s)+S_1(s)n+\frac{p(s)}{2z(s)}n^2\right)} \begin{pmatrix} e^{-i\frac{\theta-\gamma}{2}} & e^{-i\frac{\theta+\gamma}{2}} \\ e^{i\frac{\theta+\gamma}{2}} & e^{i\frac{\theta-\gamma}{2}} \end{pmatrix} \frac{A(\gamma)d\gamma}{\sqrt{z(s)}} \tag{23}$$

$$(1 + O(\hbar^{1/2})), \quad \alpha = 1, 2,$$

where $A(\gamma)$ is unknown amplitude. This integral can be evaluated numerically, and the corresponding algorithm is very simple. The rectangular or Simpson formula may be used. The basic idea of the approximation is that the total fan of classical trajectories corresponding to the discrete set of angular parameter $\gamma \in [0, 2\pi]$ must stretch for the values of s as large as possible thus securing total and uniform covering of the observation point $\mathbf{x}$. Then, all the components of the Gaussian beam asymptotic solution (22), that is, $S_0(s), S_1(s), a(s), z(s), p(s)$ must be computed for various values of the discrete set of $\gamma \in [0, 2\pi]$. This includes the coordinates s, n of the observation point with respect to every trajectory determined by γ. The parameter w is used in the construction of the complex $z(s), p(s)$

$$\begin{pmatrix} z(s) \\ p(s) \end{pmatrix} = \begin{pmatrix} z_1(s) \\ p_1(s) \end{pmatrix} + iw \begin{pmatrix} z_2(s) \\ p_2(s) \end{pmatrix}$$

where the real functions $z_1(s), p_1(s), z_2(s), p_2(s)$ satisfy (21), and the initial conditions

$$\begin{pmatrix} z_1(0) \\ p_1(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} z_2(0) \\ p_2(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The parameter w determines the width of localized Gaussian beams. The thinner Gaussian beams, the more accurate approximation for solution may be obtained ((16)), ((17)). For example, for the case $U(\mathbf{x}) = 0$, we obtain the equation in variations in the form

$$\ddot{z} + R^{-2} z = 0,$$

and the corresponding solution

$$z = \cos \frac{s}{R} + iw \sin \frac{s}{R}, \quad w > 0,$$

leads to

$$Im(\Gamma) = a Im(\frac{\dot{z}}{z}) = a \frac{s}{R[\cos^2 \frac{s}{R} + w^2 \sin^2 \frac{s}{R}]} > 0, \quad a = E/v_F.$$

The amplitude $A(\gamma)$ can be determined by the steepest descent method (see ((16)), ((17))). In the region close to $\mathbf{x}^{(0)}$, where the structure of electron classical trajectories is regular away from caustics, the approximation (23) has to coincide with the ray asymptotic solution

$$G(\mathbf{x}, \mathbf{x}^{(0)}) = \frac{1}{2\hbar} \sqrt{\frac{k}{2\pi}} \frac{e^{\frac{i}{\hbar} S(t, \gamma_0) + i\pi/4}}{\sqrt{J_\alpha(t, \gamma_0)}} \begin{pmatrix} e^{-i\frac{\theta - \gamma_0}{2}} & e^{-i\frac{\theta + \gamma_0}{2}} \\ e^{i\frac{\theta + \gamma_0}{2}} & e^{i\frac{\theta - \gamma_0}{2}} \end{pmatrix} (1 + O(\hbar)), \tag{24}$$

where γ_0 determines the trajectory connecting $\mathbf{x}^{(0)}$ and $\mathbf{x}$. Taking into account that asymptotically small neighbourhood of trajectories close to the trajectory $\gamma = \gamma_0$ contribute into the integral (23) as $\hbar \to 0$, and using inside this neighbourhood the following approximations (see (17))

$$S = S_0 + S_1 n + \frac{1}{2} \frac{\tilde{p}(s)}{\tilde{z}(s)} n^2 + O(n^3),$$

$$n = \tilde{z}(s)(\gamma - \gamma_0) + O((\gamma - \gamma_0)^2),$$

where real functions $\tilde{z}(s), \tilde{p}(s)$ satisfy (21) with initial conditions $\tilde{z}(0) = 0, \tilde{p}(0) = |a(0)|$, we obtain

$$G(x, x^{(0)}, E) = e^{\frac{i}{\hbar}S(t,\gamma_0)} \frac{A(\gamma_0)}{\sqrt{z(s)}} \begin{pmatrix} e^{-i\frac{\theta-\gamma_0}{2}} & e^{-i\frac{\theta+\gamma_0}{2}} \\ e^{i\frac{\theta+\gamma_0}{2}} & e^{i\frac{\theta-\gamma_0}{2}} \end{pmatrix}$$

$$\int_{-\Delta_1}^{\Delta_1} \exp\Big(- \frac{i}{2\hbar}\frac{a(0)\tilde{z}(s)}{z(s)}(\gamma-\gamma_0)^2\Big) d(\gamma-\gamma_0) + ...$$

$$= e^{\frac{i}{\hbar}S(t,\gamma_0)} \frac{A(\gamma_0)}{\sqrt{\tilde{z}(s)}} \begin{pmatrix} e^{-i\frac{\theta-\gamma_0}{2}} & e^{-i\frac{\theta+\gamma_0}{2}} \\ e^{i\frac{\theta+\gamma_0}{2}} & e^{i\frac{\theta-\gamma_0}{2}} \end{pmatrix} \sqrt{\frac{2\pi\hbar}{|a(0)|}} e^{\mp i\pi/4},$$

where Δ_1 is a positive constant. Since $J(s,\gamma_0) = \tilde{z}(s)$, matching the leading term for $G(x, x^{(0)}, E)$ given in (24) leads to

$$A(\gamma_0) = \frac{ik}{4\pi\hbar}$$

for electrons,

$$A(\gamma_0) = \frac{-ik}{4\pi\hbar}$$

for holes. Thus, we obtain

$$A(\gamma) = \frac{i|k|}{4\pi\hbar}.$$

4. Testing the method of Gaussian beams summation for electron-hole waveguide motion in magnetic field

In this section the method of Gaussian beams summation for electron-hole motion in magnetic field is tested for a special case with linear electrostatic potential $U = \beta x_2$ in (2), and we assume that $v_F = 1$. For this case we compare applicability of both asymptotic representations (10) and (23) for the Green's tensor component $G_{11}(x, x^{(0)}, E)$. The hamiltonian dynamics of electrons motion is determined by the Hamilton function in Landau gauge $\mathbf{A} = B(-x_2, 0, 0)$

$$h_1 = \beta x_2 + \sqrt{(p_1 - \alpha x_2)^2 + p_2^2},$$

in the domain $\Omega_e = \{\mathbf{x} : E > \beta x_2\}$ on the level set $h_1 = E$, or

$$H^e = \frac{1}{2}\Big((p_1 - \alpha x_2)^2 + p_2^2 - (E - \beta x_2)^2\Big),$$

on the level set $H^e = 0$. The hamiltonian dynamics of holes motion is determined by the Hamiltilton function

$$h_2 = \beta x_2 - \sqrt{(p_1 - \alpha x_2)^2 + p_2^2},$$

in the domain $\Omega_e = \{\mathbf{x} : E < \beta x_2\}$ on the level set $h_2 = E$, or

$$H^h = \frac{1}{2}\Big(- (p_1 - \alpha x_2)^2 - p_2^2 + (E - \beta x_2)^2\Big),$$

on the level set $H^h = 0$.

In the case $|\beta| < |\alpha|$, a drift motion of electrons and holes takes place in the right direction of the axis x_1. For electrons $E > 0$, the family of classical drift trajectories are given by

$$x_1(t,\gamma) = (\pi_1 - \frac{\pi_1\alpha^2 - \alpha\beta E}{\Omega^2})t + \frac{\alpha\pi_2}{\Omega^2}(\cos\Omega t - 1) + \frac{\pi_1\alpha^2 - \alpha\beta E}{\Omega^3}\sin\Omega t,$$

$$x_2(t,\gamma) = \frac{\beta E - \pi_1\alpha}{\Omega^2}(\cos\Omega t - 1) + \frac{\pi_2}{\Omega}\sin\Omega t,$$

where $\Omega = \sqrt{\alpha^2 - \beta^2}$, $t \geq 0$, $0 \leq \gamma < 2\pi$, and

$$p_1|_{t=0} = \pi_1 = E\cos\gamma, \quad p_2|_{t=0} = \pi_2 = E\sin\gamma, \quad E = \sqrt{\pi_1^2 + \pi_2^2} > 0.$$

For holes $E < 0$, the family of classical drift trajectories are given by

$$x_1(t,\gamma) = -(\pi_1 - \frac{\pi_1\alpha^2 - \alpha\beta E}{\Omega^2})t + \frac{\alpha\pi_2}{\Omega^2}(\cos\Omega t - 1) - \frac{\pi_1\alpha^2 - \alpha\beta E}{\Omega^3}\sin\Omega t,$$

$$x_2(t,\gamma) = \frac{\beta E - \pi_1\alpha}{\Omega^2}(\cos\Omega t - 1) - \frac{\pi_2}{\Omega}\sin\Omega t,$$

and

$$p_1|_{t=0} = \pi_1 = |E|\cos\gamma, \quad p_2|_{t=0} = \pi_2 = |E|\sin\gamma, \quad E = -\sqrt{\pi_1^2 + \pi_2^2} < 0.$$

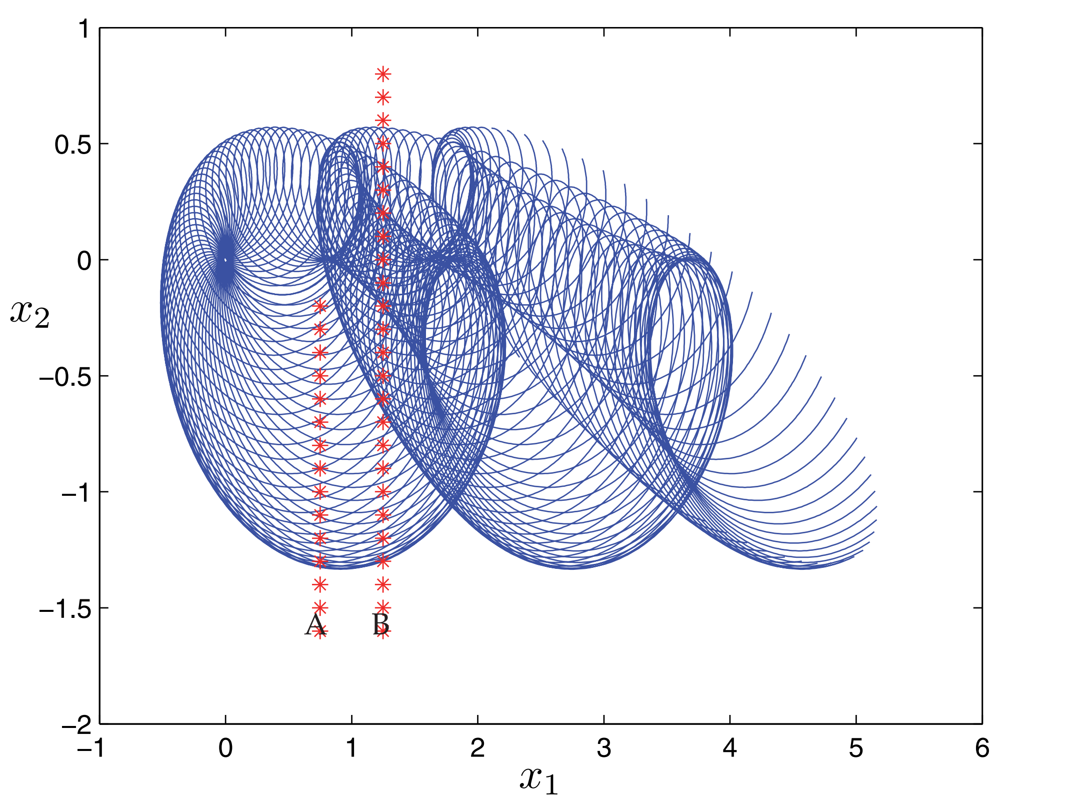


Fig. 2. Classical trajectories of electronic waveguide in magnetic and electrostatic fields.

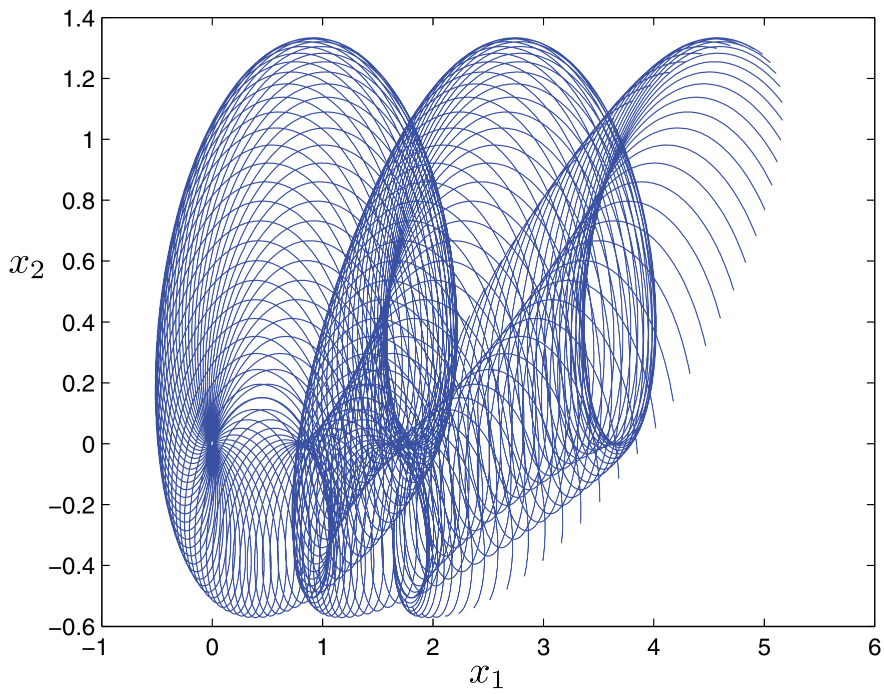


Fig. 3. Classical trajectories of holes waveguide in magnetic and electrostatic fields.

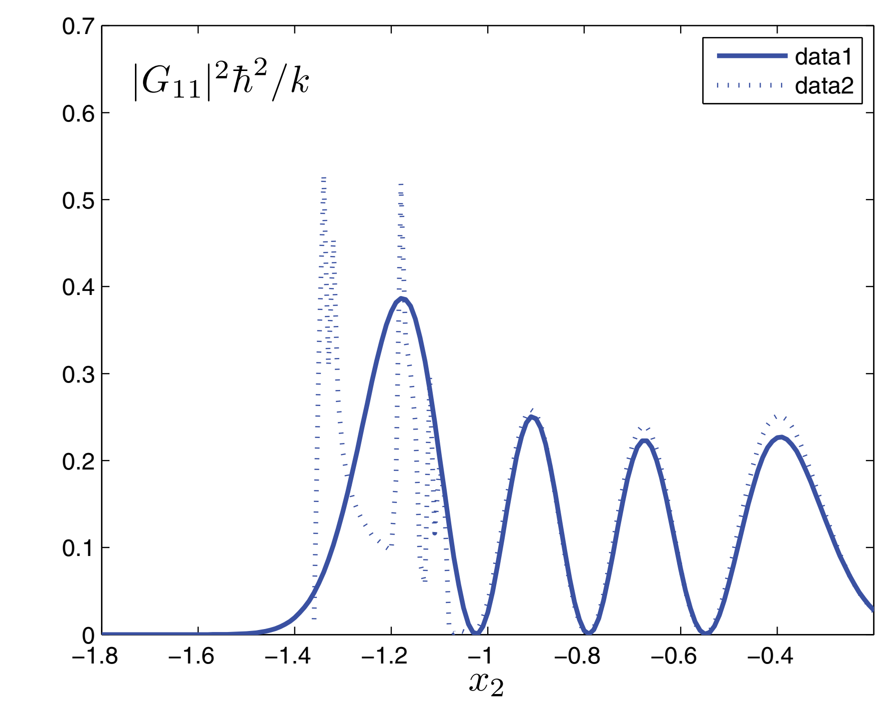


Fig. 4. The values of $|G_{11}(x, x^{(0)}, E)|^2\hbar^2/k$ at the points of vertical cut A for electronic waveguide in magnetic and electrostatic fields (data 1 - Gaussian beams summation, data 2 - ray asymptotics).

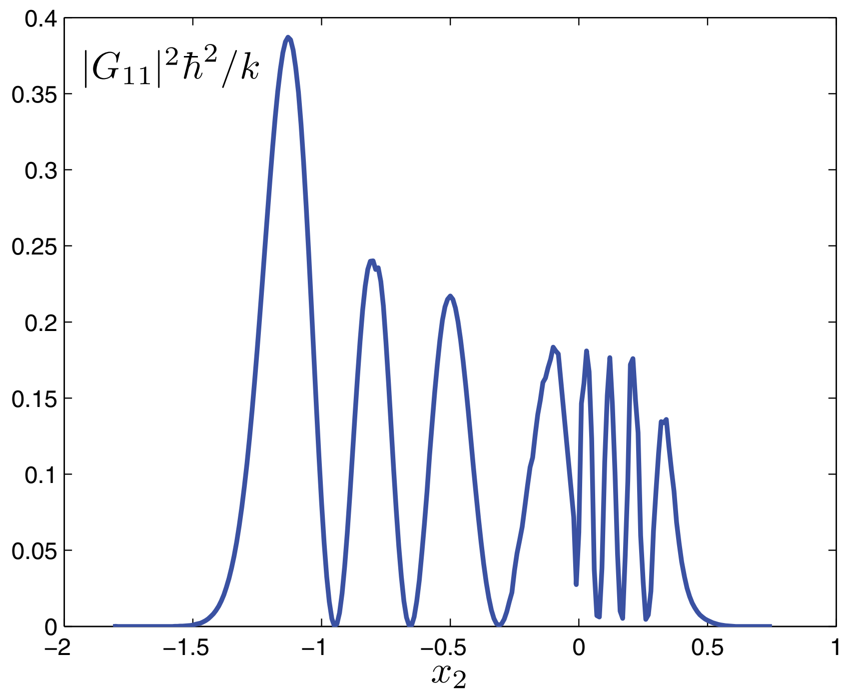


Fig. 5. The values of $|G_{11}(x, x^{(0)}, E)|^2\hbar^2/k$ at the points of vertical cut B for electronic waveguide in magnetic and electrostatic fields, Gaussian beams summation.

For both families of the classical trajectories, it can be shown rigorously that all of them are bounded from the corresponding turning lines. That is, for electrons it is always $E > \beta x_2(t, \gamma)$, and for holes $E < \beta x_2(t, \gamma)$, for arbitrary (t, γ).
Consider the case with following values of the dimensionless parameters of the problem $E = 1$, $\alpha = 2.5$, $\beta = 1$, $\hbar = 0.05$, $w = 2$. The structure of trajectories for holes and electrons is shown in Fig. 2, 3. It is worth to remark that in both cases shown in Fig. 2 and 3, the electron-hole waveguide propagation is clearly seen to be isolated from the potential turning lines, for electrons $x_2 \leq 1$, for holes $x_2 \geq -1$. This waveguide propagation (drift) takes place to the right from the source ($\mathbf{x}^{(0)} = (0, 0)$). In Fig. 4 the values of electronic Green's tensor normalised component $|G_{11}(x, x^{(0)}, E)|^2\hbar^2/k$ at the points of vertical cut $A = \{\mathbf{x} : x_1 = 0.75, -1.7 < x_2 < -0.2\}$ are presented that were computed by means of Gaussian beams summation approximation (23) and the ray asymptotics (10). Both graphs again show a good agreement within the domain that is away from caustics. It is clear that near to caustics the ray asymptotics blows up. Instead, Gaussian beams summation approximation shows a smooth transition through the caustic line with exponential decay into geometrical shadow domain. Discretizing the integral (23) by means of 128 Gaussian beams was used. In Fig. 5 the values of electronic Green's tensor normalised component $|G_{11}(x, x^{(0)}, E)|^2\hbar^2/k$ at the points of the second vertical cut $B = \{\mathbf{x} : x_1 = 1.25, -1.8 < x_2 < 0.75\}$ are presented that are computed only by means of Gaussian beams summation approximation (23). One should observe the oscillatory behaviour of Green's tensor components between caustic lines confining the waveguide and exponential decal away from the waveguide. Similar results could be expected for the hole Green's tensor normalised components.

5. Conclusion

Using the basic steps of techniques of Gaussian beams summation, known for acoustic wave propagation, this method was applied for electron-holes motion described by Dirac system in magnetic field and arbitrary potential in graphene to construct the Green's tensor semiclassical uniform approximation. This approximation was tested for a special cases of waveguide excitation by point source for electron-hole motion in magnetic and linear electric fields. The asymptotic results for the Green's tensor computed by Gaussian beams summation were found to be in a very good agreement with data obtained by the ray asymptotic solution. The method of Gaussian beams summation is efficient for construction of WKB approximation describing electron-hole motion in magnetic field and any scalar potential including problems of electron-hole waveguide transport through resonators.

It is worth to remark that the semiclassical analysis for the Dirac system considered in this chapter corresponds to the case of the first K Diract point in the first Brillouine zone. The case of the second K' Dirac point is treated in a similar way.

6. Acknowledgments

The authors would like to thank Dr A.Vagov, Prof M.Popov, Prof F.Kusmartsev for constructive discussions and valuable remarks.

7. References

[1] Datta, S., 1995 *Electronic transport in mesoscopic systems*, Cambridge University Press, Cambridge.

[2] Mello, P. A., Kumar, N., 2004 *Quantum Transport in Mesoscopic SyStem*, Oxford University Press, New York.

[3] Stockmann, H. J., 2000, *Quantum Chaos. An Introduction*, Cambridge University Press, Cambridge.

[4] V. V. Belov and S.Yu. Dobrokhotov, Sov. Math. Doclady 37, 264 (1988).

[5] Castro Neto, A.H., Guinea, F., Peres, N.M.R., Geim, A.K., and Novoselov, K.S. Rev. Mod. Phys. 81, Jan-March, (2009).

[6] Cheianov, V.V., Fal'ko, V.I. Phys.Rev. B. 74, 041403(R)(2006).

[7] Fistul, M.V., Efetov, K.B. PRL 98, 256803 (2007).

[8] Silvestrov, P.G., Efetov, K.B. PRL 98, 016802 (2007).

[9] Sonin, E.B. Phys.Rev. B. 79, 195438 (2009).

[10] Schwieters, C.D., Alford, J.A. and Delos, J.B. Phys.Rev.B. 54, N15, 10652 (1996).

[11] Beenaker, C.W.J. Rev. Mod. Phys. 69, 731 (1997).

[12] Blomquist, T. and Zozoulenko, I. V. Phys.Rev.B. 61, N3, 1724 (2000).

[13] Jalabert, R. A., Baranger, H. U., Stone, A. D. Phys.Rev.Lett. 65, N19, 2442 (1990).

[14] Carmier, P., Ullmo, D. Phys.Rev. B. 77, N24, 245413 (2008).

[15] Maslov, V. P. and M.V.Fedoriuk, 1981, *Semiclassical approximation in quantum mechanics*, Reidel, Dordrecht.

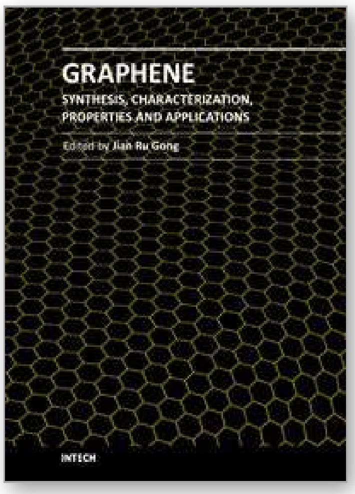
[16] Popov, M.M., Wave Motion 61, N3, 1724 (1981).

[17] Popov, M.M., 2002, *Method Gaussian beams*, Petroleum Brazil.

[18] V. V. Zalipaev, F. V. Kusmartsev, and M. M. Popov, J. Phys. A: Math. Theor. 41, 065101 (2008).

[19] V. V. Zalipaev, The Gaussian beams summation method in the quantum problems of electronic motion in a magnetic field, J.Phys. A: Math. Theor. 42, 205302, 14pp, (2009).
[20] Babich, V. M., Buldyrev, V.S. 1991, *Asymptotic methods in shortwave diffraction problems*, Springer-Verlag, New York.
[21] Babich, V. M., Kirpichnikova, N. Ya., 1979, *The boundary-layer method in diffraction problems*, Springer-Verlag, Berlin.

IntechOpen



Graphene - Synthesis, Characterization, Properties and Applications
Edited by Prof. Jian Gong

ISBN 978-953-307-292-0
Hard cover, 184 pages
Publisher InTech
Published online 15, September, 2011
Published in print edition September, 2011

The discovery of graphene has led to a deluge of international research interest, and this new material in the field of materials science and condensed-matter physics has revealed a cornucopia of new physics and potential applications. This collection gives a roughly review on the recent progress on the synthesis, characterization, properties and applications of graphene, providing useful information for researchers interested in this area.