The Gaussian beams summation method in the quantum problems of electronic motion in a magnetic field

2009 J. Phys. A: Math. Theor. 42 205302

(http://iopscience.iop.org/1751-8121/42/20/205302)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 205302 (14pp) doi:10.1088/1751-8113/42/20/205302

The Gaussian beams summation method in the quantum problems of electronic motion in a magnetic field

V V Zalipaev

Department of Mathematical Sciences, University of Liverpool, Liverpool, L69 7ZL, UK

E-mail: v.zalipaev@liv.ac.uk

Received 26 August 2008, in final form 31 March 2009
Published 28 April 2009
Online at stacks.iop.org/JPhysA/42/205302

Abstract
In this paper the Gaussian beams summation method, developed earlier for acoustic wave propagation, is generalized and applied to electron motion in a magnetic field and arbitrary potential in the case of shortwave approximation. It provides semiclassical uniform approximation for Green's function for stationary two-dimensional quantum problems. The approximation is valid near the caustics of an arbitrary geometrical structure and focal points. This approach is tested for two special cases of waveguide excitation by a point source for electron motion in a magnetic field with linear or parabolic potentials.

PACS numbers: 03.65.−w, 03.65.−sq, 04.40.−fa, 04.30.−db

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The recent development of semiclassical analysis has been demonstrated in various fields of modern physics such as nano-structures [1, 2], electronic transport in mesoscopic systems [3, 4], quantum chaotic dynamics of acoustic, optical and electronic resonators [5] and many others. One of the examples of the application of semiclassical analysis is quantum electronic waveguides and resonators. In modern mesoscopic electronic devices, two-dimensional conductors with controllable geometric features are much smaller than inelastic scattering length. Thus, electronic motion is ballistic (see [6–9]). Similar effects take place in nanotubes. It is of particular interest when electron motion is controlled by an external magnetic field.

Constructions of semiclassical approximations of Green's function inside electronic waveguides or resonators have been a key problem in the analysis of electronic transport problems in mesoscopic systems (see [6–9]). It is worth mentioning a semiclassical approach in computing the density of eigenlevels for a resonator with chaotic dynamics. It is also based on the WKB asymptotic expansion of Green's function [5].

However, the structure of classical trajectories 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 is not valid. In this case, one of the possibilities of tackling the problem of computing Green's function is Maslov's canonical operator method. It was developed to solve the problems in the construction of semiclassical asymptotics for elliptic PDEs and quantum mechanics equations [10]. The method gives a cumbersome universal asymptotic construction depending on the 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 the Airy function for smooth caustic and Piercy integral in the case of casp.

On the other hand, there exists an alternative method of the summation of Gaussian beams (integral over Gaussian beams) which was developed in [11] for acoustic and later for electromagnetic and elastic wave propagation [12]. The theoretical foundations of the method are rather simple in comparison with Maslov's canonical operator method. The Gaussian beam as a localized asymptotic solution is always regular near the caustics or focal point. Realization of the method does not require any knowledge about the geometrical properties of caustics. 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 the caustics or focal points of an arbitrary geometric structure. The application of the method to the computations of high-frequency acoustic and elastic wave fields was proved to be very efficient and robust [12].

This method is convenient for constructing a semiclassical uniform approximation for Green's function for the interior of waveguides quantum stationary problems. But the application of this method to the problems of electron motion in magnetic fields required a generalization of the approach originally developed for acoustic wave propagation problems. The first step in this direction has been done in [15], where a semiclassical analysis was developed for electron motion inside a closed resonator in the presence of a homogeneous magnetic field and arbitrary scalar potential.

In this paper using the basic techniques described in [11, 12] and in [15], we develop the Gaussian beams summation method for electron motion in a magnetic field and arbitrary scalar potential $u(\mathbf{x})$ stationary problems to construct Green's function semiclassical approximation (electron spin effects are not taken into account). This approach has been tested for two classical cases of separation of variables, namely

$$\frac{1}{2m}\left\{(\hat{p}_1+\alpha x_2)^2+\hat{p}_2^2\right\}G+e_2x_2G=EG+\delta(\mathbf{x}-\mathbf{x}^{(0)}), \tag{1}$$

for linear potential (electric field with component e_2), and

$$\frac{1}{2m}\left\{(\hat{p}_1+\alpha x_2)^2+\hat{p}_2^2\right\}G+\beta\frac{x_2^2}{2}G=EG+\delta(\mathbf{x}-\mathbf{x}^{(0)}), \tag{2}$$

for parabolic potential with parameter $\beta > 0$, where

$$\mathbf{x}=(x_1,x_2),\qquad \hat{p}_1=\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x_1},\qquad \hat{p}_2=\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x_2},\qquad \alpha=\frac{eB}{c},$$

with magnetic potential in the Landau gauge $\mathbf{A} = B(-x_2, 0, 0)$, where $\delta(\mathbf{x})$ is the Dirac delta function, e is the particle charge, c is the speed of light and $\hbar$ is the Plank constant. Both cases deal with electronic waveguide propagation excited by point source $\mathbf{x}^{(0)}$ as their solutions represent propagating waves confined to a strip formed by the interior between two turning lines or a turning line and caustics. A similar situation takes place for an acoustic wave field of depth waveguide in the ocean acoustics made by local internal minimum of the speed of wave propagation with respect to the depth coordinate (a waveguide without reflecting boundaries). The corresponding exact mode decompositions for Green's functions are derived. Numerical results obtained by the Gaussian beams summation method were tested against data computed by the exact mode decompositions. It is shown that for both approaches, numerical results are in a very good agreement. However, it is necessary to remark that the Gaussian beams summation method has a significant drawback. It is unable to provide an accurate approximation for Green's function near the turning line where $E = u(\mathbf{x})$.

It is important to note that the Gaussian beam asymptotic solution used as the main tool in the Gaussian beams summation method differs from the well-known quantum mechanics and quantum field theory coherent states introduced earlier by Schrödinger and Glauber. Both are different types of Gaussian wave packet solutions.

The paper is organized as follows. First, in section 2, a description of the boundary layer semiclassical method used to construct a localized asymptotic solution of the Gaussian beam in the presence of a magnetic field and a scalar potential is given. Subsequently, in section 3, the techniques of the Gaussian beams summation method are presented. Finally, in section 4, exact mode decompositions for Green's functions for cases (1) and (2) are derived. Here, the comparison of numerical results obtained by the Gaussian beams summation method and the mode decompositions is discussed.

2. Electronic Gaussian beams

First, the basic steps of the ray method recurrence relations (see [13, 14]) are considered for the stationary problem of Green's function for the Schrödinger operator describing an electron in the presence of a homogeneous magnetic field and arbitrary scalar potential

$$\frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2 G + u(\mathbf{x})G = EG + \delta(\mathbf{x} - \mathbf{x}^{(0)}). \tag{3}$$

These results are used in the derivation of the electronic Gaussian beam asymptotic expansion. A ray asymptotic solution is the principal part of the method of the summation of Gaussian beams.

2.1. Ray asymptotic solutions

Consider the axial gauge of a magnetic field: $\mathbf{A} = B/2(-x_2, x_1, 0)$. The WKB ray solution is sought in the form of formal asymptotic expansion with respect to small parameter $\hbar$:

$$G(\mathbf{x}, \mathbf{x}^{(0)}) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(\mathbf{x})} \sum_{j=0}^{+\infty} G_j(\mathbf{x})(\mathrm{i}\hbar)^j. \tag{4}$$

Substituting this series into (3), and equating to zero the corresponding coefficients of successive degrees of $\hbar$, we obtain a recurrent system of equations which determines the unknown $S(\mathbf{x})$ and $G_j(\mathbf{x})$. Classical action $S(\mathbf{x})$ satisfies the Hamilton–Jacobi equation

$$\langle \nabla S, \nabla S\rangle + \alpha x_2 S_{x_1} - \alpha x_1 S_{x_2} + \frac{\alpha^2}{4}\left(x_1^2 + x_2^2\right) - 2m(E - u(\mathbf{x})) = 0, \tag{5}$$

where symbol $\langle , \rangle$ means the scalar product and amplitudes G_j satisfy the transport equations

$$2\langle \nabla S, \nabla G_j\rangle + \alpha\left(x_2 G_{jx_1} - x_1 G_{jx_2}\right) + \Delta S G_j = \Delta G_{j-1}, \qquad G_{-1} = 0.$$

Taking into account the method of by-characteristics [10] and solving the corresponding Hamilton system

$$\dot{\mathbf{x}} = \mathcal{H}_{\mathbf{p}}, \qquad \dot{\mathbf{p}} = -\mathcal{H}_{\mathbf{x}}, \qquad \mathbf{x} = (x_1, x_2), \qquad \mathbf{p} = (p_1, p_2),$$

with the Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) + u(\mathbf{x}) - E \tag{6}$$

and initial conditions

$$\mathbf{x}|_{t=0} = \mathbf{x}^{(0)}, \qquad \mathbf{p}|_{t=0} = \frac{1}{\sqrt{2m(E - u(\mathbf{x}^{(0)}))}}(\cos\gamma, \sin\gamma)^T,$$

we obtain the classical trajectories in the phase space $R^4_{x,p}$ in the form of functions $\mathbf{x} = \mathbf{x}(t,\gamma), \mathbf{p} = \mathbf{p}(t,\gamma)$, parametrized by the so-called ray coordinates, time and polar angle t, γ. In the coordinate space R^2_x, the classical trajectories (rays) connect $\mathbf{x}$ and $\mathbf{x}^{(0)}$. It yields solution S in the form of integral

$$\begin{aligned} S &= \int_{\mathbf{x}^{(0)}}^{\mathbf{x}} \sqrt{2m(E - u(\mathbf{x}(s)))}\,\mathrm{d}s + \frac{e}{c}\int_{\mathbf{x}^{(0)}}^{\mathbf{x}} \mathbf{A}\,\mathrm{d}\mathbf{x} \\ &= \int_{\mathbf{x}^{(0)}}^{\mathbf{x}} \left(\sqrt{2m(E - u(\mathbf{x}(s))\big(\dot{x}_1^2 + \dot{x}_2^2\big)} + \frac{\alpha}{2}(-x_2\dot{x}_1 + x_1\dot{x}_2)\right)\mathrm{d}t. \end{aligned} \tag{7}$$

The transport equations may be written as follows:

$$2m\frac{\mathrm{d}G_j}{\mathrm{d}t} + \Delta S G_j = \Delta G_{j-1},$$

where $\frac{\mathrm{d}}{\mathrm{d}t}$ is a derivative with respect to the Hamiltonian system. Following [10], we obtain

$$\Delta S = m\frac{\mathrm{d}}{\mathrm{d}t}\ln J(t,\gamma), \qquad J(t,\gamma) = \left|\frac{\partial(x_1, x_2)}{\partial(t,\gamma)}\right|,$$

where J is geometrical spreading. Now the transport equation can be integrated:

$$G_j(\mathbf{x}, \mathbf{x}^{(0)}) = \sqrt{\frac{J(0,\gamma)}{J(t,\gamma)}}\left(g_j(\gamma) + \frac{1}{2m}\int_0^t \Delta G_{j-1}\,\mathrm{d}\tau\right), \tag{8}$$

where $g_j(\gamma)$ are constants of integration. These constants should be determined by the boundary layer method (see [14, chapter 6]) matching the outer asymptotic expansion (8) with a solution constructed in an asymptotically small neighbourhood of the point source $\mathbf{x}^{(0)}$.

Finally, taking into account a finite number of trajectories connecting $\mathbf{x}$ and $\mathbf{x}^{(0)}$, up to the leading order the ray asymptotic solution is given by

$$G(\mathbf{x}, \mathbf{x}^{(0)}) = \sum_n \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t^{(n)},\gamma^{(n)}) - \mathrm{i}\frac{\pi}{2}\mu_n}\sqrt{\frac{J(0,\gamma^{(n)})}{J(t^{(n)},\gamma^{(n)})}}g_0(\gamma^{(n)})(1 + O(\hbar)), \tag{9}$$

where μ_n is the Maslov index of the nth trajectory [10]. This solution is singular near the caustics or focal points where $J(t,\gamma) = 0$.

Here is an example of the WKB asymptotic expansion of Green's function of an electron in a magnetic field with $u(\mathbf{x}) = 0$:

$$G = \sum_{n=1,2}\frac{1}{2\sqrt{2\pi k|J_n|}}\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_n - \frac{\mathrm{i}\pi}{4} - \frac{\mathrm{i}\pi}{2}\mu_n}}{1 + \mathrm{e}^{\mathrm{i}mR^2\omega\pi/\hbar}}(1 + O(k^{-1})), \qquad k = \frac{\sqrt{2mE}}{\hbar} \gg 1, \tag{10}$$

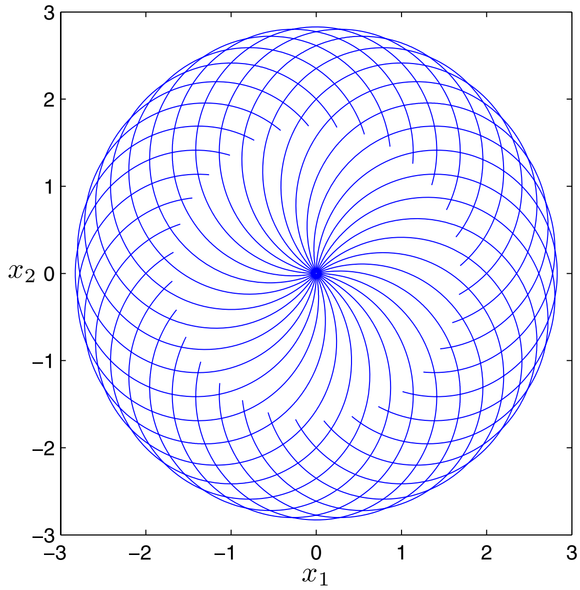

Figure 1. Family of classical trajectories for the problem of Green's function of an electron in a magnetic field with $u(\mathbf{x}) = 0$ and $\mathbf{x}^{(0)} = (0, 0)$.

where

$$S = \frac{mR^2\omega}{2}\left(\frac{s}{R} + \sin\frac{s}{R}\right), \qquad J = R\sin\frac{s}{R},$$
$$R = \frac{\sqrt{2E/m}}{\omega}, \qquad \omega = \frac{eB}{mc}, \qquad \mu_1 = 0, \qquad \mu_2 = 1,$$

where s is the arc length being chosen instead of t and measured along the trajectory from $\mathbf{x}^{(0)}$. This formula includes an infinite sum of multiple traversals of the circular orbits that is a sum of geometrical progression. This WKB asymptotic expansion was constructed with the help of the ray coordinates

$$x_1 = R\left[\sin\left(\frac{s}{R} - \gamma\right) + \sin\gamma\right] + x_1^{(0)}, \qquad x_2 = R\left[\cos\left(\frac{s}{R} - \gamma\right) - \cos\gamma\right] + x_2^{(0)}.$$

The property of the solution being singular at

$$E = E_l = \hbar\omega\big(l + \tfrac{1}{2}\big), \qquad l \in N,$$

gives the quantization of the energy spectrum (Landau levels). This solution is singular at $s = \pi\nu R$, $\nu \in N$ (see figure 1). The set of singular points are the circle $\nu = (2n + 1)$ which is a smooth caustic, and the focal point $\mathbf{x}^{(0)}$, where $\nu = 2n$ $(n \in N)$.

Frequently, in practice while applying the ray asymptotic method, the structure of classical trajectories looks very complicated. This is due to the presence of caustics and focal points. This situation takes place for a charged particle moving in strong magnetic fields. Thus, the ray asymptotic expansion is not effective as it is not valid inside domains asymptotically close to caustics and focal points.

As stated earlier, the method of Gaussian beams summation provides effective asymptotic approximation valid near caustics and focal points. In the following section, a generalization of the method is described for the wavefunction of electron motion in a magnetic field and arbitrary scalar potential. It gives analytical representation of Green's function as an integral over Gaussian beams.

2.2. Localized asymptotic solution—Gaussian beam

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

$$\mathbf{x} = \mathbf{x}_0(s) + \mathbf{e_n}(s)n, \tag{11}$$

where $\mathbf{e_n}(s)$ is the unit vector normal to the trajectory.

Following [14], we apply the asymptotic boundary-layer method to the homogeneous Schrödinger equation (3). 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

$$\psi = \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S_0+S_1 n+\Gamma(s)n^2/2)}}{\sqrt{a(s)}} \sum_{j=0}^{+\infty} \psi_j(s, \nu)\hbar^{j/2}. \tag{12}$$

Here $S_0(s), S_1(s), \Gamma(s)$ are coefficients of asymptotic expansion of S with respect to small n:

$$S = S_0(s) + S_1(s)n + \Gamma(s)n^2/2 + \cdots.$$

Substituting this expansion into the Hamilton–Jacobi equation (5), we obtain

$$S_0 = \int_0^s \left(a(s) - \frac{\alpha}{2}\left(x_1^{(0)}\gamma_1 + x_2^{(0)}\gamma_2\right)\right)\mathrm{d}s, \qquad S_1 = \frac{\alpha}{2}\left(x_1^{(0)}\gamma_2 - x_2^{(0)}\gamma_1\right),$$

$$a(s) = \sqrt{2m(E - u_0(s))}, \qquad u(\mathbf{x}) = u_0(s) + u_1(s)n + u_2(s)n^2 + \cdots,$$

and $\gamma_i(s), i = 1, 2$, are the Cartesian components of the vector $\mathbf{e_n}(s)$. The coefficient Γ satisfies the Ricatti equation (see [13, 14])

$$\dot{\Gamma} + \frac{1}{a}\Gamma^2 + ad = 0, \tag{13}$$

where the symbol $\dot{\Gamma}$ means the derivative with respect to s:

$$d(s) = \frac{u_2}{E - u_0} + \frac{u_1^2}{4(E - u_0)^2} - \frac{u_1}{\rho(E - u_0)} - \frac{\alpha}{\rho a}.$$

By means of the substitute $\Gamma = a\frac{\dot{z}}{z}$, the Ricatti equation is reduced to

$$\frac{\mathrm{d}}{\mathrm{d}s}(a(s)\dot{z}) + a(s)d(s)z = 0. \tag{14}$$

It is worth remarking that the solution $z(s)$ satisfies the so-called equation 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

$$\mathbf{x}(s) = \mathbf{x}_0(s) + n(s)\,\mathbf{e_n}(s).$$

The equation in variations may be written as the following Hamiltonian system:

$$\dot{z} = p/a(s), \qquad \dot{p} = -a(s)d(s)z, \tag{15}$$

with the Hamiltonian function

$$H_2(s, p, z) = \frac{p^2}{2a(s)} + \frac{a(s)d(s)}{2}z^2.$$

For the zero-order amplitude, we have the transport equation

$$2m\frac{\mathrm{d}\psi_0}{\mathrm{d}t} + \Delta S\psi_0 = 0.$$

Taking into account the expansion

$$\psi_0 = \psi_0^{(0)} + \psi_0^{(1)}n + O(n^2),$$

for the leading term, we obtain ODE for $\psi_0^{(0)}$:

$$\frac{\mathrm{d}\psi_0^{(0)}}{\mathrm{d}s} + \frac{1}{2a}\left(\frac{\mathrm{d}\dot{S}_0}{\mathrm{d}s} + \Gamma - \frac{S_1}{\rho}\right)\psi_0^{(0)} = 0$$

and

$$\frac{\mathrm{d}\psi_0^{(0)}}{\mathrm{d}s} + \frac{1}{2a}\left(\frac{\mathrm{d}a}{\mathrm{d}s} + \frac{a\dot{z}}{z}\right)\psi_0^{(0)} = 0.$$

Its solution is $\psi_0^{(0)} = \frac{\text{const}}{\sqrt{az}}$.

It is very important that solutions of the system of equations in variations (15) may be chosen complex $z(s) = z_1(s) + \mathrm{i}z_2(s)$ and $p(s) = p_1(s) + \mathrm{i}p_2(s)$, where $z_1(s)$, $p_1(s)$ and $z_2(s)$, $p_2(s)$ are, respectively, the real and linear independent solutions to (15). This leads to $\mathrm{Im}(\Gamma(s)) > 0$ for $0 < s < s*$, thus providing asymptotic localization of the solution ψ. The localization and regularity near the caustics are due to the fact that

$$\mathrm{Im}(\Gamma(s)) = \mathrm{Im}\left(a\frac{\dot{z}}{z}\right) = a\frac{z_1\dot{z}_2 - \dot{z}_1 z_2}{z_1^2 + z_2^2} = \frac{\text{const}}{z_1^2 + z_2^2}.$$

Thus, we obtain that to the leading order the Gaussian beam asymptotic solution is given by

$$\psi = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S_0(s) + S_1(s)n + \frac{p(s)}{2z(s)}n^2)}\frac{1}{\sqrt{a(s)z(s)}}(1 + O(\hbar^{1/2})). \qquad (16)$$

It is always regular near caustics and focal points regardless of its complicated geometrical structure. However, it is clear that this asymptotic solution is not valid near potential turning lines where $a(s)$ vanishes.

3. Asymptotic expansion of Green's function for an electron in a magnetic field in the form of an integral over Gaussian beams

The theory of the method of Gaussian beams summation was originally developed for acoustic wave fields. For electron motion in a magnetic field, general points of theoretical basis of the method are the same. In this section, the desired uniform approximation of an electron wavefunction valid near caustics and focal points is described briefly. For electron Green's function stationary problem (3), two types of approximations are being discussed.

The first one is the integral over all Gaussian beams irradiated from the point source $\mathbf{x}^{(0)}$:

$$G(\mathbf{x}, \mathbf{x}^{(0)}, E) = \int_0^{2\pi} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S_0(s) + S_1(s)n + \frac{p(s)}{2z(s)}n^2)}\frac{A(\gamma)\,\mathrm{d}\gamma}{\sqrt{a(s)z(s)}}(1 + O(\hbar^{1/2})), \qquad (17)$$

where $A(\gamma)$ is an unknown amplitude. This integral can be evaluated numerically, and the corresponding algorithm is very simple. The rectangular or Simpson formulae may be used. The basic idea of the approximation is that the total fan of classical trajectories corresponding to the discrete set of an 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 $\mathbf{x}$. For each trajectory fixed by a value of γ, a set of local coordinates (s, n) (see (11)) of the observation point **x** has to be determined. Then, all the components of the Gaussian beam asymptotic solution (16), 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 $\gamma \in [0, 2\pi]$. The parameter w is used in the construction of the complex solution $z(s)$, $p(s)$ in such a way that

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

where the real $z_1(s)$, $p_1(s)$, $z_2(s)$, $p_2(s)$ satisfy (15) and the following initial conditions:

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

The parameter w determines the width of the localized Gaussian beams. The thinner the Gaussian beams, the more accurate an approximation for a solution may be obtained numerically (see [11, 12]).

The amplitude $A(\gamma)$ is to be determined by the steepest descent method (see [11, 12]). In the region close to $\mathbf{x}^{(0)}$, where the structure of electron classical trajectories is regular away from the caustics, the approximation (17) must coincide with the ray asymptotic solution

$$G(\mathbf{x}, \mathbf{x}^{(0)}, E) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S} \sqrt{\frac{J(0, \gamma_0)}{J(s, \gamma_0)}} g_0(\gamma_0)(1 + O(\hbar)), \tag{18}$$

where γ_0 determines the trajectory connecting $\mathbf{x}^{(0)}$ and **x**. Taking into account the fact that only an asymptotically small ($\hbar \to 0$) neighbourhood of trajectories, close to the trajectory with $\gamma = \gamma_0$, contributes to the integral (17), we may use in this neighbourhood the following approximations:

$$S = S_0 + S_1 n + \frac{1}{2}\frac{\tilde{p}(s)}{\tilde{z}(s)} n^2 + O(n^3), \qquad n = \tilde{z}(s)(\gamma - \gamma_0) + O((\gamma - \gamma_0)^2),$$

where real $\tilde{z}(s)$ and $\tilde{p}(s)$ satisfy (15) with initial conditions $\tilde{z}(0) = 0$ and $\tilde{p}(0) = a(0)$ respectively. Thus, to the leading order we obtain

$$\begin{aligned} G(\mathbf{x}, \mathbf{x}^{(0)}, E) &= \frac{A(\gamma_0)}{\sqrt{a(s)z(s)}} \int_{-\Delta_1}^{\Delta_1} \exp\left(-\frac{\mathrm{i}}{2\hbar} \frac{a(0)\tilde{z}(s)}{z(s)} (\gamma - \gamma_0)^2 \right) + \cdots \\ &= \frac{A(\gamma_0)}{\sqrt{a(s)\tilde{z}(s)}} \sqrt{\frac{2\pi\hbar}{a(0)}}\, \mathrm{e}^{-\mathrm{i}\pi/4}, \end{aligned}$$

where Δ_1 is a positive constant. Since $J(s, \gamma_0) = a(s)\tilde{z}(s)$, matching the leading term for $G(\mathbf{x}, \mathbf{x}^{(0)}, E)$ with (18) leads to

$$A(\gamma_0) = \frac{\mathrm{e}^{\mathrm{i}\pi/4}}{2\pi\hbar} g_0(\gamma_0)\sqrt{J(0, \gamma_0)a(0)}.$$

The second type of approximation for electron Green's function problem (3) combines a contribution of ray asymptotic solutions computed for trajectories arriving at **x**, which are not effected by caustics (their $J(t, \gamma)$ does not vanish), and a Gaussian beam integral performed in the finite interval of $\gamma \in [\gamma_0 - \Delta_2, \gamma_0 + \Delta_2]$ representing trajectories tangent to caustics

$$\begin{aligned} G(\mathbf{x}, \mathbf{x}^{(0)}, E) = &\sum_n \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t^{(n)}, \gamma^{(n)}) - \mathrm{i}\frac{\pi}{2}\mu_n} \sqrt{\frac{J(0, \gamma^{(n)})}{J(t^{(n)}, \gamma^{(n)})}} g_0(\gamma^{(n)})(1 + O(\hbar)) \\ &+ \int_{\gamma_0 - \Delta_2}^{\gamma_0 + \Delta_2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S_0(s) + S_1(s)n + \frac{p(s)}{2z(s)}n^2)} \frac{A(\gamma)\,\mathrm{d}\gamma}{\sqrt{a(s)z(s)}} (1 + O(\hbar^{1/2})). \end{aligned} \tag{19}$$

Here, γ_0 determines the trajectory connecting $\mathbf{x}^{(0)}$ and $\mathbf{x}$, and corresponding $J(t, \gamma_0)$ vanishes as $\mathbf{x}$ close to caustics. The positive constant Δ_2 must be chosen in such a way that the corresponding dense fan of trajectories totally covers the observation point $\mathbf{x}$. However, it is worth remarking that although the corresponding numerical algorithm is faster than the code for the previous case, its structure is considerably more complicated logically. This fact takes place due to the complex behaviour of the classical trajectories of an electron in a magnetic field with caustics and focal points (see figures 3 and 7).

4. Numerical tests of Gaussian beams summation for electronic waveguide motion in a magnetic field

In this section, the method of Gaussian beams summation for electronic motion in magnetic field is tested for two special cases (1) and (2). For both cases owing to separation variables, Green's function is represented by exact mode decomposition. This gives the possibility of comparing numerical results obtained by two independent methods and, thus, determining a region of applicability of the Gaussian beams summation method, its advantages and drawbacks.

First, consider the case of an electron in magnetic and electric fields (1). Let $m = 1$, and let us rewrite this problem as follows:

$$\left(-\Delta - \frac{2\mathrm{i}\alpha}{\hbar} x_2 \frac{\partial}{\partial x_1} + \frac{\alpha^2 x_2^2}{\hbar^2} - \frac{2e_2 x_2}{\hbar^2} - k^2\right) G(\mathbf{x}, \mathbf{x}^{(0)}, E) = \delta(\mathbf{x} - \mathbf{x}^{(0)}), \quad (20)$$

where the wave number is given by $k = \frac{\sqrt{2E}}{\hbar}$. The solution $G(\mathbf{x}, \mathbf{x}^{(0)}, E)$ is sought in the form of a Fourier integral

$$G(x_1, x_2, \mathbf{x}^{(0)}, E) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}k_1 x_1} \tilde{G}(k_1, x_2, \mathbf{x}^{(0)}, E)\, \mathrm{d}k_1, \quad (21)$$

where $\tilde{G}(k_1, x_2, \mathbf{x}^{(0)}, E)$ is the fundamental solution to

$$\left(-\frac{\partial^2}{\partial x_2^2} - \frac{2k_1 x_2 \alpha}{\hbar} + \frac{\alpha^2 x_2^2}{\hbar^2} + k_1^2 - \frac{2e_2 x_2}{\hbar^2} - k^2\right) \tilde{G}(k_1, x_2, \mathbf{x}^{(0)}, E) = \delta\big(x_2 - x_2^{(0)}\big).$$

Its Fourier series with respect to corresponding eigenfunctions is given by

$$\tilde{G}(k_1, x_2, \mathbf{x}^{(0)}, E) = \sqrt{\frac{\hbar}{\alpha}} \sum_{n=0}^{\infty} \frac{\Phi_n(x_2, k_1)\Phi_n\big(x_2^{(0)}, k_1\big)}{2n + 1 - \Lambda(k_1)},$$

where

$$\Lambda(k_1) = \frac{\hbar}{\alpha}\left(k^2 + 2\frac{k_1 e_2}{\hbar\alpha} + \frac{e_2^2}{\hbar^2\alpha^2}\right),$$

$$\Phi_n(x_2, k_1) = \phi_n\left(x_2\sqrt{\frac{\alpha}{\hbar}} - \left(\frac{\hbar}{\alpha}\right)^{3/2}\left(\frac{\alpha k_1}{\hbar} + \frac{e_2}{\hbar^2}\right)\right).$$

Here, $\phi_n(x)$ are Hermitian functions $\phi_n(x) = \mathrm{e}^{-x^2/2} H_n(x)$ with Hermitian polynomials $H_n(x)$. Taking into account the fact that the contour of integration in (21) is shifted into the complex plane of k_1 shown in figure 2(a), the Fourier integral for $G(\mathbf{x}, \mathbf{x}^{(0)}, E)$ can be calculated as a sum of residues in the poles

$$k_1^{(n)} = \left((2n + 1)\frac{\alpha}{\hbar} - k^2 - \frac{e_2^2}{\hbar^2\alpha^2}\right)\frac{\hbar\alpha}{2e_2}.$$

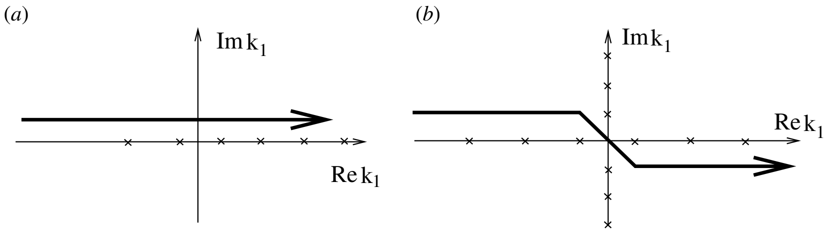

Figure 2. The poles and the integration contours in the complex plane k_1 for the Fourier integral of Green's function. (*a*) electron in the magnetic and electric fields and (*b*) electron in an magnetic field and parabolic potential.

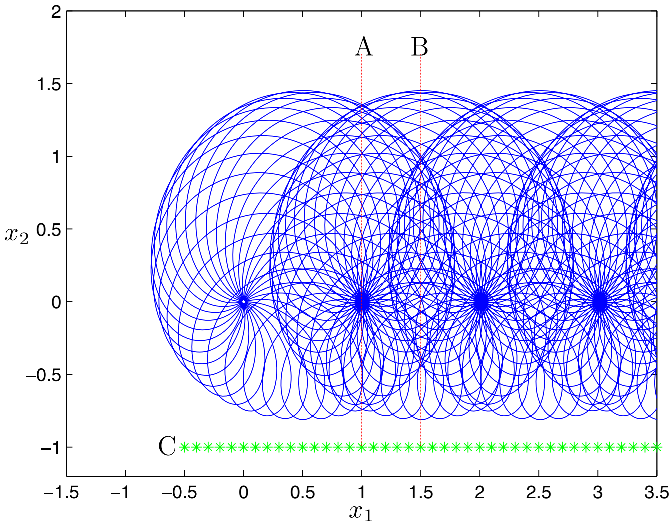

Figure 3. The structure of the classical trajectories of an electronic waveguide in magnetic and electric fields.

Thus, we obtain

$$G(\mathbf{x}, \mathbf{x}^{(0)}, E) = \mathrm{i}\sqrt{\hbar}\frac{\alpha^{3/2}}{2e_2}\sum_{n=0}^{\infty} \mathrm{e}^{-\mathrm{i}k_1^{(n)}x_1}\Phi_n\big(x_2, k_1^{(n)}\big)\Phi_n\big(x_2^{(0)}, k_1^{(n)}\big). \tag{22}$$

This formula describes Green's function presentation as a sum of propagating modes inside a waveguide above a turning line (line C is given by $E = u(\mathbf{x}) = e_2x_2$) and between two external caustic lines (see figure 3). This waveguide propagation to the right from the source ($\mathbf{x}^{(0)} = (0, 0)$) takes place due to the presence of a magnetic field. On the left side of the source, Green's function decays exponentially. Smooth caustic lines and focal points are seen clearly inside the waveguide. We observe three types of zones separated by caustics since at any observation point we have six incoming trajectories (the most dense zone), then four and finally two (less dense zone). In figures 4 and 5, the values of $|G(\mathbf{x}, \mathbf{x}^{(0)}, E)|^2/\hbar$ at the points of vertical cuts A and B are presented. These data were computed by means of the Gaussian summation (17) and the mode decomposition (22) for the following values of parameters: $\alpha = 2.5, e_2 = 1, E = 1, \hbar = 0.05, w = 2$. The vertical cut A goes through the focal point. Both graphs show a good agreement. Discretizing the integral (17), 128 Gaussian beams were

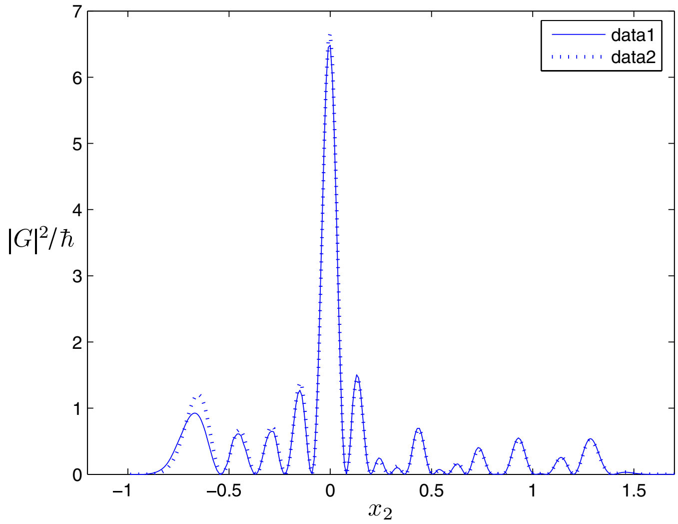

Figure 4. The values of $|G(\mathbf{x}, \mathbf{x}^{(0)}, E)|^2$ at the points of vertical cut A for an electronic waveguide in magnetic and electric fields (data 1—Gaussian beams summation and data 2—mode decomposition).

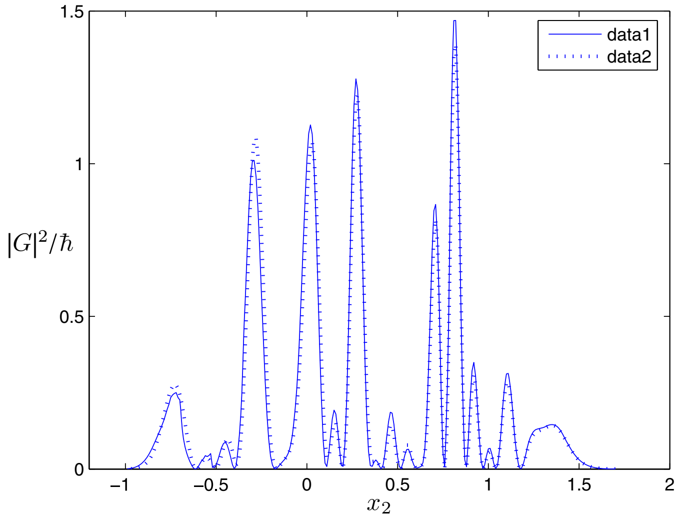

Figure 5. The values of $|G(\mathbf{x}, \mathbf{x}^{(0)}, E)|^2$ at the points of vertical cut B for an electronic waveguide in magnetic and electric fields (data 1—Gaussian beams summation and data 2—mode decomposition).

used. Approximation (19) is also effective in this case. It provides the same order of error compared with (22).

Consider the second case of electron motion in a magnetic field and parabolic potential (2). Using the same notations, let us rewrite this problem as follows:

$$\left(-\Delta - \frac{2i\alpha}{\hbar}x_2\frac{\partial}{\partial x_1} + \frac{\alpha^2 x_2^2}{\hbar^2} + \frac{\beta x_2^2}{\hbar^2} - k^2\right)G(\mathbf{x}, \mathbf{x}^{(0)}, E) = \delta(\mathbf{x} - \mathbf{x}^{(0)}). \tag{23}$$

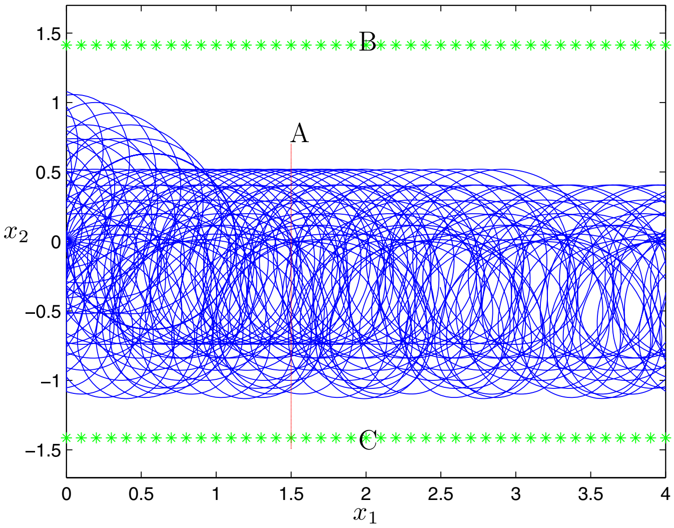

Figure 6. The structure of the classical trajectories of an electronic waveguide in a magnetic field and parabolic potential.

The solution $G(\mathbf{x}, \mathbf{x}^{(0)}, E)$ is sought in the form of Fourier integral (21), where $\tilde{G}(k_1, x_2, \mathbf{x}^{(0)}, E)$ is the fundamental solution of

$$\left(-\frac{\partial^2}{\partial x_2^2} - \frac{2k_1x_2\alpha}{\hbar} + \frac{\alpha^2x_2^2}{\hbar^2} + k_1^2 + \frac{\beta x_2^2}{\hbar^2} - k^2\right)\tilde{G}(k_1, x_2, \mathbf{x}^{(0)}, E) = \delta\big(x_2 - x_2^{(0)}\big).$$

Its Fourier series with respect to the corresponding eigenfunctions is given by

$$\tilde{G}(k_1, x_2, \mathbf{x}^{(0)}, E) = \frac{\sqrt{\mu}}{1 - \left(\frac{\alpha}{\mu\hbar}\right)^2} \sum_{n=0}^{\infty} \frac{\Phi_n(x_2, k_1)\Phi_n\big(x_2^{(0)}, k_1\big)}{k_1^2 - \big(k_1^{(n)}\big)^2},$$

where

$$k_1^{(n)} = \sqrt{\frac{\alpha^2 + \beta}{\beta}}\sqrt{k^2 - \mu(2n+1)},$$

$$\Phi_n(x_2, k_1) = \phi_n\left(x_2\sqrt{\mu} - \frac{\alpha k_1}{\hbar\mu^{3/2}})\right), \qquad \mu = \frac{\sqrt{\alpha^2 + \beta}}{\hbar}.$$

Taking into account the fact that the contour of integration in (21) in the complex plane of k_1 is chosen in a way as shown in figure 2(*b*), the Fourier integral for $G(\mathbf{x}, \mathbf{x}^{(0)}, E)$ can be calculated as a sum of residues in the poles $k_1^{(n)}$ leading to

$$G(\mathbf{x}, \mathbf{x}^{(0)}, E) = \frac{\mathrm{i}}{2}\frac{\sqrt{\mu}}{1 - \left(\frac{\alpha}{\mu\hbar}\right)^2} \sum_{n=0}^{\infty} \mathrm{e}^{\mathrm{i}k_1^{(n)}|x_1|}\Phi_n\big(x_2, k_1^{(n)}\big)\frac{\Phi_n\big(x_2^{(0)}, k_1^{(n)}\big)}{k_1^{(n)}}. \tag{24}$$

This is Green's function presentation described as a sum of propagating modes inside a waveguide between the two turning lines B, C $\big(E = u(\mathbf{x}) = \beta x_2^2/2\big)$ and confined by two external caustic lines (see figure 6). This waveguide propagation takes place to the right and left from the source $(\mathbf{x}^{(0)} = (0, 0))$. The structure of trajectories is symmetric with respect to $x_1 = 0$. Thus, only the right part of the picture is chosen. In figure 7, the values of $|G(\mathbf{x}, \mathbf{x}^{(0)}, E)|^2$ at the points of vertical cut A (see figure 6) are presented. These data were

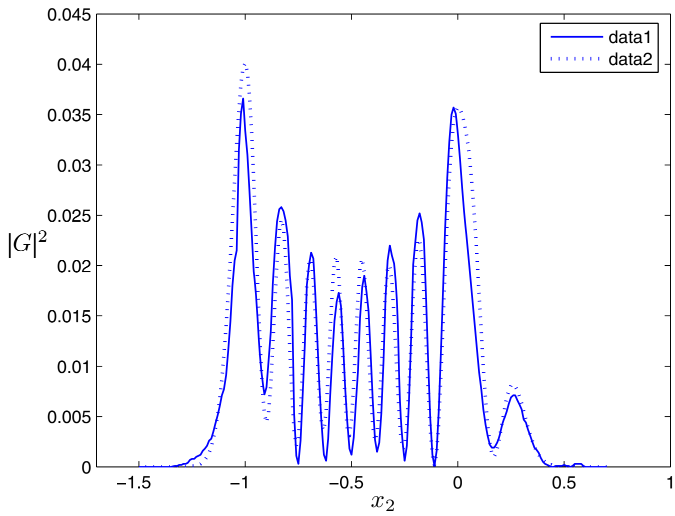

Figure 7. The values of $|G(\mathbf{x}, \mathbf{x}^{(0)}, E)|^2$ at the points of vertical cut A for an electronic waveguide in a magnetic field and parabolic potential (data 1—Gaussian beams summation and data 2—mode decomposition).

computed by means of the Gaussian summation (17) and the mode decomposition (22) for the following values of parameters: $\alpha = 2, \beta = 1, E = 1, \hbar = 0.05, w = 2$. Both graphs again show a good agreement. Discretizing the integral (17), 128 Gaussian beams were used. Application of (19) in this case seems to be ineffective as the structure of the trajectories looks very complicated.

It is worth remarking that in both cases shown in figures 3 and 6, the electronic waveguide propagation is clearly seen to be isolated from the potential turning lines (line C in figure 3 and lines B, C in figure 6) where the Gaussian beams approximation is not valid.

5. Conclusion

Using the basic steps of the techniques of Gaussian beams summation developed for acoustic wave propagation in the case of shortwave approximation, this method was generalized and applied for electron motion in a magnetic field and arbitrary potential $u(\mathbf{x})$. It provides semiclassical uniform approximation for Green's function in stationary problems describing electronic wave propagation. This approximation was tested for two special cases of waveguide excitation by a point source for electron motion in a magnetic field for linear and parabolic potentials. The asymptotic approximations for Green's functions computed by the Gaussian beams summation method were found to be in a very good agreement with data obtained by the separation of variables (exact mode decomposition of Green's function). Thus, the method of Gaussian beams summation is efficient for the construction of the WKB approximation describing electron motion in a magnetic field and any scalar potential. It may be applied to the problems of electronic waveguide transport through resonators. However, there is a drawback of the method. The corresponding asymptotic approximation is not valid near the potential turning line as a single Gaussian beam asymptotic solution breaks down in this case. This fact may be considered as a future prospect towards the generalization of the Gaussian beam summation method which is uniformly valid near the potential turning line.

Acknowledgments

The authors would like to thank the ESF network AQDJJ for the financial support, and Professor M Popov, Dr A Vagov and Dr H Shumerus for constructive discussions and valuable remarks.

References

[1] Belov V V, Dobrokhotov S Yu and Tudorovskii T Ya 2004 *Theor. Math. Phys.* **141** 1562–92
[2] Bruning J, Yu Dobrokhotov S, Nekrasov R V and Tudorovskii T Ya 2008 *Russ. J. Math. Phys.* **15** 1–15
[3] Datta S 1995 *Electronic Transport in Mesoscopic Systems* (Cambridge: Cambridge University Press)
[4] Mello P A and Kumar N 2004 *Quantum Transport in Mesoscopic Systems* (New York: Oxford University Press)
[5] Stockmann H J 2000 *Quantum Chaos. An Introduction* (Cambridge: Cambridge University Press)
[6] Schwieters C D, Alford J A and Delos J B 1996 *Phys. Rev.* B **54** 10652
[7] Beenaker C W J 1997 *Rev. Mod. Phys.* **69** 731
[8] Blomquist T and Zozoulenko I V 2000 *Phys. Rev.* B **61** 1724
[9] Jalabert R A, Baranger H U and Stone A D 1990 *Phys. Rev. Lett.* **65** 2442
[10] Maslov V P and Fedoriuk M V 1981 *Semiclassical Approximation in Quantum Mechanics* (Dordrecht: Reidel)
[11] Popov M M 1981 *Wave Motion* **61** 1724
[12] Popov M M 2002 *Ray Theory and Gaussian Beam Method for Geophysicists* (Bahia: EDUFBA Publishing)
[13] Babich V M and Buldyrev V S 1991 *Asymptotic Methods in Shortwave Diffraction Problems* (New York: Springer)
[14] Babich V M and Ya Kirpichnikova N 1979 *The Boundary-Layer Method in Diffraction Problems* (Berlin: Springer)
[15] Zalipaev V V, Kusmartsev F V and Popov M M 2008 *J. Phys. A: Math. Theor.* **41** 065101