Analysis of a Stratified Quantum Waveguide with Interactions at Interface Planes

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Abstract. In this paper we consider a quantum waveguide that consists of three strata $\Pi_0 = \{(x, x_3) \in \mathbb{R}^2 : x_3 < 0\}$, $\Pi_{0,h} = \{(x, x_3) \in \mathbb{R}^2 : 0 < x_3 < h\}$, $\Pi_h = \{(x, x_3) \in \mathbb{R}^2 : x_3 > h\}$, where $x = (x_1, x_2) \in \mathbb{R}^2$. A potential of the form $q = q_r + q_s$ is established in this structure, where $q_r$ is a regular bounded potential depending on only the coordinate $x_3$, and $q_s$ is the singular potential $q_s = \alpha_1 \delta(x_3) + \beta_1 \delta'(x_3) + \alpha_2 \delta(x_3 - h) + \beta_2 \delta'(x_3 - h)$ with support at the planes $x_3 = 0$ and $x_3 = h$. The Green’s function of the waveguide is constructed as an expansion involving the eigenfunctions and generalized eigenfunctions of an auxiliary one-dimensional Schrödinger operator. The asymptotic analysis of the Green’s function is carried out by means of the stationary phase method. This gives the leading contribution of the Green’s function far from the point source. Finally some numerical examples are considered for the application of the present analysis.

1. Introduction

In this work it is studied a stratified quantum waveguide consisting of an inhomogeneous core enclosed by a homogeneous cladding. In the system of rectangular coordinates $r = (x_1, x_2, x_3) \in \mathbb{R}^3$ this structure is governed by the stationary Schrödinger equation

$$S_q \psi(r) := -\Delta \psi(r) + q(r) \psi(r) = \mu^2 \psi(r),$$

where $\Delta := \partial^2_{x_1} + \partial^2_{x_2} + \partial^2_{x_3}$ is the Laplacian operator, $\mu^2 \in \mathbb{R}$ is an energy parameter, and $\psi$ is the wavefunction. The units are chosen so that $\hbar^2 = 1 = 2m$. By $q$ we denote the potential established in the waveguide and $S_q$ denotes its corresponding Schrödinger operator. The potential $q = q_r + q_s$ is assumed to depend on only the vertical coordinate $x_3$. By $q_r \in L^\infty(\mathbb{R})$ we denote a regular attractive potential with compact support on $(0, h)$,

$$q_r(x_3) = \begin{cases} V(x_3), & 0 < x_3 < h \\ 0, & \text{elsewhere} \end{cases},$$

with $V$ a real-valued function that satisfies certain smoothness conditions. By $q_s$ we denote the singular potential $q_s(x_3) = \alpha_1 \delta(x_3) + \beta_1 \delta'(x_3) + \alpha_2 \delta(x_3 - h) + \beta_2 \delta'(x_3 - h)$, $\alpha_i, \beta_i \in \mathbb{R}$ ($i = 1, 2$), supported at the planes $x_3 = \{0, h\}$. In the waveguide these planes represent...
interfaces between the core $\Pi_{0,h} := \{ r = (x, x_3) \in \mathbb{R}^3 : 0 < x_3 < h \}$ and the cladding $\Pi_0 := \{ r = (x, x_3) \in \mathbb{R}^3 : x_3 < 0 \}$, $\Pi_0 := \{ r = (x, x_3) \in \mathbb{R}^3 : x_3 > h \}$, where $x = (x_1, x_2) \in \mathbb{R}^2$ denotes the horizontal coordinates. The study of Schrödinger operators with potentials involving Dirac deltas and their derivatives has been widely considered in the literature, see, e.g., [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]. Such singular potentials have been used in the Kronig-Penney model [16], for modeling bipolar interactions, and to analyze the Casimir effect [17, 18].

We obtain the Green’s function of the waveguide as an eigenfunction expansion. The Green’s function is defined by the differential expression

$$\left( S_q - \mu^2 \right) g(x, x_3; x', x'_3) = \delta(x - x', x_3 - x'_3), \quad (x, x_3) \in \mathbb{R}^3,$$

subjected to suitable boundary conditions, where $(x', x'_3) \in \mathbb{R}^3$ is the position of a point source. This source emits particles that interact with the waveguide. As is shown later, the Green’s function gives a wave-packet solution for Schrödinger equation (1). Indeed, outside the point source above equation is equivalent to Schrödinger equation (1). Hence, the mathematical study of the Green’s function provides a description of the bound and scattering states, all at once.

For approaching the Schrödinger operator $S_q$ involving a singular potential, we will construct a self-adjoint extension based on the work of Kurasov [19]. Then, we will use the Fourier transform with respect to $x \in \mathbb{R}^2$ on the resulting self-adjoint boundary-value problem, which gives a one-dimensional spectral problem depending on only the coordinate $x_3$. The eigenfunctions and generalized eigenfunctions of this spectral problem will serve as a basis for the expansion of the Green’s function of the waveguide. The solution thus obtained will consist of a superposition of bound states and lateral waves. The asymptotics of the Green’s function far from the point source will be analyzed by means of the stationary phase method.

The content of this work is organized as follows. In Section 2 we construct the eigenfunctions and generalized eigenfunctions of an auxiliary one-dimensional spectral problem. Also a dispersion equation for calculating its eigenvalues is obtained in a closed-form. In Section 3 the Green’s function of the quantum waveguide is obtained as an expansion involving the eigenfunction of the auxiliary problem. In Section 4 we obtain the leading term of the asymptotics of the Green’s function by means of the stationary phase method. In Section 5 we consider the numerical implementation of the leading term of the Green’s function based on the spectral parameter power series (SPPS for short) method. Finally in Section 6 we draw some conclusions.

2. Spectral analysis of an auxiliary one-dimensional problem

Let us consider the one-dimensional Schrödinger equation

$$\mathcal{L}_q(x, \frac{d}{dx}) u(x) := \left( -\frac{d^2}{dx^2} + q(x) \right) u(x) = \lambda u(x), \quad x \in \mathbb{R},$$

(2)

where $q = q_r + q_s$, and $\lambda \in \mathbb{R}$ is the spectral parameter. The singular potential is $q_s(x) = \alpha_1 \delta(x) + \beta_1 \delta'(x) + \alpha_2 \delta(x-h) + \beta_2 \delta'(x-h)$ with $\alpha_i, \beta_i \in \mathbb{R}$ ($i = 1, 2$), and $q_r \in L^\infty(\mathbb{R})$ is a regular potential. In the work [20] the action of distributions $\delta$ and $\delta'$ is properly continued for their use on discontinuous functions. This continuation replaces the singular potential by certain boundary conditions at the points $x = \{0, h\}$. More precisely, let $H_{q_r}$ be a Schrödinger operator defined by the differential expression $\mathcal{L}_{q_r} u(x) := \left( -\frac{d^2}{dx^2} + q_r(x) \right) u(x)$, $x \in \mathbb{R} \setminus \{0, h\}$, together with the point conditions

$$\begin{pmatrix} u(0^+) \\ u'(0^+) \end{pmatrix} = A_1 \begin{pmatrix} u(0^-) \\ u'(0^-) \end{pmatrix}, \quad \begin{pmatrix} u(h^+) \\ u'(h^+) \end{pmatrix} = A_2 \begin{pmatrix} u(h^-) \\ u'(h^-) \end{pmatrix},$$

where $A_1$ and $A_2$ are matrices that depend on the boundary conditions at $x = 0$ and $x = h$, respectively. These matrices are determined by the boundary conditions and the eigenvalues of the auxiliary problem.

The analysis of the Schrödinger equation (2) is based on the following steps:

1. **Construction of the Eigenfunctions:** We construct the eigenfunctions of the auxiliary problem $\mathcal{L}_{q_r}$, which are solutions of the differential equation $\mathcal{L}_{q_r} u(x) = \lambda u(x)$. These eigenfunctions are characterized by their regularity and their behavior at the points $x = \{0, h\}$.

2. **Regularization of the Potential:** We regularize the singular potential $q_s(x)$ by means of a compact support function $\mathcal{R}(x)$, which is equal to 1 in a neighborhood of $x = 0$ and $x = h$, and equals 0 outside a large enough interval. This regularization allows us to use standard techniques for solving the Schrödinger equation with a regular potential.

3. **Spectral Analysis:** We analyze the spectrum of the Schrödinger operator $\mathcal{L}_q$, which is the set of all eigenvalues $\lambda$ of the equation $\mathcal{L}_q u(x) = \lambda u(x)$. The spectrum is characterized by its discrete and continuous parts, and it is related to the asymptotic behavior of the Green’s function.

4. **Asymptotic Behavior:** We study the asymptotic behavior of the Green’s function $g(x, x_3; x', x'_3)$ as $x \to \pm \infty$, $x_3 \to \pm \infty$, $x' \to \pm \infty$, and $x'_3 \to \pm \infty$. This behavior is determined by the properties of the eigenfunctions of the auxiliary problem and the boundary conditions.

5. **Numerical Implementation:** We implement the asymptotic expansion of the Green’s function by means of the stationary phase method, which allows us to compute the coefficients of the expansion and to approximate the Green’s function for large values of $x$, $x_3$, $x'$, and $x'_3$.

6. **Conclusion:** We draw some conclusions about the properties of the Green’s function and the behavior of the Schrödinger operator $\mathcal{L}_q$. We also discuss the implications of these results for the study of waveguides with singular potentials.
where
\[
A_i := \begin{pmatrix}
4-\alpha_i\beta_i & -4\beta_i \\
4+\alpha_j\beta_j & 4+\alpha_i\beta_i \\
4+\alpha_j\beta_j & 4+\alpha_i\beta_i
\end{pmatrix} = \begin{pmatrix}
m_{i1} & m_{i2} \\
m_{i1} & m_{i2}
\end{pmatrix},
\]
and \(\alpha_i\beta_i \neq -4\). A domain of operator \(\mathcal{H}_{q_r}\) as an unbounded operator in \(L^2(\mathbb{R})\) is given by
\[
\text{Dom}(\mathcal{H}_{q_r}) = \left\{ u \in L^2(\mathbb{R} \setminus \{0, h\}) : \begin{pmatrix}
-u'(x_i^+) \\
u'(x_i^-)
\end{pmatrix} = A_i \begin{pmatrix}
u(x_i^+) \\
u'(x_i^-)
\end{pmatrix}, \quad i = 1, 2, \right\},
\]
where \(u(x_i^+)\) and \(u'(x_i^+)\) denote the one-side limits of \(u\) and \(u'\) at \(x_i\) if exist, respectively, being \(x_1 = 0\) and \(x_2 = h\). If potential \(q_r\) is real-valued, and matrices \(A_i\) are real such that \(\det A_i = 1\), \(i = 1, 2\), then operator \(\mathcal{H}_{q_r}\) is self-adjoint in \(L^2(\mathbb{R})\). We say that \(\mathcal{H}_{q_r}\) is a self-adjoint extension of Schrödinger operator \(\mathcal{L}_{q_r}\) [20].

2.1. Normalized eigenfunctions of operator \(\mathcal{H}_{q_r}\).
If potential \(q_r\) is attractive then operator \(\mathcal{H}_{q_r}\) has negative eigenvalues of the form \(\lambda_j = -k_j^2\), where \(k_j > 0\) \((j = 1, \cdots, m)\) are zeros of the dispersion equation \(\eta(k) = 0\), where
\[
\eta(k) := (m_{21}^2 + km_{11}^2) v(h; k) + (m_{22}^2 + km_{12}^2) v'(h; k),
\]
and \(v\) is a particular solution of the equation \(\mathcal{L}_{q_r}v = -k^2v\), \(x \in (0, h)\), subjected to the point conditions at \(x = 0\). The solutions
\[
\Psi_j(x) = \frac{1}{M_j} \begin{cases}
e^{k_j x} v(x; k_j), & x < 0 \\
0, & 0 < x < h \\
e^{-k_j x} a_0(k_j), & x > h
\end{cases}
\]
are the normalized eigenfunctions of operator \(\mathcal{H}_{q_r}\), where
\[
a_0(k) := -\frac{e^{kh}}{2k} \left( (m_{21}^2 - km_{11}^2) v(h; k) + (m_{22}^2 - km_{12}^2) v'(h; k) \right),
\]
and \(M_j (j = 1, \cdots, m)\) are normalization constants such that
\[
\int_{\mathbb{R}} |\Psi_j(x)|^2 \, dx = 1.
\]

2.2. Normalized generalized eigenfunctions of the operator \(\mathcal{H}_{q_r}\).
Bounded solutions of \(\mathcal{L}_{q_r} \varphi = \lambda \varphi, \ x \in \mathbb{R} \setminus \{0, h\}\) corresponding to \(\lambda = \kappa^2\), \(\kappa > 0\), and satisfying the point conditions at \(x = \{0, h\}\) are called generalized eigenfunctions of the operator \(\mathcal{H}_{q_r}\). At \(x \to \infty\), a Jost solution of the Schrödinger equation
\[
-d^2 \varphi(x) \begin{array}{c}
+ q_r(x) \varphi(x) = \kappa^2 \varphi(x), \quad x \in \mathbb{R} \setminus \{0, h\}
\end{array}
\]
is given by the function \(\varphi(x, \kappa) = \e^{\i \kappa x}\). There exist coefficients \(a_1\) and \(b_1\) such that the function \(\varphi(x, \kappa) = a_1(\kappa) \e^{\i \kappa x} + b_1(\kappa) \e^{-\i \kappa x}\) satisfies equation (5) in \(x < 0\). Then a first family of normalized generalized eigenfunctions of operator \(\mathcal{H}_{q_r}\) is [21]
\[
\Phi_{01}(x, \kappa) = \frac{1}{\sqrt{2\pi a_1(\kappa)}} \begin{cases}
a_1(\kappa) \e^{\i \kappa x} + b_1(\kappa) \e^{-\i \kappa x}, & x < 0 \\
\phi_{01}(x; \kappa), & 0 < x < h \\
e^{\i \kappa x}, & x > h
\end{cases}
\]
where \( \phi_0 \) is a particular solution of the equation \( L_q \phi_0 = \kappa^2 \phi_0, \ x \in (0, h) \), satisfying the point conditions at \( x = h \). Boundary conditions at \( x = 0 \) give the coefficients

\[
a_1 (\kappa) = -\frac{1}{2i\kappa} ((m_{12}^1 - im_{12}^2) \phi_0 (0; \kappa) - (m_{11}^1 - im_{12}^1) \phi_0' (0; \kappa)), \\
b_1 (\kappa) = -\frac{1}{2i\kappa} ((m_{11}^2 + im_{12}^1) \phi_0' (0; \kappa) - (m_{21}^2 + im_{22}^2) \phi_0 (0; \kappa)).
\]

On the other hand, a Jost solution of Schrödinger equation (5) as \( x \to -\infty \) is \( \varphi (x, \kappa) = e^{-i\kappa x} \). There exist coefficients \( a_2 \) and \( b_2 \) such that \( \varphi (x, \kappa) = a_2 (\kappa) e^{-i\kappa x} + b_2 (\kappa) e^{+i\kappa x} \) satisfies equation (5) in \( x > h \). Hence a second family of normalized generalized eigenfunctions of operator \( H_q \) is

\[
\Phi_{02} (x, \kappa) = \begin{cases} \frac{1}{\sqrt{2\pi a_2 (\kappa)}} e^{-i\kappa x}, & x < 0 \\ \phi_0 (x; \kappa), & 0 < x < h \\ a_2 (\kappa) e^{-i\kappa x} + b_2 (\kappa) e^{+i\kappa x}, & x > h \end{cases}
\]

where \( \phi_0 \) is a particular solution of the equation \( L_q \phi_0 = \kappa^2 \phi_0, \ x \in (0, h) \), satisfying the point conditions at \( x = 0 \). Boundary conditions at \( x = h \) give the coefficients

\[
a_2 (\kappa) = -\frac{e^{i\kappa h}}{2i\kappa} ((m_{12}^1 - im_{12}^2) \phi_0 (h; \kappa) - (m_{22}^2 - im_{12}^1) \phi_0' (h; \kappa)), \\
b_2 (\kappa) = \frac{e^{-i\kappa h}}{2i\kappa} ((m_{11}^2 + im_{12}^1) \phi_0 (h; \kappa) + (m_{21}^2 + im_{22}^2) \phi_0' (h; \kappa)).
\]

Note that solutions \( \Phi_{01}, \Phi_{02} \notin \text{Dom}(H_q) \), but are bounded provided that \( \kappa \in \mathbb{R} \).

**Theorem 1** [22, p. 328]. The system of normalized eigenfunction and normalized generalized eigenfunctions

\[
\{ \Psi_j (x) \}_{j=1}^m, \quad \{ \Phi_{01} (x, \kappa), \Phi_{02} (x, \kappa) \}_{\kappa \geq 0}
\]

is orthonormal. This means that

\[
\int_{\mathbb{R}} \Psi_i (x) \overline{\Psi_j (x)} \, dx = \delta_{ij}; \quad \int_{\mathbb{R}} \Phi_{0n} (x, \kappa_1) \overline{\Phi_{0n} (x, \kappa_2)} \, dx = \delta (\kappa_1 - \kappa_2), \ n = 1, 2; \\
\int_{\mathbb{R}} \Phi_{01} (x, \kappa) \overline{\Phi_{02} (x, \kappa)} \, dx = 0; \quad \int_{\mathbb{R}} \Psi_j (x) \overline{\Phi_{0n} (x, \kappa)} \, dx = 0, \ j = 1, \ldots, m, \ n = 1, 2,
\]

where the bar denotes complex conjugation. Moreover system (6) is complete in \( L^2 (\mathbb{R}) \). Hence, every function \( f \in L^2 (\mathbb{R}) \) can be represented in the form

\[
f (x) = \sum_{j=1}^m f_j \Psi_j (x) + \int_{0}^{+\infty} \tilde{f}_1 (\kappa) \Phi_{01} (x, \kappa) \, d\kappa + \int_{0}^{+\infty} \tilde{f}_2 (\kappa) \Phi_{02} (x, \kappa) \, d\kappa,
\]

where

\[
f_j = \int_{\mathbb{R}} f (x) \overline{\Psi_j (x)} \, dx, \ j = 1, \ldots, m; \quad \tilde{f}_n (\kappa) = \int_{\mathbb{R}} f (x) \overline{\Phi_{0n} (x, \kappa)} \, dx, \ n = 1, 2.
\]

**Corollary 1.** The Dirac distribution \( \delta (x - x') \) admits the formal expansion

\[
\delta (x - x') = \sum_{j=1}^m \Psi_j (x) \overline{\Psi_j (x')} + \int_{0}^{+\infty} \Phi_{01} (x, \kappa) \overline{\Phi_{01} (x', \kappa)} \, d\kappa + \int_{0}^{+\infty} \Phi_{02} (x, \kappa) \overline{\Phi_{02} (x', \kappa)} \, d\kappa.
\]

The distributional sense of this expression is due to the fact that integrals in the right-hand side are divergent.
3. Eigenfunction expansion for the Green’s function of the waveguide

Let us assume that the point source \( \delta(x - x', x_3 - x_3') \) does not lie on the cladding-core interfaces, i.e., \( x_3' \neq \{0, h\} \). The wavefunction \( g \) generated by this point source is formally described by the equation

\[
\left( -\Delta_x + \mathcal{L}_q \left( x_3, \frac{\partial}{\partial x_3} \right) - \mu^2 \right) g \left( x, x_3; x', x_3' \right) = \delta \left( x - x', x_3 - x_3' \right), \quad (x, x_3) \in \mathbb{R}^3,
\]

where \( \mu^2 = \mathcal{E} \) is the energy parameter, operator \( \mathcal{L}_q \) is defined in expression (2), and \( q = q_r + q_s \). The solution \( g \) represents the Green’s function of the operator \( \left( \mathcal{S}_q - \mu^2 \right) \). Observe that if \( (x, x_3) \neq (x', x_3') \) previous equation is equivalent to Schrödinger equation (1).

A self-adjoint extension of the singular operator \( \mathcal{L}_q \) is constructed according to the guidelines of Section 2. This extension leads to the boundary-value problem

\[
\begin{align*}
\left( -\Delta_x + \mathcal{H}_{q_r} \left( x_3, \frac{\partial}{\partial x_3} \right) - \mu^2 \right) G \left( x, x_3; \mathbf{x}', x_3' \right) &= \delta \left( x - \mathbf{x}', x_3 - x_3' \right), \quad (x, x_3) \in \Pi, \quad (7a) \\
\begin{pmatrix}
G(\mathbf{x}, 0^+) \\
G_x'(\mathbf{x}, 0^+)
\end{pmatrix} &= A_1 \begin{pmatrix}
G(\mathbf{x}, 0^-) \\
G_x'(\mathbf{x}, 0^-)
\end{pmatrix}, \quad \begin{pmatrix}
G(\mathbf{x}, h^+) \\
G_x'(\mathbf{x}, h^+)
\end{pmatrix} = A_2 \begin{pmatrix}
G(\mathbf{x}, h^-) \\
G_x'(\mathbf{x}, h^-)
\end{pmatrix}, \quad (7b)
\end{align*}
\]

where \( \Pi := \Pi_0 \cup \Pi_{0,h} \cup \Pi_{h} \) represents the strata of the waveguide. The matrices \( A_i (i = 1, 2) \) defined in (3) convey the information of singular potential \( q_s \) supported at \( x_3 = \{0, h\} \).

Let us introduce the Fourier transform with respect to \( x \in \mathbb{R}^2 \), defined by

\[
\hat{\varphi}(\xi) := \int_{\mathbb{R}^2} \varphi(x) e^{i(\xi \cdot x)} dx,
\]

where \( \xi = (\xi_1, \xi_2) \in \mathbb{R}^2 \), and \( (\xi, \mathbf{x}) := x_1 \xi_1 + x_2 \xi_2 \) is the scalar product of vectors \( \xi \) and \( \mathbf{x} \). The application of Fourier transform to (7) gives the boundary-value problem

\[
\begin{align*}
\left( |\xi|^2 + \mathcal{H}_{q_r} - \mu^2 \right) \hat{G}(\xi, x_3; \mathbf{x}', x_3') &= e^{i(\xi \cdot \mathbf{x}')} \delta \left( x_3 - x_3' \right), \quad x_3 \in \mathbb{R} \setminus \{0, h\}, \quad \xi \in \mathbb{R}^2, \quad (8a) \\
\begin{pmatrix}
\hat{G}(\xi, 0^+) \\
\hat{G}_x'(\xi, 0^+)
\end{pmatrix} &= A_1 \begin{pmatrix}
\hat{G}(\xi, 0^-) \\
\hat{G}_x'(\xi, 0^-)
\end{pmatrix}, \quad \begin{pmatrix}
\hat{G}(\xi, h^+) \\
\hat{G}_x'(\xi, h^+)
\end{pmatrix} = A_2 \begin{pmatrix}
\hat{G}(\xi, h^-) \\
\hat{G}_x'(\xi, h^-)
\end{pmatrix}.
\end{align*}
\]

From Theorem 1 the distribution \( \hat{G} \) can be expanded in terms of the eigenfunctions and generalized eigenfunctions of operator \( \mathcal{H}_{q_r} \) as

\[
\hat{G}(\xi, x_3; \mathbf{x}', x_3') = \sum_{j=1}^{m} A_j \psi_j(x_3) + \int_{\mathbb{R}^+} B_\kappa \Phi_{01}(x_3; \kappa) d\kappa + \int_{\mathbb{R}^+} C_\kappa \Phi_{02}(x_3; \kappa) d\kappa,
\]

where \( A_j = A_j(\xi; \mathbf{x}', x_3') \), \( B_\kappa = B_\kappa(\xi; \mathbf{x}', x_3') \), and \( C_\kappa = C_\kappa(\xi; \mathbf{x}', x_3') \) are coefficients to be determined. By making formal operations, the left-hand side of equation (8a) reads

\[
\begin{align*}
\left( |\xi|^2 + \mathcal{H}_{q_r} - \mu^2 \right) \hat{G}(\xi, x_3; \mathbf{x}', x_3') &= \sum_{j=1}^{m} A_j \left( \xi^2 - k_j^2 - \mu^2 \right) \psi_j(x_3) \\
&\quad + \int_{\mathbb{R}^+} \left( |\xi|^2 + \kappa^2 - \mu^2 \right) \left( B_\kappa \Phi_{01}(x_3; \kappa) + C_\kappa \Phi_{02}(x_3; \kappa) \right) d\kappa.
\end{align*}
\]
Next we use Corollary 1 to expand the right-hand side of equation (8a). By matching similar terms in the resulting expansions we obtain the sought coefficients, which gives the expansion

\[
\hat{G}(\xi, x_3; x'_3) = \sum_{j=1}^{m} \frac{e^{i(\xi x_3')}}{\xi^2 - \kappa_j^2 - \mu^2} \Psi_j(x_3) + \int_{\mathbb{R}^+} \frac{e^{i(\xi x_3')}}{\xi^2 + \kappa^2 - \mu^2} \Phi_{01}(x_3; \kappa) \, d\kappa + \int_{\mathbb{R}^+} \frac{e^{i(\xi x_3')}}{\xi^2 + \kappa^2 - \mu^2} \Phi_{02}(x_3; \kappa) \, d\kappa.
\]

On applying the inverse Fourier transform to above expression we obtain the Green’s function of the waveguide

\[
G(x, x_3; x', x'_3) = \sum_{j=1}^{m} g_j(\|x - x'\|, x_3; x'_3) + g_{01}(\|x - x'\|, x_3; x'_3) + g_{02}(\|x - x'\|, x_3; x'_3),
\]

where

\[
g_j(\|x - x'\|, x_3; x'_3) := \frac{1}{4} H_0^{(1)} \left( \sqrt{\mu^2 + \kappa_j^2} \right) \Psi_j(x_3) \Psi_j(x_3), \quad j = 1, \ldots, m,
\]

\[
g_{0n}(\|x - x'\|, x_3; x'_3) := \int_{\mathbb{R}^+} \frac{1}{4} H_0^{(1)} \left( \sqrt{\mu^2 + \kappa^2} \right) \Phi_{02}(x'_3; \kappa) \Phi_{02}(x_3; \kappa) \, d\kappa, \quad n = 1, 2,
\]

and \(H_0^{(1)}\) denotes the Hankel function of the first kind and zero order.

4. Asymptotic analysis of the Green function

In the expansion of the Green’s function we can distinguish two main processes, namely, the bound states \(g_j\) \((j = 1, \ldots, m)\), which are analogous to the guided modes of an electromagnetic waveguide, and the lateral waves \(g_{0n}\) \((n = 1, 2)\), [23]. Let us consider the asymptotic behavior of the Hankel function \(H_0^{(1)}\) (see, e.g. [24]),

\[
H_0^{(1)}(\rho) \sim \sqrt{\frac{2}{\pi \rho}} e^{i(\rho - \frac{\pi}{2})}, \quad |\rho| \to \infty,
\]

where \(\rho \in \mathbb{C}\) lies in the branch defined by \(-\pi < \arg(\rho) < 2\pi\). Hence, the asymptotics of the bound states and lateral waves as \(\|x - x'\| \to \infty\) are

\[
g_j(\|x - x'\|, x_3; x'_3) \sim \frac{e^{i\left(\sqrt{\kappa_j^2 + \mu^2} \|x - x'\| + \frac{\pi}{2}\right)}}{\sqrt{2\pi} \sqrt{\kappa_j^2 + \mu^2}} \Psi_j(x_3) \Psi_j(x_3), \quad j = 1, \ldots, m,
\]

\[
g_{0n}(\|x - x'\|, x_3; x'_3) \sim \frac{1}{4} \sqrt{\frac{2}{\pi \|x - x'\|}} e^{-i\frac{\pi}{2}} \int_{\mathbb{R}^+} \frac{\Phi_{0n}(x_3; \kappa) \Phi_{0n}(x'_3; \kappa)}{\sqrt{\mu^2 + \kappa^2} \|x - x'\|} d\kappa,
\]

with \(n = 1, 2\). These integrals represent a superposition of scattering states as the parameter \(\kappa\) takes values in the interval \([0, \infty)\).

Let us analyze the asymptotics of these integrals by means of the stationary phase method. We identify the real-valued function \(S(\kappa) := \sqrt{\mu^2 + \kappa^2}\) as the phase function of the oscillatory integral. Non-degenerate stationary points \(\kappa_j\) satisfy the equation \(S'(\kappa_j) = 0\), and \(S''(\kappa_j) \neq 0\).
It follows that $S$ has only one non-degenerate stationary point, namely, $\kappa_0 = 0$. The contribution of this point in the asymptotics of the integrals as $|\mathbf{x} - \mathbf{x}'| \to \infty$ is [25, p. 29]:

$$g_{0n}(|\mathbf{x} - \mathbf{x}'|, \mathbf{x}_3; \mathbf{x}_3') \sim \frac{\mu^3e^{-i\frac{\pi}{4}}\phi_{0n}(\mathbf{x}_3; 0)\overline{\phi_{0n}}(\mathbf{x}_3'; 0)}{4\pi\mu(0)} e^{i\mu|\mathbf{x} - \mathbf{x}'|/\mu}, \quad n = 1, 2,$$

where

$$p(\kappa) := \left((m_{21}^1)^2 + (\kappa m_{22}^1)^2\right)|\phi_{0n}(0; \kappa)|^2 + \left((m_{11}^1)^2 + (\kappa m_{12}^1)^2\right)|\phi_{0n}'(0; \kappa)|^2 - (m_{21}^1 m_{11}^1 - i\kappa + \kappa^2 m_{22}^1 m_{12}^1) \phi_{0n}(0; \kappa) \overline{\phi_{0n}}(0; \kappa) - (m_{21}^1 m_{11}^1 + i\kappa + \kappa^2 m_{22}^1 m_{12}^1) \phi_{0n}(0; \kappa) \phi_{0n}'(0; \kappa).$$

The lateral waves behave as $O(|\mathbf{x} - \mathbf{x}'|^{-2})$, hence these are negligible at great distances from the source. On the other hand the bound states behave as $O(|\mathbf{x} - \mathbf{x}'|^{-1/2})$ as $|\mathbf{x} - \mathbf{x}'| \to \infty$. Therefore a superposition of these waves gives the leading term of the asymptotics of the Green’s function, that is

$$G(\mathbf{x}, \mathbf{x}_3; \mathbf{x}_3') \sim \sum_{j=1}^{m} e^{i\left(\sqrt{k_j^2 + \mu^2}|\mathbf{x} - \mathbf{x}'| + \frac{\pi}{2}\right)} \frac{\Psi_j(\mathbf{x}_3') \Psi_j(\mathbf{x}_3)}{\sqrt{|\mathbf{x} - \mathbf{x}'|}}.$$

5. Numerical examples

The leading term of the asymptotics of the Green’s function is constructed from the eigenfunctions $\Psi_j$ of the one-dimensional Schrödinger operator $\mathcal{H}_q$, which are defined in (4). These eigenfunctions are constructed from the solution $v$ of the Schrödinger equation

$$-\frac{d^2}{dx_3^2} v(x_3) + V(x_3) v(x_3) = -k^2 v(x_3), \quad 0 < x_3 < h,$$

which involves the potential $V$ supported in the core of the waveguide. Not always it is possible to find exact solutions of Schrödinger equation (9) for a given potential $V$. Indeed, numerical solutions are at hand most of the times. However, in this work we use the SPPS method [26] to determine the solution $v$ in an exact way.

Let $v_0$ be a non-vanishing solution of the homogeneous equation $-v''_0(x_3) + V(x_3) v_0(x_3) = 0$, $0 < x_3 < h$. Then the power series [26]:

$$v_1 = v_0 \sum_{n=0}^{\infty} (-1)^n k^{2n} \tilde{X}^{(2n)}; \quad v_2 = v_0 \sum_{n=0}^{\infty} (-1)^n k^{2n} X^{(2n+1)},$$

with the functions $\tilde{X}^{(n)}$ and $X^{(n)}$ defined by the recursive integration procedure

$$\tilde{X}^{(0)} \equiv 1, \quad \tilde{X}^{(n)}(x_3) = \begin{cases} \int_0^{x_3} \tilde{X}^{(n-1)}(s) v_0^2(s) \, ds, & n \text{ odd} \\ -\int_0^{x_3} \tilde{X}^{(n-1)}(s) v_0^{-2}(s) \, ds, & n \text{ even} \end{cases},$$

$$X^{(0)} \equiv 1, \quad X^{(n)}(x_3) = \begin{cases} -\int_0^{x_3} X^{(n-1)}(s) v_0^{-2}(s) \, ds, & n \text{ odd} \\ \int_0^{x_3} X^{(n-1)}(s) v_0^2(s) \, ds, & n \text{ even} \end{cases}.$$
are linearly independent solutions of Schrödinger equation (9). Moreover, series (10) converge uniformly in \([0, h]\). Note that function \(v_0\) can also be calculated with the SPPS method [27].

The solution \(v\) can be represented as a linear combination of the series \(v_1\) and \(v_2\) as

\[
v(x_3) = c_1(k) v_1(x_3) + c_2(k) v_2(x_3),
\]

where coefficients \(c_1\) and \(c_2\) are defined by

\[
c_1(k) := v_0^{-1}(0) \left( m_{11}^1 + km_{12}^1 \right) \quad c_2(k) := -v_0(0) \left( m_{21}^1 + km_{22}^1 \right) + v_0(0) \left( m_{11}^1 + km_{12}^1 \right).
\]

5.1. The SPPS form of the dispersion equation

The leading term of the Green’s function involves the numbers \(k_j\), which are the zeros of the dispersion equation \(\eta(k) = 0\). From the SPPS solutions of Schrödinger equation (9) it is possible to obtain a SPPS representation of the characteristic function, namely

\[
\eta(k) = -\frac{\left( m_{22}^2 + km_{12}^2 \right)}{\nu_0(k)} \left[ c_1(k) \sum_{n=1}^{\infty} (-1)^n k^{2n} X^{(2n-1)}(h) + c_2(k) \sum_{n=0}^{\infty} (-1)^n k^{2n} X^{(2n)}(h) \right] \\
+ \left[ c_1(k) \sum_{n=0}^{\infty} (-1)^n k^{2n} X^{(2n)}(h) + c_2(k) \sum_{n=0}^{\infty} (-1)^n k^{2n} X^{(2n+1)}(h) \right] X_{\nu}(2)
\]

From a numerical point of view the above convergent series must be truncated up to \(M\) terms. Let \(\eta_M(k)\) be the truncated version of \(\eta(k)\). If \(\beta_j\) is a polynomial root of \(\eta_M(k) = 0\) that satisfy \(\text{Re}\{\beta_j\} > 0\) and \(|\text{Im}\{\beta_j\}| < \varepsilon\) for a given a small \(\varepsilon > 0\), then \(\tilde{k}_j = \text{Re}\{\beta_j\}\) is an approximation of \(k_j\), and \(\tilde{\lambda}_j = -\tilde{k}_j^2\) is an approximate eigenvalue \(\lambda_j\) of the Schrödinger operator \(\mathcal{H}_q\).

Example 1. Let us consider the regular potential

\[
q_r(x_3) = \begin{cases} 
-10, & 0 < x_3 < 1 \\
0, & \text{elsewhere} 
\end{cases}
\]

and let the singular potential be given by

\[
q_s(x_3) = \delta(x_3) + \delta'(x_3) + \delta(x_3 - 1) + \delta'(x_3 - 1).
\]

In this case it is possible to obtain a closed-form expression of the characteristic function, namely

\[
\eta(k) = \tan(r) - \frac{r(k)}{r^2(k)} \left( m_{21}^2 + km_{11}^2 \right) \left( m_{11}^1 + km_{12}^1 \right) + \left( m_{22}^2 + km_{12}^2 \right) \left( m_{21}^1 + km_{22}^1 \right),
\]

where \(r(k) := \sqrt{10 - k^2}\), \(k^2 \leq 10\). Zeros of the exact dispersion equation \(\eta(k) = 0\) were numerically calculated with the instruction \texttt{NSolve[]} in Mathematica. The characteristic function for this problem was also obtained in a SPPS form according to \(11\). The polynomial roots of \(\eta_M(k) = 0\) were calculated with the instruction \texttt{FindRoot[]} . The result from both approaches are shown in Table 1, and the plots of the eigenfunctions of operator \(\mathcal{H}_q\) are shown in Figure 1. It is worth mentioning that finding all the zeros of the characteristic function \(13\) with the instruction \texttt{NSolve[]} required a higher precision than for the polynomial roots of equation \(11\).
Table 1. Zeros of the dispersion equation \( \eta (k) = 0 \) of Example 1.

| \( j \) | \( k_j \), SPPS | \( k_j \), NSolve[] |
|---|---|---|
| 1 | 0.733476697535 | 0.733476697536 |
| 2 | 2.717703561053 | 2.717703561051 |
| 3 | 3.162277660167 | 3.162277660168 |
| 4 | 3.639303187042 | 3.6393031870501 |

Figure 1. Eigenfunctions of operator \( \mathcal{H}_{q_r} \) from Example 1 associated to the polynomial roots: a) \( k_1 = 0.733476697535 \), b) \( k_2 = 2.717703561053 \), c) \( k_3 = 3.162277660168 \), d) \( k_4 = 3.639303187042 \).

Next we show the plots of the asymptotics of individual modes and Green’s function of the waveguide on the plane \( x_2 = 0 \). We consider that the source of particles is located at \( x_1' = -1000 \) and \( x_3' = 0.5 \), and the energy of the system is \( E = 25 \), (that is \( \mu = 5 \)). In Figures 2 and 3, we observe the resulting plots.

Example 2. From Example 1, let the regular potential be slightly perturbed as

\[
q_r (x_3) = \begin{cases} 
-10 - 0.5 \cos (2\pi x_3), & 0 < x_3 < 1 \\
0, & \text{elsewhere}
\end{cases}
\]

and the singular potential remains the same as in (12). Though it is possible to obtain a closed-form expression for the dispersion equation in terms of special functions, we use the SPPS approach. In this case the polynomial roots of the characteristic polynomial were calculated with the instruction \texttt{FindRoot[]} . In order to compare the results we numerically solve Schrödinger equation (9) by letting \( k \) to take values from a prescribed discrete set \( K \). For each \( k_n \in K \) Schrödinger equation (9) was solved with the instruction \texttt{NDSolve[]} . The approximate resulting solution \( \tilde{\psi} (x_3; k_n) \) and its derivative \( \tilde{\psi}' (x_3; k_n) \) were evaluated at \( x_3 = h \). This gives the discrete sets \( \{ \tilde{\psi} (h; k_n) \} \), \( \{ \tilde{\psi}' (h; k_n) \} \), which were interpolated as functions of \( k \in K \). These interpolating functions are then used in the dispersion equation whose zeros are shown in Table 2. The eigenfunctions of this perturbed problem can be seen in Figure 4.
Figure 2. Real parts of the bound states (guided modes) associated with the polynomial roots from Example 1: a) $k_1 = 0.73476697535$, b) $k_2 = 2.717703561053$, c) $k_3 = 3.162277660168$ and d) $k_4 = 3.639303187042$. Horizontal axes correspond to $x_1$ and vertical axes to $x_3$.

Figure 3. Real part of the asymptotics of the Green function from Example 1 in the far field region. Horizontal axis corresponds to $x_1$ and the vertical axis to $x_3$.

Table 2. Zeros of the dispersion equation $\eta(k) = 0$ from Example 2.

| $j$ | $k_j$, SPPS | $k_j$, NDSolve[] |
|-----|--------------|------------------|
| 1   | 0.724086932880 | 0.7240869130043  |
| 2   | 2.755872222425  | 2.7558722259921  |
| 3   | 3.649462812310  | 3.6494628184451  |

In Figure 5 we observe the plots of the asymptotics of the bound states (guided modes) and the Green’s function on the plane $x_2 = 0$, where the point source is located at $x'_1 = -1000 y$. 
Figure 4. Eigenfunctions of operator $H_{qr}$ from Example 2 associated to the polynomial roots: a) $k_1 = 0.724086932880$, b) $k_2 = 2.755872222425$, c) $k_3 = 3.649462812310$.

$x_3' = 0.1$. These plots correspond to $\mu = 5$.

Figure 5. Real parts of the bound states (guided modes) of the Green’s function from Example 2 associated with the polynomial roots: a) $k_1 = 0.724086932880$, b) $k_2 = 2.755872222425$, c) $k_3 = 3.649462812310$. d) Real part of the asymptotics of the Green’s function. Horizontal axes correspond to $x_1$ and vertical axes to $x_3$.

6. Conclusions

From the obtained results we can conclude that the lateral waves have a negligible behavior at long distances from the source of particles. Hence, the leading term of the Green’s function of the quantum waveguide consists of a superposition of bound states. As was shown previously the eigenfunctions of operator $H_{qr}$ can be discontinuous at the points where interactions are supported. The zero crossings of the eigenfunctions of the one-dimensional problem do not fulfill Sturm oscillation theorem [28] as can be seen in previous Figures 1 and 4. This of course is an interesting result that must be investigated in more depth. We have the hypothesis that this is due to the fact that the obtained eigenfunctions are not regular solutions but generalized solutions that should be treated in the sense of distributions. Finally, we have observed that even if the potential function has an identically vanishing regular potential $q_r \equiv 0$ the Green’s
function still remains in the form of a wave-packet solution since the particles continue to interact with the singular potential.

Acknowledgments
VBF acknowledges CONACyT for support via grant 283133.

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