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Green's function for the Schrödinger equation with a generalized point interaction and stability of superoscillations

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Abstract

In this paper we study the time dependent Schrödinger equation with all possible self-adjoint singular interactions located at the origin, which include the δ and δ'-potentials as well as boundary conditions of Dirichlet, Neumann, and Robin type as particular cases. We derive an explicit representation of the time dependent Green's function and give a mathematical rigorous meaning to the corresponding integral for holomorphic initial conditions, using Fresnel integrals. Superoscillatory functions appear in the context of weak measurements in quantum mechanics and are naturally treated as holomorphic entire functions. As an application of the Green's function we study the stability and oscillatory properties of the solution of the Schrödinger equation subject to a generalized point interaction when the initial datum is a superoscillatory function.

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Contents

1. Introduction

The main purpose of this paper is to study the Green's function of the time dependent Schrödinger equation subject to general self-adjoint point interactions located at the origin, and to prove stability results for the solutions corresponding to superoscillating initial data. As a consequence of our detailed analysis we also obtain an explicit expression and asymptotic expansion of the time dependent plane wave solution, which allows to discuss the oscillatory properties of the time evolution of superoscillations under generalized point interactions.

Strongly localized potentials, also called pseudo-potentials or nowadays better known as δ-potentials, were already considered by Kronig and Penney in [46] and Fermi in [40]. Heuristically speaking, these δ-potentials are represented by the Hamiltonian

$$H = -\Delta + \sum_{y \in Y} c_y \, \delta(x - y), \tag{1.1}$$

where $c_y \, \delta(x - y)$ is a point source of strength c_y located at the point $y \in \mathbb{R}^d$, $d \geq 1$. The δ-potentials may form a discrete set, e.g., a periodic lattice $Y = \mathbb{Z}^d$, or a single point $Y = \{0\}$. The rigorous mathematical meaning of the Hamiltonian (1.1) was given only much later by Berezin and Faddeev in [22].

In this paper we will restrict ourselves to a single point interaction in $\mathbb{R}$ and hence assume $Y = \{0\}$ and $d = 1$ from now on. In this context H in (1.1) is defined as a proper self-adjoint extension of the symmetric operator $-\Delta$ on $C_0^\infty(\mathbb{R} \setminus \{0\})$ which corresponds to interface (or jump) conditions at the origin of the form

$$\begin{aligned} u(0^+) &= u(0^-), \\ u'(0^+) - u'(0^-) &= c_0 \, u(0); \end{aligned} \tag{1.2}$$

a detailed discussion can be found in the standard monograph [16]. Besides the δ-potential also other types of self-adjoint interface conditions can be treated (see [13,32,35,36,38,44,51,53] and [21,39,50] for interactions on hypersurfaces), among them so-called δ'-potentials and further generalizations, as well as decoupled systems with Dirichlet, Neumann, or Robin conditions. There are various ways to describe the complete family of self-adjoint interface conditions at the origin and for our purposes it is convenient to use the parametrization

$$(I - J) \begin{pmatrix} u(0^+) \\ u(0^-) \end{pmatrix} = i(I + J) \begin{pmatrix} u'(0^+) \\ -u'(0^-) \end{pmatrix} \tag{1.3}$$

with unitary 2×2-matrices J (see Example 3.2 for identifying (1.2) as a special case of (1.3)) and I denoting the 2×2 identity matrix. To be more precise: The class of jump conditions (1.3) coincides with the class of self-adjoint interface conditions at the point 0. In other words, each unitary matrix $J \in \mathbb{C}^{2\times 2}$ leads to a self-adjoint realization of the Laplacian in $L^2(\mathbb{R})$ with a generalized point interaction supported at the point 0, and conversely, for each self-adjoint Laplacian in $L^2(\mathbb{R})$ with a generalized point interaction supported at the point 0 there exists a unitary matrix $J \in \mathbb{C}^{2\times 2}$ such that the interface condition has the form (1.3); cf. [20, Chapter 2.2].

An important problem we study in this paper is the time dependent Schrödinger equation with holomorphic initial datum F subject to a general self-adjoint singular interaction supported at the origin, that is, we consider

$$i\frac{\partial}{\partial t}\Psi(t,x) = -\frac{\partial^2}{\partial x^2}\Psi(t,x), \qquad t > 0,\ x \in \mathbb{R}\setminus\{0\}, \tag{1.4a}$$

$$(I-J)\begin{pmatrix}\Psi(t,0^+)\\ \Psi(t,0^-)\end{pmatrix} = i(I+J)\begin{pmatrix}\frac{\partial}{\partial x}\Psi(t,0^+)\\ -\frac{\partial}{\partial x}\Psi(t,0^-)\end{pmatrix}, \qquad t > 0, \tag{1.4b}$$

$$\Psi(0^+,x) = F(x), \qquad x \in \mathbb{R}\setminus\{0\}. \tag{1.4c}$$

It will be shown in Section 2 that the corresponding Green's function is given by

$$\begin{aligned} G(t,x,y) = &\left(\mu_+^{(x,y)}\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}} + \omega_+\sqrt{it}\right) + \mu_-^{(x,y)}\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}} + \omega_-\sqrt{it}\right)\right)e^{-\frac{(|x|+|y|)^2}{4it}} \\ &+ \frac{1}{2\sqrt{i\pi t}}\left(\mu_0^{(x,y)}e^{-\frac{(|x|+|y|)^2}{4it}} + e^{-\frac{(x-y)^2}{4it}}\right), \qquad t>0,\ x,y \in \mathbb{R}\setminus\{0\}, \end{aligned} \tag{1.5}$$

where the entire function Λ is defined in (2.2) and the coefficients $\mu_\pm$, μ_0, and $\omega_\pm$ are explicitly determined in terms of the entries of the unitary matrix J in the jump condition (1.4b); cf. Theorem 2.4, the examples in Section 3, and [14,15,43,49,54] for related results. Using the Green's function (1.5) the solution Ψ of (1.4) can be written as the integral

$$\Psi(t,x) = \int_{\mathbb{R}} G(t,x,y)F(y)dy, \qquad t>0,\ x \in \mathbb{R}\setminus\{0\}. \tag{1.6}$$

While this integral is well defined for compactly supported continuous functions F, one has difficulties in making sense of (1.6) already for plane waves $F(x) = e^{ikx}$. A mathematically rigorous analysis of this issue for a certain class of holomorphic functions with growth condition is provided in Section 4, where the main tool is the Fresnel integral approach.

The general results in Section 2 and Section 4 are applied to superoscillations in Section 5. Superoscillating functions are band-limited functions that can oscillate faster than their fastest Fourier component. They appear in quantum mechanics as results of weak measurements and, in particular, their time evolution under the Schrödinger equation is of crucial importance, see [1,10,12,31]. For a rigorous treatment of this subject we refer to [2–7,18,19,33] and [8]. These kinds of functions also appear in antenna theory [55] (see also [25]), and various applications in optics were studied by M.V. Berry and many others, see, e.g., [24,26–30,41,42,47,48]. More information can also be found in the introductory papers [9,11,17,45] and in the *Roadmap on superoscillations* [23].

A weak measurement of a quantum observable represented by the self-adjoint operator A, involving a pre-selected state ψ_0 and a post-selected state ψ_1, leads to the weak value

$$A_{weak} := \frac{(\psi_1, A\psi_0)}{(\psi_1, \psi_0)} \in \mathbb{C},$$

where the real part of A_{weak} can be interpreted as the shift and the imaginary part as the momentum of the pointer recording the measurement. An important feature of the weak measurement is that, in contrast with strong measurements $A_{strong} := (\psi, A\psi)/(\psi, \psi)$, the real part of A_{weak} may become very large when the states ψ_0 and ψ_1 are almost orthogonal; this leads to superoscillations. A typical superoscillatory function is

$$F_n(x,k) = \sum_{l=0}^{n} C_l(n,k) e^{i(1-\frac{2l}{n})x}, \qquad x \in \mathbb{R}, \tag{1.7}$$

where $|k| > 1$ and

$$C_l(n,k) = \binom{n}{l} \left(\frac{1+k}{2}\right)^{n-l} \left(\frac{1-k}{2}\right)^{l}.$$

If we let n tend to infinity, we obtain $\lim_{n\to\infty} F_n(x,k) = e^{ikx}$ uniformly for x in compact subsets of $\mathbb{R}$. The notion superoscillations comes from the fact that the frequencies $(1 - \frac{2l}{n})$ in (1.7) are in modulus bounded by 1, but the frequency k of the limit function can be arbitrarily large.

As a consequence of the representation (1.6) of the solution of the Schrödinger equation subject to a general self-adjoint singular interaction we ask: When does a convergent sequence of initial conditions

$$\lim_{n\to\infty} F_n = F \tag{1.8}$$

also lead to a convergent sequence of solutions

$$\lim_{n\to\infty} \Psi(t,x;F_n) = \Psi(t,x;F), \tag{1.9}$$

and which type of convergence should be considered in (1.8) and (1.9)? Our abstract result Theorem 4.6, which is also the bridge to investigate the time evolution of superoscillations in Section 5, shows that (1.9) holds uniformly on compact subsets of $(0,\infty) \times \mathbb{R}$, whenever the sequence $(F_n)_n$ satisfy some exponential boundedness conditions and the convergence in (1.8) is such that

$$\lim_{n\to\infty} \sup_{z \in S_\alpha \cup (-S_\alpha)} \left|F_n(z) - F(z)\right| e^{-C|z|} = 0$$

for some $C \geq 0$ and certain sectors S_α and $-S_\alpha$ in the complex plane; cf. Section 4 for more details. These abstract assumptions are in accordance with the convergence properties of (holomorphic extensions of) superoscillating functions in spaces of entire functions with exponential growth that have been clarified just in the recent years, see [37]. The case of superoscillatory initial data is then discussed in Corollary 5.2 and the explicit form, oscillatory behaviour, and long time asymptotics of the corresponding limit in (1.9) are provided in Proposition 5.3 and Theorem 5.5.

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2. Green's function for the Schrödinger equation with a generalized point interaction

In this section we derive the Green's function of the time dependent Schrödinger equation (1.4) with a generalized singular interaction located at the origin. That is, we construct a function G which depends on the matrix J, such that the solution Ψ of (1.4) can be written in the form

$$\Psi(t,x) = \int_{\mathbb{R}} G(t,x,y)F(y)dy, \qquad t>0,\ x \in \mathbb{R}\setminus\{0\}. \tag{2.1}$$

In Section 4 we shall clarify for which initial conditions F and in which sense this integral is understood. Here, we only want to derive the explicit form and some properties of the Green's function G itself.

We start by defining the entire function

$$\Lambda(z) := e^{z^2}(1-\operatorname{erf}(z)), \qquad z \in \mathbb{C}, \tag{2.2}$$

where $\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-\xi^2}d\xi$ is the well known error function. Some important properties of this function are collected in the following lemma; cf. [19, Lemma 3.1].

Lemma 2.1. *The function Λ in (2.2) has the following properties:*

(i) *The function Λ satisfies the differential equation*

$$\frac{d}{dz}\Lambda(z) = 2z\Lambda(z) - \frac{2}{\sqrt{\pi}}, \qquad z \in \mathbb{C}. \tag{2.3}$$

(ii) *The value of the function Λ at $-z$ is given by*

$$\Lambda(-z) = 2e^{z^2} - \Lambda(z), \qquad z \in \mathbb{C}. \tag{2.4}$$

(iii) *The absolute value of* $\Lambda(z)$ *can be estimated by*

$$|\Lambda(z)| \leq \Lambda(\mathrm{Re}(z)), \qquad z \in \mathbb{C}. \tag{2.5}$$

(iv) *The function* Λ *is monotonically decreasing on* $\mathbb{R}$ *and asymptotically on* $\mathbb{C}$ *one has*

$$\Lambda(z) = \begin{cases} \mathcal{O}\big(\frac{1}{|z|}\big), & \text{if } \mathrm{Re}(z) \geq 0, \\ 2e^{z^2} + \mathcal{O}\big(\frac{1}{|z|}\big), & \text{if } \mathrm{Re}(z) \leq 0, \end{cases} \qquad \text{as } |z| \to \infty. \tag{2.6}$$

(v) *For all* $a > 0$ *and* $b, c \in \mathbb{C}$ *one has the integral identities*

$$\int_0^\infty e^{-ax^2-bx}dx = \frac{\sqrt{\pi}}{2\sqrt{a}}\Lambda\Big(\frac{b}{2\sqrt{a}}\Big), \tag{2.7a}$$

$$\int_0^\infty e^{-ax^2-bx}\Lambda\big(\sqrt{a}\,x + c\big)dx = -\frac{1}{2\sqrt{a}}\begin{cases} \frac{\Lambda(c)-\Lambda(\frac{b}{2\sqrt{a}})}{c-\frac{b}{2\sqrt{a}}}, & \text{if } c \neq \frac{b}{2\sqrt{a}}, \\ \Lambda'(c), & \text{if } c = \frac{b}{2\sqrt{a}}. \end{cases} \tag{2.7b}$$

Proof. (i) and (ii) are contained in [19, Lemma 3.1].

(iii) Using $\int_0^\infty e^{-\xi^2}d\xi = \frac{\sqrt{\pi}}{2}$ in the definition (2.2) gives

$$\Lambda(z) = \frac{2}{\sqrt{\pi}}e^{z^2}\left(\int_0^\infty e^{-\xi^2}d\xi - \int_0^z e^{-\xi^2}d\xi\right). \tag{2.8}$$

Now we use that the complex integral over the entire function $e^{-\xi^2}$ is path independent and that $\lim_{x\to\infty}\int_x^{x+z} e^{-\xi^2}d\xi = 0$. Hence, the two integrals on the right-hand side of (2.8) can be replaced by a path integral from z to ∞, parallel to the real axis. This gives

$$\Lambda(z) = \frac{2}{\sqrt{\pi}}e^{z^2}\int_0^\infty e^{-(z+s)^2}ds = \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-s^2-2zs}ds. \tag{2.9}$$

This representation can now be used to estimate the absolute value

$$|\Lambda(z)| \leq \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-s^2-2\,\mathrm{Re}(z)s}ds = \Lambda(\mathrm{Re}(z)).$$

(iv) The monotonicity is a direct consequence of the representation (2.9) and the asymptotics were shown in [19, Lemma 3.1].

(v) Substituting $t = \frac{s}{\sqrt{a}}$ in the integral (2.9) gives

$$\Lambda(z) = \frac{2\sqrt{a}}{\sqrt{\pi}} \int_0^\infty e^{-at^2 - 2z\sqrt{a}\,t}\, dt,$$

which is exactly (2.7a) if we evaluate at $z = \frac{b}{2\sqrt{a}}$. In order to check (2.7b) we first use (2.3) to obtain for $c \neq \frac{b}{\sqrt{a}}$ the primitive

$$e^{-ax^2-bx}\Lambda\big(\sqrt{a}\,x + c\big) = \frac{1}{2\sqrt{a}}\frac{d}{dx} e^{-ax^2-bx}\,\frac{\Lambda\big(\sqrt{a}\,x+c\big) - \Lambda\big(\sqrt{a}\,x + \frac{b}{2\sqrt{a}}\big)}{c - \frac{b}{2\sqrt{a}}}.$$

The assertion on the integral in (2.7b) now simply follows by evaluating at $x = 0$ and $x \to \infty$; observe that by (2.6) the limit $x \to \infty$ vanishes. Similarly, also in the case $b = 2\sqrt{a}\,c$ we get the primitive

$$e^{-ax^2-2\sqrt{a}\,cx}\Lambda\big(\sqrt{a}\,x + c\big) = \frac{1}{2\sqrt{a}}\frac{d}{dx} e^{-ax^2-bx}\Lambda'\big(\sqrt{a}\,x + c\big)$$

and we also get the second case of the integral (2.7b) by evaluating the primitive at $x = 0$ and $x \to \infty$. □

Using (2.2) we now define for every $t > 0$, $x \in \mathbb{R} \setminus \{0\}$, $z \in \mathbb{C}$, and $\omega \in \mathbb{R}$, the functions

$$G_0(t,x,z) := \frac{1}{2\sqrt{i\pi t}} e^{-\frac{(|x|+z)^2}{4it}}, \tag{2.10a}$$

$$G_1(t,x,z) := \Lambda\left(\frac{|x|+z}{2\sqrt{it}} + \omega\sqrt{it}\right) e^{-\frac{(|x|+z)^2}{4it}}, \tag{2.10b}$$

$$G_{\text{free}}(t,x,z) := \frac{1}{2\sqrt{i\pi t}} e^{-\frac{(x-z)^2}{4it}}, \tag{2.10c}$$

which will appear as components of the Green's function (1.5) later on. In the following preparatory lemma we check that each of these components is a solution of the free Schrödinger equation on $\mathbb{R} \setminus \{0\}$.

Lemma 2.2. *For every $t > 0$, $x \in \mathbb{R} \setminus \{0\}$, $z \in \mathbb{C}$, the functions in* (2.10) *satisfy the differential equations*

$$i\frac{\partial}{\partial t} G_j(t,x,z) = -\frac{\partial^2}{\partial x^2} G_j(t,x,z), \qquad j \in \{0, 1, \text{free}\}. \tag{2.11}$$

Proof. In order to verify (2.11) we compute the derivatives of the functions (2.10) explicitly. For G_0 we get

$$\frac{\partial}{\partial t}G_0(t,x,z)=\frac{i}{4t\sqrt{i\pi t}}\left(i-\frac{(|x|+z)^2}{2t}\right)e^{-\frac{(|x|+z)^2}{4it}}, \tag{2.12a}$$

$$\frac{\partial}{\partial x}G_0(t,x,z)=-\operatorname{sgn}(x)\frac{|x|+z}{4it\sqrt{i\pi t}}e^{-\frac{(|x|+z)^2}{4it}}, \tag{2.12b}$$

$$\frac{\partial^2}{\partial x^2}G_0(t,x,z)=\frac{1}{4t\sqrt{i\pi t}}\left(i-\frac{(|x|+z)^2}{2t}\right)e^{-\frac{(|x|+z)^2}{4it}}. \tag{2.12c}$$

For G_1 we use (2.3) to obtain

$$\frac{\partial}{\partial t}G_1(t,x,z)=i\left(\omega^2\Lambda\left(\frac{|x|+z}{2\sqrt{it}}+\omega\sqrt{it}\right)+\frac{1}{it\sqrt{\pi}}\left(\frac{|x|+z}{2\sqrt{it}}-\omega\sqrt{it}\right)\right)e^{-\frac{(|x|+z)^2}{4it}}, \tag{2.13a}$$

$$\frac{\partial}{\partial x}G_1(t,x,z)=\operatorname{sgn}(x)\left(\omega\Lambda\left(\frac{|x|+z}{2\sqrt{it}}+\omega\sqrt{it}\right)-\frac{1}{\sqrt{i\pi t}}\right)e^{-\frac{(|x|+z)^2}{4it}}, \tag{2.13b}$$

$$\frac{\partial^2}{\partial x^2}G_1(t,x,z)=\left(\omega^2\Lambda\left(\frac{|x|+z}{2\sqrt{it}}+\omega\sqrt{it}\right)+\frac{1}{it\sqrt{\pi}}\left(\frac{|x|+z}{2\sqrt{it}}-\omega\sqrt{it}\right)\right)e^{-\frac{(|x|+z)^2}{4it}}. \tag{2.13c}$$

Finally, for G_{free} we get, in a similar way as for G_0, the derivatives

$$\frac{\partial}{\partial t}G_{\text{free}}(t,x,z)=\frac{i}{4t\sqrt{i\pi t}}\left(i-\frac{(x-z)^2}{2t}\right)e^{-\frac{(x-z)^2}{4it}}, \tag{2.14a}$$

$$\frac{\partial}{\partial x}G_{\text{free}}(t,x,z)=-\frac{x-z}{4it\sqrt{i\pi t}}e^{-\frac{(x-z)^2}{4it}}, \tag{2.14b}$$

$$\frac{\partial^2}{\partial x^2}G_{\text{free}}(t,x,z)=\frac{1}{4t\sqrt{i\pi t}}\left(i-\frac{(x-z)^2}{2t}\right)e^{-\frac{(x-z)^2}{4it}}. \tag{2.14c}$$

In all three cases it is obvious that the differential equation (2.11) is satisfied. □

Next we will collect some elementary estimates of the functions G_0, G_1, and G_{free}, which will be needed throughout the paper.

Lemma 2.3. *For every $t>0$, $x\in\mathbb{R}\setminus\{0\}$, and $z\in\mathbb{C}$ with $\operatorname{Arg}(z)\in[0,\frac{\pi}{2}]$ the following estimates for the functions (2.10) hold:*

$$\left|G_j(t,x,z)\right|\leq c_j(t)\,e^{-\frac{\operatorname{Im}(z^2)}{4t}-\frac{|x|\operatorname{Im}(z)}{2t}},\qquad j\in\{0,1\}, \tag{2.15a}$$

$$\left|G_{\text{free}}(t,x,z)\right|\leq c_{\text{free}}(t)\,e^{-\frac{\operatorname{Im}(z^2)}{4t}+\frac{x\operatorname{Im}(z)}{2t}}, \tag{2.15b}$$

where $c_0(t)=c_{\text{free}}(t)=\frac{1}{2\sqrt{\pi t}}$ and $c_1(t)=\Lambda\left(\frac{\omega\sqrt{t}}{\sqrt{2}}\right)$. In particular, the functions (2.10) satisfy the common estimate

$$\left|G_j(t,x,z)\right|\leq c_j(t)\,e^{-\frac{\operatorname{Im}(z^2)}{4t}+\frac{|x|\operatorname{Im}(z)}{2t}},\qquad j\in\{0,1,\text{free}\}. \tag{2.16}$$

Proof. The estimates (2.15a) and (2.15b) for G_0 and G_{free} are obvious. For the estimate (2.15a) of G_1 we use Lemma 2.1 (iii) and (iv) to get

$$\left|\Lambda\left(\frac{|x|+z}{2\sqrt{it}}+\omega\sqrt{it}\right)\right| \le \Lambda\left(\frac{|x|+\text{Re}(z)+\text{Im}(z)}{2\sqrt{2t}}+\frac{\omega\sqrt{t}}{\sqrt{2}}\right) \le \Lambda\left(\frac{\omega\sqrt{t}}{\sqrt{2}}\right),$$

where the monotonicity of Λ is applicable since $\text{Re}(z), \text{Im}(z) \ge 0$ due to $\text{Arg}(z) \in [0, \frac{\pi}{2}]$. Finally, the estimate (2.16) follows immediately from (2.15) by further estimating the exponents. □

Now we turn to our main objective in this section and introduce the Green's function

$$\begin{aligned} G(t,x,y) &= \mu_+^{(x,y)} G_1(t,x,|y|;\omega_+) + \mu_-^{(x,y)} G_1(t,x,|y|;\omega_-) \\ &\quad + \mu_0^{(x,y)} G_0(t,x,|y|) + G_{\text{free}}(t,x,y), \qquad t>0,\ x,y \in \mathbb{R}\setminus\{0\}, \end{aligned} \tag{2.17}$$

which is expressed in terms of the functions (2.10) and we have added the additional argument $\omega_\pm$ in G_1 to emphasize the dependence of the parameter ω in (2.10b). The function in (2.17) coincides with the Green's function (1.5) mentioned in the Introduction. We prove in Theorem 2.4 below that for a proper choice of coefficients $\mu_\pm$, μ_0, and $\omega_\pm$ the function (2.17) satisfies the differential equation (1.4a) as well as the jump condition (1.4b) for a fixed unitary matrix J. The connection to the initial value (1.4c) is postponed to Lemma 4.2 and Theorem 4.4 in Section 4, where the precise meaning of the integral (2.1) is clarified first.

Next we provide the coefficients $\omega_\pm$ and the piecewise constant functions $\mu_\pm$ and μ_0 explicitly in terms of the unitary 2×2-matrix J in (1.4b). Note that every unitary 2×2-matrix can be written in the form

$$J = e^{i\phi}\begin{pmatrix} \alpha & -\bar{\beta} \\ \beta & \bar{\alpha} \end{pmatrix} \tag{2.18}$$

with parameters $\phi \in [0,\pi)$ and $\alpha, \beta \in \mathbb{C}$ satisfying $|\alpha|^2+|\beta|^2=1$. It is convenient to use

$$\eta^{(x,y)} := \frac{1}{\sqrt{1-\text{Re}(\alpha)^2}} \begin{cases} -\text{Im}(\alpha), & \text{if } x,y>0, \\ -i\bar{\beta}, & \text{if } x>0,\ y<0, \\ i\beta, & \text{if } x<0,\ y>0, \\ \text{Im}(\alpha), & \text{if } x,y<0, \end{cases} \qquad \text{if } |\text{Re}(\alpha)| \ne 1, \tag{2.19a}$$

$$\eta^{(x,y)} := 0, \qquad \text{if } |\text{Re}(\alpha)| = 1, \tag{2.19b}$$

the step function

$$\Theta(x) = \begin{cases} 1, & \text{if } x>0, \\ 0, & \text{if } x<0, \end{cases}$$

and to distinguish the following three cases.

Case I: If $\text{Re}(\alpha) \ne -\cos(\phi)$, then

$$\omega_\pm = \frac{-\sin(\phi) \pm \sqrt{1-\text{Re}(\alpha)^2}}{\cos(\phi)+\text{Re}(\alpha)}, \qquad \mu_\pm^{(x,y)} = -\frac{\omega_\pm}{2}\left(\Theta(xy) \pm \eta^{(x,y)}\right), \qquad \mu_0^{(x,y)} = \text{sgn}(xy).$$

Case II: If $\mathrm{Re}(\alpha) = -\cos(\phi) \neq -1$, then $\omega_- = \mu_-^{(x,y)} = 0$ and

$$\omega_+ = \cot(\phi), \quad \mu_+^{(x,y)} = -\frac{\omega_+}{2}\big(\Theta(xy) + \eta^{(x,y)}\big), \quad \mu_0^{(x,y)} = \eta^{(x,y)} - \Theta(-xy).$$

Case III: If $\mathrm{Re}(\alpha) = -\cos(\phi) = -1$, then $\omega_\pm = \mu_\pm^{(x,y)} = 0$ and $\mu_0^{(x,y)} = -1$.

These three cases correspond to the rank of the matrix $I + J$ on the right hand side of the jump conditions (1.4b) or (2.21). More precisely, in Case I we have $\mathrm{rank}(I + J) = 2$, in Case II we have $\mathrm{rank}(I + J) = 1$, and finally, in Case III we have $\mathrm{rank}(I + J) = 0$.

Theorem 2.4. *For every fixed $y \in \mathbb{R} \setminus \{0\}$ the Green's function (2.17) satisfies the differential equation*

$$i\frac{\partial}{\partial t}G(t,x,y) = -\frac{\partial^2}{\partial x^2}G(t,x,y), \qquad t > 0,\ x \in \mathbb{R} \setminus \{0\}, \tag{2.20}$$

as well as the jump condition

$$(I - J)\begin{pmatrix} G(t,0^+,y) \\ G(t,0^-,y) \end{pmatrix} = i(I + J)\begin{pmatrix} \frac{\partial}{\partial x}G(t,0^+,y) \\ -\frac{\partial}{\partial x}G(t,0^-,y) \end{pmatrix}, \qquad t > 0. \tag{2.21}$$

Proof. Note first that the coefficients $\mu_\pm^{(x,y)}$ and $\mu_0^{(x,y)}$ in the representation (2.17) of the function G only depend on the signs of x and y. In particular, the coefficients are constant on the half lines $x > 0$ and $x < 0$, and hence it follows from Lemma 2.2 that the function G in (2.17) is a solution of the differential equation (2.20).

In the following we will verify that the jump condition (2.21) is satisfied. Using (2.12b), (2.13b), and (2.14b) we find that the spatial derivative of the function G is given by

$$\begin{aligned}
\frac{\partial}{\partial x}G(t,x,y) &= \mu_+^{(x,y)}\,\mathrm{sgn}(x)\left(\omega_+\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}} + \omega_+\sqrt{it}\right) - \frac{1}{\sqrt{i\pi t}}\right)e^{-\frac{(|x|+|y|)^2}{4it}} \\
&\quad + \mu_-^{(x,y)}\,\mathrm{sgn}(x)\left(\omega_-\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}} + \omega_-\sqrt{it}\right) - \frac{1}{\sqrt{i\pi t}}\right)e^{-\frac{(|x|+|y|)^2}{4it}} \\
&\quad - \frac{1}{4it\sqrt{i\pi t}}\left(\mu_0^{(x,y)}\,\mathrm{sgn}(x)\big(|x|+|y|\big)e^{-\frac{(|x|+|y|)^2}{4it}} + (x-y)e^{-\frac{(x-y)^2}{4it}}\right).
\end{aligned}$$

For the jump condition (2.21) we have to evaluate G and $\frac{\partial}{\partial x}G$ at $x = 0^\pm$. As in (2.21) this will be done in a vector form, where the first entry is the limit $x = 0^+$ and the second entry the limit $x = 0^-$. We have

$$\begin{aligned}
\begin{pmatrix} G(t,0^+,y) \\ G(t,0^-,y) \end{pmatrix} &= \left(\begin{pmatrix} \mu_+^{(0^+,y)} \\ \mu_+^{(0^-,y)} \end{pmatrix}\Lambda\left(\frac{|y|}{2\sqrt{it}} + \omega_+\sqrt{it}\right) + \begin{pmatrix} \mu_-^{(0^+,y)} \\ \mu_-^{(0^-,y)} \end{pmatrix}\Lambda\left(\frac{|y|}{2\sqrt{it}} + \omega_-\sqrt{it}\right)\right. \\
&\quad \left. + \frac{1}{2\sqrt{i\pi t}}\begin{pmatrix} \mu_0^{(0^+,y)} + 1 \\ \mu_0^{(0^-,y)} + 1 \end{pmatrix}\right)e^{-\frac{y^2}{4it}},
\end{aligned}$$

$$\begin{pmatrix} \frac{\partial}{\partial x}G(t,0^+,y) \\ -\frac{\partial}{\partial x}G(t,0^-,y) \end{pmatrix} = \Bigg(\begin{pmatrix} \mu_+^{(0^+,y)} \\ \mu_+^{(0^-,y)} \end{pmatrix} \omega_+ \Lambda\left(\frac{|y|}{2\sqrt{it}} + \omega_+\sqrt{it}\right)$$

$$+ \begin{pmatrix} \mu_-^{(0^+,y)} \\ \mu_-^{(0^-,y)} \end{pmatrix} \omega_- \Lambda\left(\frac{|y|}{2\sqrt{it}} + \omega_-\sqrt{it}\right)$$

$$- \frac{1}{\sqrt{i\pi t}} \begin{pmatrix} \mu_+^{(0^+,y)} + \mu_-^{(0^+,y)} \\ \mu_+^{(0^-,y)} + \mu_-^{(0^-,y)} \end{pmatrix} - \frac{|y|}{4it\sqrt{i\pi t}} \begin{pmatrix} \mu_0^{(0^+,y)} - \operatorname{sgn}(y) \\ \mu_0^{(0^-,y)} + \operatorname{sgn}(y) \end{pmatrix} \Bigg) e^{-\frac{y^2}{4it}},$$

and since (2.21) has to be satisfied for all $y \in \mathbb{R} \setminus \{0\}$ it suffices to compare and match the coefficients corresponding to the terms

$$\Lambda\left(\frac{|y|}{2\sqrt{it}} + \omega_\pm\sqrt{it}\right), \quad \frac{1}{2\sqrt{i\pi t}}, \quad \text{and} \quad \frac{|y|}{4it\sqrt{i\pi t}},$$

which leads to the following four equations

$$(\mathrm{A}_\pm): \ (I-J)\begin{pmatrix} \mu_\pm^{(0^+,y)} \\ \mu_\pm^{(0^-,y)} \end{pmatrix} = i\omega_\pm(I+J)\begin{pmatrix} \mu_\pm^{(0^+,y)} \\ \mu_\pm^{(0^-,y)} \end{pmatrix},$$

$$(\mathrm{B}) \ : \ (I-J)\begin{pmatrix} \mu_0^{(0^+,y)} + 1 \\ \mu_0^{(0^-,y)} + 1 \end{pmatrix} = -2i(I+J)\begin{pmatrix} \mu_+^{(0^+,y)} + \mu_-^{(0^+,y)} \\ \mu_+^{(0^-,y)} + \mu_-^{(0^-,y)} \end{pmatrix},$$

$$(\mathrm{C}) \ : \ \begin{pmatrix} 0 \\ 0 \end{pmatrix} = (I+J)\begin{pmatrix} \mu_0^{(0^+,y)} - \operatorname{sgn}(y) \\ \mu_0^{(0^-,y)} + \operatorname{sgn}(y) \end{pmatrix}.$$

Since the variable y only appears as $\operatorname{sgn}(y)$ each equation splits up in one for $y > 0$ and one for $y < 0$. We will consider this by writing ($\mathrm{A}_\pm$), (B), and (C) as matrix equations, where the first column is for $y > 0$ and the second column for $y < 0$. For a shorter notation we will use the matrices

$$\mathbb{1} := \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad N := \begin{pmatrix} \eta^{(0^+,0^+)} & \eta^{(0^+,0^-)} \\ \eta^{(0^-,0^+)} & \eta^{(0^-,0^-)} \end{pmatrix}, \quad M_j := \begin{pmatrix} \mu_j^{(0^+,0^+)} & \mu_j^{(0^+,0^-)} \\ \mu_j^{(0^-,0^+)} & \mu_j^{(0^-,0^-)} \end{pmatrix}, \tag{2.23}$$

where $j \in \{0, \pm\}$. Note that the matrix N satisfies the identity

$$\sqrt{1-\operatorname{Re}(\alpha)^2}\, N = \begin{pmatrix} -\operatorname{Im}(\alpha) & -i\bar{\beta} \\ i\beta & \operatorname{Im}(\alpha) \end{pmatrix} \tag{2.24}$$

by (2.19a) for $|\operatorname{Re}(\alpha)| \neq 1$ and also for $|\operatorname{Re}(\alpha)| = 1$, since then $\operatorname{Im}(\alpha) = \beta = 0$ due to $|\alpha|^2 + |\beta|^2 = 1$. From (2.24) and $|\alpha|^2 + |\beta|^2 = 1$ it immediately follows that

$$N^2 = \frac{1}{1-\operatorname{Re}(\alpha)^2}\begin{pmatrix} -\operatorname{Im}(\alpha) & -i\bar{\beta} \\ i\beta & \operatorname{Im}(\alpha) \end{pmatrix}^2 = \frac{\operatorname{Im}(\alpha)^2 + |\beta|^2}{1-\operatorname{Re}(\alpha)^2}\, I = I \qquad \text{if } |\operatorname{Re}(\alpha)| \neq 1,$$

and, consequently,

$$(N+I)(N-I) = N^2 - N + N - I = N^2 - I = 0 \qquad \text{if } |\mathrm{Re}(\alpha)| \neq 1, \tag{2.25}$$

to which we will refer throughout the proof. With the help of the matrices (2.23) we now rewrite the equations ($\mathrm{A}_\pm$), (B), and (C) above in the matrix form

$$\begin{aligned}
(\mathrm{A}_\pm) &: \ (I-J)M_\pm = i\omega_\pm (I+J)M_\pm, \\
(\mathrm{B}) &: \ (I-J)(M_0 + \mathbb{1}) = -2i(I+J)(M_+ + M_-), \\
(\mathrm{C}) &: \ 0 = (I+J)(M_0 + \mathbb{1} - 2I).
\end{aligned}$$

Plugging in the matrix J from (2.18) and multiplying by $e^{-i\phi}$ these equations turn into

$$(\mathrm{A}_\pm): \begin{pmatrix} e^{-i\phi}-\alpha & \bar\beta \\ -\beta & e^{-i\phi}-\bar\alpha \end{pmatrix} M_\pm = i\omega_\pm \begin{pmatrix} e^{-i\phi}+\alpha & -\bar\beta \\ \beta & e^{-i\phi}+\bar\alpha \end{pmatrix} M_\pm, \tag{2.26a}$$

$$(\mathrm{B}) \ : \begin{pmatrix} e^{-i\phi}-\alpha & \bar\beta \\ -\beta & e^{-i\phi}-\bar\alpha \end{pmatrix} (M_0+\mathbb{1}) = -2i \begin{pmatrix} e^{-i\phi}+\alpha & -\bar\beta \\ \beta & e^{-i\phi}+\bar\alpha \end{pmatrix} (M_+ + M_-), \tag{2.26b}$$

$$(\mathrm{C}) \ : 0 = \begin{pmatrix} e^{-i\phi}+\alpha & -\bar\beta \\ \beta & e^{-i\phi}+\bar\alpha \end{pmatrix} (M_0 + \mathbb{1} - 2I). \tag{2.26c}$$

In the following we will discuss the three cases above Theorem 2.4 separately and verify that in each case with the proper choice of the coefficients $\omega_\pm$ and $\mu_\pm, \mu_0$ the equations ($\mathrm{A}_\pm$), (B), and (C) are satisfied, that is, the jump condition (2.21) holds.

Case I. Observe first that the equation (2.26c) is satisfied since $\mu_0^{(x,y)} = \mathrm{sgn}(xy)$ in this case, and hence we conclude $M_0 = 2I - \mathbb{1}$. Next we use $|\alpha|^2 + |\beta|^2 = 1$ to compute

$$\det \begin{pmatrix} e^{-i\phi}+\alpha & -\bar\beta \\ \beta & e^{-i\phi}+\bar\alpha \end{pmatrix} = 2e^{-i\phi}\big(\cos(\phi) + \mathrm{Re}(\alpha)\big) \neq 0,$$

where we also used the assumption $\mathrm{Re}(\alpha) \neq -\cos(\phi)$ in Case I. It follows that the matrix on the right hand side of ($\mathrm{A}_\pm$) and (B) is invertible with the inverse

$$\begin{pmatrix} e^{-i\phi}+\alpha & -\bar\beta \\ \beta & e^{-i\phi}+\bar\alpha \end{pmatrix}^{-1} = \frac{e^{i\phi}}{2(\cos(\phi)+\mathrm{Re}(\alpha))} \begin{pmatrix} e^{-i\phi}+\bar\alpha & \bar\beta \\ -\beta & e^{-i\phi}+\alpha \end{pmatrix},$$

and this leads to

$$\begin{aligned}
&\begin{pmatrix} e^{-i\phi}+\alpha & -\bar\beta \\ \beta & e^{-i\phi}+\bar\alpha \end{pmatrix}^{-1} \begin{pmatrix} e^{-i\phi}-\alpha & \bar\beta \\ -\beta & e^{-i\phi}-\bar\alpha \end{pmatrix} \\
&\qquad = \frac{-i}{\cos(\phi)+\mathrm{Re}(\alpha)} \begin{pmatrix} \sin(\phi)+\mathrm{Im}(\alpha) & i\bar\beta \\ -i\beta & \sin(\phi)-\mathrm{Im}(\alpha) \end{pmatrix} \\
&\qquad = \frac{-i}{\cos(\phi)+\mathrm{Re}(\alpha)} \big(\sin(\phi)\, I - \sqrt{1-\mathrm{Re}(\alpha)^2}\, N\big),
\end{aligned}$$

where in the last line we used the identity (2.24). Hence the equations (2.26a) and (2.26b) turn into

$$(\mathrm{A}_\pm): \frac{\sin(\phi)\, I - \sqrt{1-\mathrm{Re}(\alpha)^2}\, N}{\cos(\phi) + \mathrm{Re}(\alpha)} M_\pm = -\omega_\pm M_\pm,$$
$$(\mathrm{B}) \ : \frac{\sin(\phi)\, I - \sqrt{1-\mathrm{Re}(\alpha)^2}\, N}{\cos(\phi) + \mathrm{Re}(\alpha)} (M_0 + \mathbb{1}) = 2(M_+ + M_-).$$

Using the explicit form $\omega_\pm = \frac{-\sin(\phi)\pm\sqrt{1-\mathrm{Re}(\alpha)^2}}{\cos(\phi)+\mathrm{Re}(\alpha)}$ in $(\mathrm{A}_\pm)$ and $M_0 = 2I - \mathbb{1}$ in (B) these equations reduce to

$$(\mathrm{A}_\pm): \sqrt{1-\mathrm{Re}(\alpha)^2}(N \mp I) M_\pm = 0,$$
$$(\mathrm{B}) \ : \frac{\sin(\phi)\, I - \sqrt{1-\mathrm{Re}(\alpha)^2}\, N}{\cos(\phi) + \mathrm{Re}(\alpha)} = M_+ + M_-.$$

Since we treat Case I we have $\mu_\pm^{(x,y)} = -\frac{\omega_\pm}{2}\big(\Theta(xy) \pm \eta^{(x,y)}\big)$ and from that we conclude

$$M_\pm = -\frac{\omega_\pm}{2}(I \pm N). \tag{2.27}$$

In particular, this yields

$$M_+ + M_- = -\frac{(\omega_+ + \omega_-)I + (\omega_+ - \omega_-)N}{2} = \frac{\sin(\phi)I - \sqrt{1-\mathrm{Re}(\alpha)^2}\, N}{\cos(\phi) + \mathrm{Re}(\alpha)},$$

which shows that equation (B) is valid. It remains to check $(\mathrm{A}_\pm)$. Indeed, these equations are obviously valid if $|\mathrm{Re}(\alpha)| = 1$ and if $|\mathrm{Re}(\alpha)| \neq 1$ they follow from the identities (2.25) and (2.27).

Case II. Here we assume $\mathrm{Re}(\alpha) = -\cos(\phi) \neq -1$, which implies, in particular, $\phi \neq 0$ and consequently $\sin(\phi) \neq 0$. The matrices in the equations $(\mathrm{A}_\pm)$, (B), and (C) in (2.26) now have the form

$$\begin{pmatrix} e^{-i\phi} - \alpha & \bar{\beta} \\ -\beta & e^{-i\phi} - \bar{\alpha} \end{pmatrix} = \big(2\cos(\phi) - i\sin(\phi)\big)I + i\begin{pmatrix} -\mathrm{Im}(\alpha) & -i\bar{\beta} \\ i\beta & \mathrm{Im}(\alpha) \end{pmatrix}$$
$$= -i\sin(\phi)\big((2i\cot(\phi) + 1)I - N\big),$$
$$\begin{pmatrix} e^{-i\phi} + \alpha & -\bar{\beta} \\ \beta & e^{-i\phi} + \bar{\alpha} \end{pmatrix} = -i\sin(\phi)I - i\begin{pmatrix} -\mathrm{Im}(\alpha) & -i\bar{\beta} \\ i\beta & \mathrm{Im}(\alpha) \end{pmatrix}$$
$$= -i\sin(\phi)(I + N),$$

where in both cases we used (2.24) and $\sqrt{1-\mathrm{Re}(\alpha)^2} = \sin(\phi)$, because $\mathrm{Re}(\alpha) = -\cos(\phi)$. Using this in (2.26) leads to

$$
\begin{aligned}
(\mathrm{A}_\pm):&\ \big((2i\cot(\phi)+1)I-N\big)M_\pm = i\omega_\pm(I+N)M_\pm,\\
(\mathrm{B})\ :&\ \big((2i\cot(\phi)+1)I-N\big)(M_0+\mathbb{1}) = -2i(I+N)(M_+ + M_-),\\
(\mathrm{C})\ :&\ 0=(I+N)(M_0+\mathbb{1}-2I).
\end{aligned}
$$

Since in Case II we have $\mu_-^{(x,y)}=0$, that is, $M_-=0$, the equation (A_-) is trivially satisfied. Furthermore, with our choice $\omega_+=\cot(\phi)$ the equation (A_+) reduces to

$$
(\mathrm{A}_+):\ \ (i\cot(\phi)+1)(I-N)M_+ = 0.
$$

By our choice of $\mu_+^{(x,y)}$ we have $M_+=-\frac{\omega_+}{2}(I+N)$ as in the previous case (cf. (2.27)) and hence we conclude together with (2.25) that equation (A_+) is valid; note that we can apply (2.25) since $\mathrm{Re}(\alpha)\neq -1$ by the assumption in Case II and also $\mathrm{Re}(\alpha)=-\cos(\phi)\neq 1$ as $\phi\in[0,\pi)$. Next, we observe that also equation (C) holds by (2.25) and $\mu_0^{(x,y)}=\eta^{(x,y)}-\Theta(-xy)$, which gives $M_0=N-\mathbb{1}+I$. In order to check (B), we plug in the above values for M_0 and $M_\pm$, and obtain

$$
(\mathrm{B}):\ \ (1+i\cot(\phi))(I-N)(N+I)=0,
$$

which holds by (2.25).

Case III. Here we assume $\mathrm{Re}(\alpha)=-\cos(\phi)=-1$ and hence $\mathrm{Im}(\alpha)=\beta=\phi=0$ follows from the condition $|\alpha|^2+|\beta|^2=1$. Therefore, the equations ($\mathrm{A}_\pm$), (B), and (C) in (2.26) have the particularly simple form

$$
\begin{aligned}
(\mathrm{A}_\pm):&\ 2M_\pm = 0,\\
(\mathrm{B})\ :&\ M_0+\mathbb{1}=0,\\
(\mathrm{C})\ :&\ 0=0,
\end{aligned}
$$

and are all obviously satisfied by the definition of the coefficients in Case III. □

3. Special cases of generalized point interactions and their Green's functions

In this section we consider some particular generalized point interactions and derive the explicit form of the Green's function in these situations. As an almost trivial case we start with the free particle in Example 3.1, discuss the well-known δ and δ'-interactions afterwards in Example 3.2 and Example 3.3, respectively, and in Examples 3.4–3.6 we treat decoupled systems with Dirichlet, Neumann, and Robin boundary conditions at the origin. In each of the examples we first provide the corresponding matrix J for the interface conditions (1.4b) with parameters ϕ,α,β as in (2.18), then we determine which of the Cases I–III above Theorem 2.4 appears, and finally we compute the coefficients in the Green's function (1.5) or (2.17). The special Green's functions in this section are known from the mathematical and physical literature.

Example 3.1 *(Free particle).* The wave function corresponding to a free particle is continuous with continuous first derivative and hence at the point $x=0$ we have

$$
\Psi(t,0^-)=\Psi(t,0^+) \qquad \text{and} \qquad \frac{\partial}{\partial x}\Psi(t,0^-)=\frac{\partial}{\partial x}\Psi(t,0^+), \qquad t>0.
$$

These continuity conditions are described in (1.4b) if we consider the matrix

$$J = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

This matrix is of the form (2.18) with $\alpha = 0$, $\beta = -i$, and $\phi = \frac{\pi}{2}$. In this situation the coefficient $\eta^{(x,y)}$ in (2.19a) is

$$\eta^{(x,y)} = \begin{cases} 0, & \text{if } x, y > 0, \\ 1, & \text{if } x > 0,\ y < 0, \\ 1, & \text{if } x < 0,\ y > 0, \\ 0, & \text{if } x, y < 0, \end{cases} = \Theta(-xy).$$

Since we are in Case II the coefficients of the corresponding Green's function in (1.5) have the explicit form

$$\begin{aligned} &\omega_- = 0, && \mu_-^{(x,y)} = 0, \\ &\omega_+ = \cot\left(\frac{\pi}{2}\right) = 0, && \mu_+^{(x,y)} = -\frac{\omega_+}{2}\left(\Theta(xy) + \eta^{(x,y)}\right) = 0, \\ & && \mu_0^{(x,y)} = \eta^{(x,y)} - \Theta(-xy) = 0. \end{aligned}$$

Therefore, the Green's function of the free particle is given by

$$G(t,x,y) = \frac{1}{2\sqrt{i\pi t}} e^{-\frac{(x-y)^2}{4it}}.$$

In the next example we treat the classical δ-point interaction located at the origin. Such singular potentials were studied intensively in the mathematical and physical literature; we refer the interested reader to the standard monograph [16] for a detailed treatment and further references. The particular Green's function that appears below can also be found (sometimes in a slightly different form) in the papers [34,43,49].

Example 3.2 *(δ-potential).* We consider the standard δ-interaction of strength $2c \in \mathbb{R} \setminus \{0\}$ located at the point $x = 0$. This situation is described by the formal Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(t,x) = \left(-\frac{\partial^2}{\partial x^2} + 2c\delta(x)\right)\Psi(t,x), \qquad t > 0,\ x \in \mathbb{R},$$

and is made mathematically rigorous in the form

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi(t,x) &= -\frac{\partial^2}{\partial x^2}\Psi(t,x), && t > 0,\ x \in \mathbb{R}\setminus\{0\}, \\ \Psi(t,0^+) &= \Psi(t,0^-), && t > 0, \qquad (3.1a) \\ \frac{\partial}{\partial x}\Psi(t,0^+) - \frac{\partial}{\partial x}\Psi(t,0^-) &= 2c\,\Psi(t,0^\pm), && t > 0. \qquad (3.1b) \end{aligned}$$

The jump condition (3.1a)–(3.1b) is realized in (1.4b) by using the matrix

$$J = \frac{1}{i-c}\begin{pmatrix} c & i \\ i & c \end{pmatrix}.$$

In fact, with this choice of J and multiplication by $(c-i)$ the condition (1.4b) reads as

$$\begin{pmatrix} 2c-i & i \\ i & 2c-i \end{pmatrix}\begin{pmatrix} \Psi(t,0^+) \\ \Psi(t,0^-) \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} \frac{\partial}{\partial x}\Psi(t,0^+) \\ -\frac{\partial}{\partial x}\Psi(t,0^-) \end{pmatrix},$$

or, more explicitely, we have the two equations

$$(2c-i)\Psi(t,0^+) + i\Psi(t,0^-) = \frac{\partial}{\partial x}\Psi(t,0^+) - \frac{\partial}{\partial x}\Psi(t,0^-),$$
$$i\Psi(t,0^+) + (2c-i)\Psi(t,0^-) = \frac{\partial}{\partial x}\Psi(t,0^+) - \frac{\partial}{\partial x}\Psi(t,0^-).$$

By subtracting these equations from each other we first conclude (3.1a) and adding the equations leads to (3.1b). In order to write the matrix J in the form (2.18) we choose $\phi \in (0,\pi)$ such that $\cot(\phi) = c$. Next we set $\alpha = -\cos(\phi)$ and $\beta = -i\sin(\phi)$. It follows, in particular, that

$$\cos(\phi) = \frac{c}{\sqrt{1+c^2}} \qquad \text{and} \qquad \sin(\phi) = \frac{1}{\sqrt{1+c^2}},$$

and therefore

$$e^{i\phi}\begin{pmatrix} \alpha & -\bar{\beta} \\ \beta & \bar{\alpha} \end{pmatrix} = \frac{1}{i-c}\begin{pmatrix} c & i \\ i & c \end{pmatrix} = J.$$

Plugging these values in (2.19a) gives

$$\eta^{(x,y)} = \begin{cases} 0, & \text{if } x, y > 0, \\ 1, & \text{if } x > 0,\ y < 0, \\ 1, & \text{if } x < 0,\ y > 0, \\ 0, & \text{if } x, y < 0, \end{cases} = \Theta(-xy),$$

and since we are in Case II the coefficients of the Green's function are

$$\begin{aligned} \omega_- &= 0, & \mu_-^{(x,y)} &= 0, \\ \omega_+ &= \cot(\phi) = c, & \mu_+^{(x,y)} &= -\frac{c}{2}\big(\Theta(xy) + \Theta(-xy)\big) = -\frac{c}{2}, \\ & & \mu_0^{(x,y)} &= \Theta(-xy) - \Theta(-xy) = 0. \end{aligned}$$

With these quantities we conclude from (1.5) that the Green's function of the δ-potential is given by

$$G(t,x,y) = -\frac{c}{2}\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}} + c\sqrt{it}\right)e^{-\frac{(|x|+|y|)^2}{4it}} + \frac{1}{2\sqrt{i\pi t}}e^{-\frac{(x-y)^2}{4it}}.$$

The δ'-interaction in the next example is another popular singular potential that appears in various situations.

Example 3.3 *(δ'-potential).* Now consider the δ'-interaction of strength $\frac{2}{c} \in \mathbb{R} \setminus \{0\}$ located at the point $x = 0$. Formally one then deals with the Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(t,x) = \Big(-\frac{\partial^2}{\partial x^2} + \frac{2}{c}\delta'(x)\Big)\Psi(t,x), \qquad t>0,\ x\in\mathbb{R},$$

which in a mathematically rigorous form reads as

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi(t,x) &= -\frac{\partial^2}{\partial x^2}\Psi(t,x), && t>0,\ x\in\mathbb{R}\setminus\{0\},\\ \frac{\partial}{\partial x}\Psi(t,0^+) &= \frac{\partial}{\partial x}\Psi(t,0^-), && t>0,\\ \Psi(t,0^+)-\Psi(t,0^-) &= \frac{2}{c}\frac{\partial}{\partial x}\Psi(t,0), && t>0. \end{aligned}$$

One verifies in a similar way as in the previous example that the jump conditions are realized in (1.4b) by using the matrix

$$J = \frac{1}{i-c}\begin{pmatrix} i & -c \\ -c & i \end{pmatrix}.$$

This matrix is of the form (2.18) if we choose $\phi \in (0,\pi)\setminus\{\frac{\pi}{2}\}$ such that $\tan(\phi) = -c$ and set $\alpha = \cos(\phi)$ and $\beta = -i\sin(\phi)$. The coefficient $\eta^{(x,y)}$ in (2.19a) then becomes

$$\eta^{(x,y)} = \begin{cases} 0, & \text{if } x,y>0,\\ 1, & \text{if } x>0,\ y<0,\\ 1, & \text{if } x<0,\ y>0,\\ 0, & \text{if } x,y<0, \end{cases} = \Theta(-xy),$$

and since we are in Case I the coefficients of the Green's function are

$$\begin{aligned} \omega_- &= -\tan(\phi) = c, & \mu_-^{(x,y)} &= -\frac{c}{2}\big(\Theta(xy)-\Theta(-xy)\big) = -\frac{c\,\mathrm{sgn}(xy)}{2},\\ \omega_+ &= 0, & \mu_+^{(x,y)} &= 0,\\ & & \mu_0^{(x,y)} &= \mathrm{sgn}(xy). \end{aligned}$$

It follows that the Green's function of the δ'-potential is given by

$$\begin{aligned} G(t,x,y) = &-\frac{c\,\mathrm{sgn}(xy)}{2}\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}} + c\sqrt{it}\right)e^{-\frac{(|x|+|y|)^2}{4it}}\\ &+ \frac{1}{2\sqrt{i\pi t}}\left(\mathrm{sgn}(xy)e^{-\frac{(|x|+|y|)^2}{4it}} + e^{-\frac{(x-y)^2}{4it}}\right). \end{aligned}$$

Now we turn to generalized point interactions that lead to decoupled systems. In the following examples we discuss Dirichlet, Neumann, and Robin boundary conditions at the origin; for a characterization of all decoupled systems see also Example 5.4.

Example 3.4 *(Dirichlet boundary conditions).* We consider the free Schrödinger equation on the two half lines $\mathbb{R} \setminus \{0\}$ with Dirichlet boundary conditions

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi(t,x) &= -\frac{\partial^2}{\partial x^2}\Psi(t,x), \qquad && t>0,\ x\in\mathbb{R}\setminus\{0\}, \\ \Psi(t,0^+) &= \Psi(t,0^-) = 0, && t>0. \end{aligned}$$

These boundary conditions are realized in (1.4b) by using the matrix

$$J = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.2}$$

that is, we have $\phi = 0$, $\alpha = -1$, and $\beta = 0$ in (2.18), and hence Case III applies. The coefficients of the Green's function are given by

$$\omega_\pm = 0, \qquad \mu_\pm^{(x,y)} = 0, \quad \text{and} \quad \mu_0^{(x,y)} = -1,$$

and lead to

$$G(t,x,y) = \frac{1}{2\sqrt{i\pi t}}\left(e^{-\frac{(x-y)^2}{4it}} - e^{-\frac{(|x|+|y|)^2}{4it}}\right). \tag{3.3}$$

Example 3.5 *(Neumann boundary conditions).* We consider the free Schrödinger equation on the two half lines $\mathbb{R} \setminus \{0\}$ with Neumann boundary conditions

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi(t,x) &= -\frac{\partial^2}{\partial x^2}\Psi(t,x), \qquad && t>0,\ x\in\mathbb{R}\setminus\{0\}, \\ \frac{\partial}{\partial x}\Psi(t,0^+) &= \frac{\partial}{\partial x}\Psi(t,0^-) = 0, && t>0. \end{aligned}$$

These boundary conditions are realized in (1.4b) by using the matrix

$$J = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

that is, we have $\phi = 0$, $\alpha = 1$, and $\beta = 0$ in (2.18), and hence Case I applies. The coefficients of the Green's function are given by

$$\omega_\pm = 0, \qquad \mu_\pm^{(x,y)} = 0, \quad \text{and} \quad \mu_0^{(x,y)} = \operatorname{sgn}(xy),$$

and lead to

$$G(t,x,y) = \frac{1}{2\sqrt{i\pi t}}\left(e^{-\frac{(x-y)^2}{4it}} + \operatorname{sgn}(xy)e^{-\frac{(|x|+|y|)^2}{4it}}\right).$$

In the next example we consider Robin boundary conditions at the origin. The Neumann boundary conditions in Example 3.5 are contained as a special case and the Dirichlet boundary conditions in Example 3.4 formally appear as a limit; cf. Remark 3.7.

Example 3.6 *(Robin boundary conditions).* We consider the free Schrödinger equation on the two half lines $\mathbb{R}\setminus\{0\}$ with Robin boundary conditions

$$\begin{aligned} & i\frac{\partial}{\partial t}\Psi(t,x) = -\frac{\partial^2}{\partial x^2}\Psi(t,x), && t>0,\ x\in\mathbb{R}\setminus\{0\}, \\ & \frac{\partial}{\partial x}\Psi(t,0^+) = a\,\Psi(t,0^+), && t>0, \\ & \frac{\partial}{\partial x}\Psi(t,0^-) = b\,\Psi(t,0^-), && t>0, \end{aligned}$$

for some $a,b\in\mathbb{R}$; note that the minus sign for the derivative at $x=0^-$ on the right hand side of (1.4b) is omitted here. These boundary conditions are realized in (1.4b) by using the matrix

$$J = \begin{pmatrix} \frac{i+a}{i-a} & 0 \\ 0 & \frac{i-b}{i+b} \end{pmatrix}, \tag{3.4}$$

which is of the form (2.18) with

$$\alpha = \operatorname{sgn}(b-a)\frac{(1-ia)(1-ib)}{\sqrt{1+a^2}\sqrt{1+b^2}}, \qquad \beta = 0,$$

and $\phi\in[0,\pi)$ chosen such that

$$e^{i\phi} = \operatorname{sgn}(b-a)\frac{(1-ia)(1+ib)}{\sqrt{1+a^2}\sqrt{1+b^2}},$$

where we use $\operatorname{sgn}(0)=1$. One verifies that Case I applies and a (more technical) computation finally leads to the Green's function

$$\begin{aligned} G(t,x,y) = \Bigg(& -a\,\Theta(x)\Theta(y)\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}}+a\sqrt{it}\right) \\ & +b\,\Theta(-x)\Theta(-y)\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}}-b\sqrt{it}\right)\Bigg) e^{-\frac{(|x|+|y|)^2}{4it}} \\ & + \frac{1}{2\sqrt{i\pi t}}\left(\operatorname{sgn}(xy)e^{-\frac{(|x|+|y|)^2}{4it}} + e^{-\frac{(x-y)^2}{4it}}\right). \end{aligned} \tag{3.5}$$

Remark 3.7. It is clear that for $a=b=0$ the boundary condition and Green's function in Example 3.6 reduce to those in Example 3.5. Moreover, also the boundary condition and Green's function for the Dirichlet decoupling in Example 3.4 can be recovered from Example 3.6. In fact, for $a\to\infty$ and $b\to-\infty$ the matrix J in (3.4) tends to the one in (3.2) and using Lemma 2.1 (iv) one obtains the asymptotics

$$\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}}+a\sqrt{it}\right)\sim\frac{1}{a\sqrt{i\pi t}}\qquad\text{and}\qquad\Lambda\left(\frac{|x|+|y|}{2\sqrt{it}}-b\sqrt{it}\right)\sim\frac{1}{-b\sqrt{i\pi t}}$$

in (3.5), which then lead to the Green's function (3.3).

4. Solution of the Schrödinger equation with a generalized point interaction

In this section we continue the theme from Section 2, where in Theorem 2.4 it was already shown that the Green's function (1.5) satisfies the Schrödinger equation (2.20) and the jump condition (2.21) that represents the generalized point interaction at the origin. Now we turn our attention to the initial value (1.4c). This missing part will be provided in Theorem 4.4 below. However, the main technical issue here is to make sense of the integral (1.6). Since we want to consider, e.g., plane waves $F(x)=e^{ikx}$ as initial conditions, we have to deal with integrands that are not absolutely integrable. For this purpose the so-called Fresnel integral, discussed in Lemma 4.1, will be useful. The resulting representation of the integral then also ensures, in a mathematical rigorous way, that the properties (2.20) and (2.21) of the Green's function G carry over to the respective properties (1.4a) and (1.4b) of the wave function Ψ.

Lemma 4.1 *(Fresnel integral). Let $f:\Omega\to\mathbb{C}$ be holomorphic on an open set $\Omega\subseteq\mathbb{C}$ which contains the sector*

$$S_\alpha:=\{\,z\in\mathbb{C}:0\le\operatorname{Arg}(z)\le\alpha\,\}\tag{4.1}$$

for some $\alpha\in(0,\frac{\pi}{2})$, and assume that f satisfies the estimate

$$|f(z)|\le A\,e^{-\varepsilon\operatorname{Im}(z^2)},\qquad z\in S_\alpha,\tag{4.2}$$

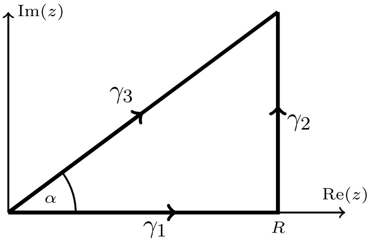
for some $A\ge 0$ and $\varepsilon>0$. Then we get

$$\lim_{R\to\infty}\int_0^R f(y)dy=e^{i\alpha}\int_0^\infty f(ye^{i\alpha})dy,\tag{4.3}$$

where the integral on the right hand side is absolutely convergent.

Proof. For simplicity we will write $k=\tan(\alpha)>0$. For every $R>0$ we consider the integration path

$$\gamma_1:=\{\,y:0\le y\le R\,\},$$
$$\gamma_2:=\{\,R+iy:0\le y\le kR\,\},$$
$$\gamma_3:=\left\{\,ye^{i\alpha}:0\le y\le R\sqrt{1+k^2}\,\right\}.$$



Since f is holomorphic, Cauchy's theorem yields

$$\int_0^R f(y)dy = \int_{\gamma_1} f(z)dz = -\int_{\gamma_2} f(z)dz + \int_{\gamma_3} f(z)dz$$
$$= -i\int_0^{kR} f(R+iy)dy + e^{i\alpha}\int_0^{R\sqrt{1+k^2}} f(ye^{i\alpha})dy. \tag{4.4}$$

From the estimate (4.2) we obtain

$$\left| -i\int_0^{kR} f(R+iy)dy \right| \le A\int_0^{\infty} e^{-2\varepsilon Ry}dy = \frac{A}{2\varepsilon R} \to 0, \quad R\to\infty,$$

and thus in the limit $R\to\infty$ we conclude from (4.4)

$$\lim_{R\to\infty}\int_0^R f(y)dy = e^{i\alpha}\lim_{R\to\infty}\int_0^R f(ye^{i\alpha})dy.$$

The estimate $|f(ye^{i\alpha})| \le Ae^{-\varepsilon\sin(2\alpha)y^2}$, $y>0$, implies that the integral on the right hand side is absolutely convergent and hence the identity (4.3) follows. □

In the next lemma we define functions Ψ_0, Ψ_1, and Ψ_{free} that are closely related to the functions G_0, G_1, and G_{free} in (2.10), which will then lead to a solution of the Schrödinger equation (1.4) in Theorem 4.4 below.

Lemma 4.2. *Let $F:\Omega\to\mathbb{C}$ be holomorphic on an open set $\Omega\subseteq\mathbb{C}$ which contains the sector S_α from (4.1) for some $\alpha\in(0,\frac{\pi}{2})$, and assume that F satisfies the estimate*

$$|F(z)| \le A\,e^{B\,\mathrm{Im}(z)}, \qquad z\in S_\alpha, \tag{4.5}$$

for some $A,B\ge 0$. For every fixed $t>0$, $x\in\mathbb{R}\setminus\{0\}$ we consider the functions

$$\Psi_j(t,x;F) = \int_0^{\infty} G_j(t,x,y)F(y)dy, \qquad j\in\{0,1,\text{free}\}. \tag{4.6}$$

Then the following assertions hold:

(i) *The integral on the right hand side in (4.6) exists as the improper Riemann integral*

$$\int_0^{\infty} G_j(t,x,y)F(y)dy := \lim_{R\to\infty}\int_0^R G_j(t,x,y)F(y)dy, \tag{4.7}$$

and the functions Ψ_j, $j\in\{0,1,\text{free}\}$, admit the absolutely integrable representation

$$\Psi_j(t,x;F) = e^{i\alpha} \int_0^\infty G_j(t,x,ye^{i\alpha})F(ye^{i\alpha})dy, \qquad j \in \{0,1,\text{free}\}. \tag{4.8}$$

(ii) *The functions* Ψ_j, $j \in \{0,1,\text{free}\}$, *in* (4.6) *are solutions of the differential equation*

$$i\frac{\partial}{\partial t}\Psi_j(t,x;F) = -\frac{\partial^2}{\partial x^2}\Psi_j(t,x;F), \qquad t>0,\ x \in \mathbb{R}\setminus\{0\}. \tag{4.9}$$

(iii) *The functions* Ψ_j, $j \in \{0,1,\text{free}\}$, *in* (4.6) *admit the initial values*

$$\Psi_0(0^+,x;F) = \Psi_1(0^+,x;F) = 0, \qquad x \in \mathbb{R}\setminus\{0\}, \tag{4.10}$$

and

$$\Psi_{\text{free}}(0^+,x;F) = \begin{cases} F(x), & \text{if } x>0, \\ 0, & \text{if } x<0. \end{cases} \tag{4.11}$$

Proof. (i) This assertion is a direct consequence of Lemma 4.1 if we verify that the functions $y \mapsto G_j(t,x,y)F(y)$, $j \in \{0,1,\text{free}\}$, satisfy an estimate of the form (4.2). In fact, the estimates (2.16) together with the assumption (4.5) leads to the bounds

$$\left|G_j(t,x,z)F(z)\right| \le Ac_j(t)e^{-\frac{\operatorname{Im}(z^2)}{4t}+(B+\frac{|x|}{2t})\operatorname{Im}(z)}, \qquad z \in S_\alpha. \tag{4.12}$$

Since for every $z \in S_\alpha$ we have $\operatorname{Im}(z) \le \tan(\alpha)\operatorname{Re}(z)$, and hence $\operatorname{Im}(z^2) \ge \frac{2}{\tan(\alpha)}\operatorname{Im}(z)^2$, the exponent in (4.12) can be further estimated by

$$-\frac{\operatorname{Im}(z^2)}{4t} + \left(B+\frac{|x|}{2t}\right)\operatorname{Im}(z) \le -\frac{\operatorname{Im}(z^2)}{8t} - \frac{\operatorname{Im}(z)^2}{4t\tan(\alpha)} + \left(B+\frac{|x|}{2t}\right)\operatorname{Im}(z).$$

Taking into account that a polynomial of the form $-a\operatorname{Im}(z)^2 + b\operatorname{Im}(z)$ with $a>0$, $b\in\mathbb{R}$, is bounded from above by $\frac{b^2}{4a}$, we find

$$-\frac{\operatorname{Im}(z^2)}{4t} + \left(B+\frac{|x|}{2t}\right)\operatorname{Im}(z) \le -\frac{\operatorname{Im}(z^2)}{8t} + t\left(B+\frac{|x|}{2t}\right)^2\tan(\alpha), \tag{4.13}$$

and thus (4.12) can be estimated by

$$\left|G_j(t,x,z)F(z)\right| \le Ac_j(t)e^{t(B+\frac{|x|}{2t})^2\tan(\alpha)}e^{-\frac{\operatorname{Im}(z^2)}{8t}}, \qquad z \in S_\alpha.$$

This shows that (4.2) indeed holds in the present context and the integral (4.6) exists in the form (4.7) and admits the absolutely integrable representation (4.8).

(ii) Now we show that the functions Ψ_0, Ψ_1, and Ψ_{free} satisfy the differential equation (4.9). Since we have already shown in Lemma 2.2 that G_0, G_1, and G_{free} solve (2.11), it remains to interchange the integral and the derivatives in the representation (4.8). We verify this property for the time derivative of G_0 and leave the analogous arguments for the spatial derivatives and the functions G_1 and G_{free} to the reader. Note that from (2.12a) with $z = ye^{i\alpha}$ one obtains

$$\Big|\frac{\partial}{\partial t}G_0\big(t,x,ye^{i\alpha}\big)\Big| \le \frac{1}{4t\sqrt{\pi t}}\Big(1+\frac{(|x|+|y|)^2}{2t}\Big)e^{-\frac{y^2\sin(2\alpha)}{4t}-\frac{|x|y\sin(\alpha)}{2t}}$$

and hence together with (4.5)

$$\Big|\frac{\partial}{\partial t}G_0(t,x,ye^{i\alpha})F(ye^{i\alpha})\Big| \le \frac{A}{4t\sqrt{\pi t}}\Big(1+\frac{(|x|+|y|)^2}{2t}\Big)e^{-\frac{y^2\sin(2\alpha)}{4t}-\frac{|x|y\sin(\alpha)}{2t}+By\sin(\alpha)}.$$

The term $e^{-\frac{y^2\sin(2\alpha)}{4t}}$ now ensures the integrability of the right hand side. Since all terms are continuous functions in t, we can also choose an integrable upper bound, which is locally uniform in t. Hence, by classical theorems for Lebesgue integral (see, e.g., [52]) the time derivative of $\Psi_0(t,x;F)$ exists and is given by

$$\frac{\partial}{\partial t}\Psi_0(t,x;F) = e^{i\alpha}\int_0^\infty \frac{\partial}{\partial t}G_0(t,x,ye^{i\alpha})F(ye^{i\alpha})dy.$$

Similar arguments also apply to the other eight derivatives in (2.12), (2.13), and (2.14), and we conclude for every $j \in \{0, 1, \text{free}\}$

$$\frac{\partial}{\partial t}\Psi_j(t,x;F) = e^{i\alpha}\int_0^\infty \frac{\partial}{\partial t}G_j(t,x,ye^{i\alpha})F(ye^{i\alpha})dy, \tag{4.14a}$$

$$\frac{\partial}{\partial x}\Psi_j(t,x;F) = e^{i\alpha}\int_0^\infty \frac{\partial}{\partial x}G_j(t,x,ye^{i\alpha})F(ye^{i\alpha})dy, \tag{4.14b}$$

$$\frac{\partial^2}{\partial x^2}\Psi_j(t,x;F) = e^{i\alpha}\int_0^\infty \frac{\partial^2}{\partial x^2}G_j(t,x,ye^{i\alpha})F(ye^{i\alpha})dy. \tag{4.14c}$$

As was already mentioned the functions G_j solve (2.11) and hence it follows that the functions Ψ_j satisfy (4.9).

(iii) To check the initial conditions (4.10) for Ψ_0 and Ψ_1, we plug in the estimates (2.15a) and (4.5) into the representation (4.8). This yields

$$\begin{aligned}\big|\Psi_j(t,x;F)\big| &\le Ac_j(t)\int_0^\infty e^{-\frac{y^2\sin(2\alpha)}{4t}+(B-\frac{|x|}{2t})y\sin(\alpha)}dy \\ &= \frac{Ac_j(t)\sqrt{\pi t}}{\sqrt{\sin(2\alpha)}}\Lambda\left(\Big(\frac{|x|}{2\sqrt{t}}-B\sqrt{t}\Big)\sqrt{\frac{\tan(\alpha)}{2}}\right)\to 0, \qquad t\to 0^+,\end{aligned} \tag{4.15}$$

for $j \in \{0, 1\}$, where we have used the integral (2.7a) in the second line; the convergence follows from the asymptotics (2.6) and the fact that $c_j(t)\sqrt{t}$ is bounded (for the precise form of the constants see Lemma 2.3). For the initial value of Ψ_{free} we distinguish two cases. For $x < 0$ we use the estimate (2.15b) and get the same convergence as in (4.15). The remaining case $x > 0$ is more involved. Here we split up the integral (4.6) into

$$\Psi_{\text{free}}(t, x; F) = \frac{1}{2\sqrt{i\pi t}} \left(\int_0^{2x} e^{-\frac{(x-y)^2}{4it}} F(y)dy + \int_{2x}^{\infty} e^{-\frac{(x-y)^2}{4it}} F(y)dy \right). \tag{4.16}$$

In the first integral we use the derivative $\frac{d}{dz}\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} e^{-z^2}$ of the error function, as well as integration by parts, to get

$$\begin{aligned} \frac{1}{2\sqrt{i\pi t}} \int_0^{2x} e^{-\frac{(x-y)^2}{4it}} F(y)dy &= -\frac{1}{2} \int_0^{2x} \frac{d}{dy} \operatorname{erf}\left(\frac{x-y}{2\sqrt{it}}\right) F(y)dy \\ &= \frac{1}{2} \left(\operatorname{erf}\left(\frac{x}{2\sqrt{it}}\right) F(0) - \operatorname{erf}\left(\frac{-x}{2\sqrt{it}}\right) F(2x) + \int_0^{2x} \operatorname{erf}\left(\frac{x-y}{2\sqrt{it}}\right) F'(y)dy \right). \end{aligned}$$

Using $\lim_{t\to 0^+} \operatorname{erf}\left(\frac{\xi}{2\sqrt{it}}\right) = \operatorname{sgn}(\xi)$, $\xi \in \mathbb{R}$, and the dominated convergence theorem we get

$$\lim_{t\to 0^+} \frac{1}{2\sqrt{i\pi t}} \int_0^{2x} e^{-\frac{(x-y)^2}{4it}} F(y)dy = \frac{1}{2} \left(F(0) + F(2x) + \int_0^{2x} \operatorname{sgn}(x-y) F'(y)dy \right) = F(x).$$

In the second integral in (4.16) we substitute $y \to y + 2x$ and obtain

$$\frac{1}{2\sqrt{i\pi t}} \int_{2x}^{\infty} e^{-\frac{(x-y)^2}{4it}} F(y)dy = \frac{1}{2\sqrt{i\pi t}} \int_0^{\infty} e^{-\frac{(x+y)^2}{4it}} F(y+2x)dy.$$

This is the same integral as the one for Ψ_0, with the initial function $F(\cdot + 2x)$ instead of F. Consequently, this integral also vanishes in the limit $t \to 0^+$. Thus, we have also shown the initial condition (4.11) for Ψ_{free}. □

As the last preparatory statement we prove the following lemma about the representation of the functions Ψ_0, Ψ_1, and Ψ_{free} at the support of the singular interaction $x = 0^\pm$.

Lemma 4.3. *Let $F : \Omega \to \mathbb{C}$ be holomorphic on an open set $\Omega \subseteq \mathbb{C}$ which contains the sector S_α from (4.1) for some $\alpha \in (0, \frac{\pi}{2})$, and assume that F satisfies the estimate*

$$|F(z)| \leq A\, e^{B\,\operatorname{Im}(z)}, \qquad z \in S_\alpha, \tag{4.17}$$

for some $A, B \geq 0$. *Then for the functions* Ψ_j, $j \in \{0, 1, \text{free}\}$, *from* (4.6) *and their spatial derivatives we are allowed to carry the limit* $x \to 0^{\pm}$ *inside the integral*

$$\Psi_j(t, 0^{\pm}; F) = \int_0^{\infty} G_j(t, 0^{\pm}, y) F(y) dy, \tag{4.18a}$$

$$\frac{\partial}{\partial x} \Psi_j(t, 0^{\pm}; F) = \int_0^{\infty} \frac{\partial}{\partial x} G_j(t, 0^{\pm}, y) F(y) dy, \tag{4.18b}$$

where, similar to (4.7)*, the integrals exist as improper Riemann integrals* $\int_0^{\infty} := \lim_{R \to \infty} \int_0^R$.

Proof. For the function Ψ_j in the representation (4.8) we have the estimate

$$\left| G_j(t, x, ye^{i\alpha}) F(ye^{i\alpha}) \right| \leq A c_j(t) e^{-\frac{y^2 \sin(2\alpha)}{4t} + y(B + \frac{|x|}{2t}) \sin(\alpha)}, \tag{4.19}$$

which follows from the assumption (4.17) on F and (2.16). Since this upper bound is continuous in x, we can choose it to be uniform for all x in a neighbourhood of 0. Now we can use the dominated convergence theorem in (4.8) to get the absolutely integrable representation

$$\Psi_j(t, 0^{\pm}; F) = e^{i\alpha} \int_0^{\infty} G_j(t, 0^{\pm}, ye^{i\alpha}) F(ye^{i\alpha}) dy. \tag{4.20}$$

Once more from (4.17) and (2.16) we get the estimate

$$\left| G_j(t, 0^{\pm}, z) F(z) \right| \leq A c_j(t)\, e^{-\frac{\operatorname{Im}(z^2)}{4t} + B \operatorname{Im}(z)}, \qquad z \in S_\alpha.$$

The estimate (4.13) for $x = 0$ allows to further estimate the integrand by

$$\left| G_j(t, 0^{\pm}, z) F(z) \right| \leq A c_j(t)\, e^{-\frac{\operatorname{Im}(z^2)}{8t} + t B^2 \tan(\alpha)}, \qquad z \in S_\alpha. \tag{4.21}$$

This estimate shows, in particular, that the assumption (4.2) of Lemma 4.1 is satisfied and hence we can use (4.3) to rewrite the absolutely integrable representation (4.20) into the improper Riemann integral (4.18a).

The same argument applies also to the spatial derivative in (4.14b). Here, the explicit representations (2.12b), (2.13b), and (2.14b) lead to a similar estimates as in (2.16), and consequently also to estimates of the form (4.19) and (4.21). □

The next theorem is the main result of this section, where a solution Ψ of the Schrödinger equation (1.4) is obtained by assembling the components Ψ_j from (4.6) based on the structure of the Green's function in (2.17). Besides the four parts of the Green's function we also have to consider that now integrals over $\mathbb{R}$ appear, whereas the integrals in (4.6) are only over the positive half line $(0, \infty)$.

Theorem 4.4. *Let $F : \Omega \to \mathbb{C}$ be holomorphic on an open set $\Omega \subseteq \mathbb{C}$ which contains the double sector*

$$S_\alpha \cup (-S_\alpha) = \{ z \in \mathbb{C} : \mathrm{Arg}(z) \in [0, \alpha] \cup [\pi, \pi + \alpha] \} \tag{4.22}$$

for some $\alpha \in (0, \frac{\pi}{2})$, and assume that F satisfies the estimate

$$|F(z)| \leq A\, e^{B|\mathrm{Im}(z)|}, \qquad z \in S_\alpha \cup (-S_\alpha), \tag{4.23}$$

for some $A, B \geq 0$. Let G be the Green's function in (1.5) or (2.17). Then the function

$$\Psi(t, x; F) = \int_{\mathbb{R}} G(t, x, y) F(y) dy, \qquad t > 0,\ x \in \mathbb{R} \setminus \{0\}, \tag{4.24}$$

exists as an improper Riemann integral of the form

$$\int_{\mathbb{R}} G(t, x, y) F(y) dy := \lim_{R_1 \to \infty} \int_{-R_1}^{0} G(t, x, y) F(y) dy + \lim_{R_2 \to \infty} \int_{0}^{R_2} G(t, x, y) F(y) dy \tag{4.25}$$

and Ψ is a solution of the Schrödinger equation (1.4).

Proof. For $y > 0$ the Green's function (2.17) can be written as

$$\begin{aligned} G(t, x, y) = {} & \mu_+^{(x,0^+)} G_1(t, x, y; \omega_+) + \mu_-^{(x,0^+)} G_1(t, x, y; \omega_-) + \mu_0^{(x,0^+)} G_0(t, x, y) \\ & + G_{\mathrm{free}}(t, x, y). \end{aligned}$$

Hence we conclude from Lemma 4.2 (i) that the limit

$$\begin{aligned} \lim_{R_2 \to \infty} \int_0^{R_2} G(t, x, y) F(y) dy = {} & \mu_+^{(x,0^+)} \Psi_1(t, x; \omega_+, F) + \mu_-^{(x,0^+)} \Psi_1(t, x; \omega_-, F) \\ & + \mu_0^{(x,0^+)} \Psi_0(t, x; F) + \Psi_{\mathrm{free}}(t, x; F) \end{aligned}$$

exists. Moreover, for $y > 0$ we also have

$$\begin{aligned} G(t, x, -y) = {} & \mu_+^{(x,0^-)} G_1(t, x, y; \omega_+) + \mu_-^{(x,0^-)} G_1(t, x, y; \omega_-) + \mu_0^{(x,0^-)} G_0(t, x, y) \\ & + G_{\mathrm{free}}(t, -x, y), \end{aligned}$$

where we have used $G_{\mathrm{free}}(t, x, -y) = G_{\mathrm{free}}(t, -x, y)$, a direct consequence of (2.10c). Again from Lemma 4.2 (i) we conclude that also the limit

$$\lim_{R_1\to\infty}\int_{-R_1}^{0} G(t,x,y)F(y)dy = \lim_{R_1\to\infty}\int_{0}^{R_1} G(t,x,-y)\widetilde{F}(y)dy$$

$$= \mu_+^{(x,0^-)}\Psi_1(t,x;\omega_+,\widetilde{F}) + \mu_-^{(x,0^-)}\Psi_1(t,x;\omega_-,\widetilde{F})$$

$$+ \mu_0^{(x,0^-)}\Psi_0(t,x;\widetilde{F}) + \Psi_{\text{free}}(t,-x;\widetilde{F})$$

exists. Here we have used the mirrored function $\widetilde{F}(z) := F(-z)$, which also satisfies the assumption (4.5), since (4.23) holds on the double sector $S_\alpha \cup (-S_\alpha)$. This leads to the existence of the function Ψ in (4.24) in the sense of (4.25), and also shows that it can be decomposed into

$$\begin{aligned}\Psi(t,x;F) = {} & \mu_+^{(x,0^-)}\Psi_1(t,x;\omega_+,\widetilde{F}) + \mu_+^{(x,0^+)}\Psi_1(t,x;\omega_+,F)\\ & + \mu_-^{(x,0^-)}\Psi_1(t,x;\omega_-,\widetilde{F}) + \mu_-^{(x,0^+)}\Psi_1(t,x;\omega_-,F)\\ & + \mu_0^{(x,0^-)}\Psi_0(t,x;\widetilde{F}) + \mu_0^{(x,0^+)}\Psi_0(t,x;F)\\ & + \Psi_{\text{free}}(t,-x;\widetilde{F}) + \Psi_{\text{free}}(t,x;F).\end{aligned} \tag{4.26}$$

Due to (4.9) the functions Ψ_0, Ψ_1, and Ψ_{free} are solutions of the differential equation, and so is its linear combination Ψ a solution of (1.4a). Note, that the coefficients $\mu_\pm$ and μ_0 only depend on the sign of x and hence do not influence the differential equation. Moreover, although the term $\Psi_{\text{free}}(t,-x,\widetilde{F})$ depends on the variable $-x$, this function also solves (1.4a) since the x-derivative is of second order.

In order to check the jump condition (1.4b) we notice that by Lemma 4.3 we are allowed to carry the limit $x \to 0^\pm$ inside the integral. Hence we get the representations

$$\Psi(t,0^\pm;F) = \int_{\mathbb{R}} G(t,0^\pm,y)F(y)dy,$$

$$\frac{\partial}{\partial x}\Psi(t,0^\pm;F) = \int_{\mathbb{R}} \frac{\partial}{\partial x}G(t,0^\pm,y)F(y)dy,$$

also for the linear combination. Again, note that the negative x argument of $\Psi_{\text{free}}(t,-x;\widetilde{F})$ does not matter, since $G_{\text{free}}(t,0^+,y) = G_{\text{free}}(t,0^-,y)$ by definition (2.10c). Since G satisfies the jump condition (2.21), the function Ψ satisfies the jump condition (1.4b). Finally, the initial values (4.10) and (4.11) imply the initial condition (1.4c) of the wave function Ψ. □

In preparation for the analysis of superoscillations in the next section we will now briefly discuss convergent sequences of initial conditions $(F_n)_n$ and the convergence of the corresponding solutions $(\Psi(t,x;F_n))_n$ of the Schrödinger equation (1.4). As before we shall first deal with the functions Ψ_j, $j \in \{0,1,\text{free}\}$, in (4.6) and assemble these components afterwards to the whole wave function Ψ; cf. (4.26) in the proof of Theorem 4.4.

Lemma 4.5. *Let $F, F_n : \Omega \to \mathbb{C}$, $n \in \mathbb{N}_0$, be holomorphic on an open set $\Omega \subseteq \mathbb{C}$ which contains the sector S_α from (4.1) for some $\alpha \in (0,\frac{\pi}{2})$, and assume that for some $A, B \geq 0$ and $A_n, B_n \geq 0$, $n \in \mathbb{N}_0$, the exponential bounds (4.5) hold. If the sequence $(F_n)_n$ converges as*

$$\lim_{n\to\infty} \sup_{z\in S_\alpha} \left|F_n(z) - F(z)\right| e^{-C|z|} = 0 \tag{4.27}$$

for some $C \geq 0$*, then also the corresponding wave functions* Ψ_j*,* $j \in \{0, 1, \text{free}\}$*, in* (4.6) *converge as*

$$\lim_{n\to\infty} \Psi_j(t, x; F_n) = \Psi_j(t, x; F), \qquad j \in \{0, 1, \text{free}\}, \tag{4.28}$$

uniformly on compact subsets of $(0, \infty) \times \mathbb{R}$.

Proof. First of all, we have the estimate

$$\left|F_n(z) - F(z)\right| \leq C_n e^{C|z|}, \qquad z \in S_\alpha,$$

where $C_n := \sup_{z\in S_\alpha} |F_n(z) - F(z)|e^{-C|z|}$. Using the representation (4.8), this inequality together with the estimate (2.16) of the Green's function, leads to

$$\begin{aligned}\left|\Psi_j(t, x; F_n) - \Psi_j(t, x; F)\right| &= \left|\int_0^\infty G_j(t, x, ye^{i\alpha})\big(F_n(ye^{i\alpha}) - F(ye^{i\alpha})\big)dy\right| \\ &\leq C_n c_j(t) \int_0^\infty e^{-\frac{y^2\sin(2\alpha)}{4t} + \frac{|x|y\sin(\alpha)}{2t}} e^{Cy} dy \\ &= C_n \frac{c_j(t)\sqrt{\pi t}}{\sqrt{\sin(2\alpha)}} \Lambda\Big(-\frac{|x|\sqrt{\tan(\alpha)}}{2\sqrt{2t}} - \frac{C\sqrt{t}}{\sqrt{\sin(2\alpha)}}\Big),\end{aligned}$$

where in the last line we have used the integral (2.7a). Since the right hand side of this inequality is continuous in $t \in (0, \infty)$ and $x \in \mathbb{R}$, and we have $C_n \to 0$ by the assumption (4.27), the uniform convergence (4.28) on compact subsets of $(0, \infty) \times \mathbb{R}$ follows. □

Lemma 4.5 now leads to the following theorem, which is an important ingredient in the next section.

Theorem 4.6. *Let* $F, F_n : \Omega \to \mathbb{C}$*,* $n \in \mathbb{N}_0$*, be holomorphic on an open set* $\Omega \subseteq \mathbb{C}$ *which contains the double sector* $S_\alpha \cup (-S_\alpha)$ *from* (4.22) *for some* $\alpha \in (0, \frac{\pi}{2})$*, and assume that for some* $A, B \geq 0$ *and* $A_n, B_n \geq 0$*,* $n \in \mathbb{N}_0$*, the exponential bounds* (4.23) *hold. If the sequence* $(F_n)_n$ *converges as*

$$\lim_{n\to\infty} \sup_{z\in S_\alpha\cup(-S_\alpha)} \left|F_n(z) - F(z)\right| e^{-C|z|} = 0 \tag{4.29}$$

for some $C \geq 0$*, then also the corresponding wave functions* Ψ *in* (4.24) *converge as*

$$\lim_{n\to\infty} \Psi(t, x; F_n) = \Psi(t, x; F), \tag{4.30}$$

uniformly on compact subsets of $(0, \infty) \times \mathbb{R}$.

Proof. It is clear that the convergence (4.29) of the functions F_n, $n \in \mathbb{N}_0$, implies the same convergence of the mirrored functions $\widetilde{F}_n(z) = F_n(-z)$, $n \in \mathbb{N}_0$, and $\widetilde{F}(z) = F(-z)$. Since the function Ψ can be decomposed in the form (4.26), the convergence (4.30) follows immediately from Lemma 4.5. □

5. Superoscillatory initial data and plane wave asymptotics

In this section we allow superoscillatory functions as initial data in the Schrödinger equation (1.4) and we show that the corresponding solutions converge uniformly on compact sets. To discuss the oscillatory properties of these solutions we study the long time asymptotics of the plane wave solution in Theorem 5.5 and Remark 5.7, where the expected oscillatory behaviour and also possible stationary terms, reflecting negative bound states of the singular potential, are identified.

Superoscillating functions are band-limited functions that can oscillate faster than their fastest Fourier component. This is made precise in the next definition.

Definition 5.1 *(Superoscillations).* A *generalized Fourier sequence* is a sequence of functions $(F_n)_n$, $n \in \mathbb{N}_0$, of the form

$$F_n(x) = \sum_{j=0}^{n} c_j(n) e^{ik_j(n)x}, \qquad x \in \mathbb{R}, \tag{5.1}$$

with $k_j(n) \in \mathbb{R}$ and $c_j(n) \in \mathbb{C}$, $j \in \{0, \dots, n\}$. A generalized Fourier sequence $(F_n)_n$ is said to be *superoscillating*, if:

(i) There exists some $k \in \mathbb{R}$ such that

$$\sup_{n \in \mathbb{N}_0,\, j \in \{0,\dots,n\}} |k_j(n)| < |k|.$$

(ii) There exists a compact subset $K \subset \mathbb{R}$, called *superoscillation set*, such that

$$\lim_{n\to\infty} \sup_{x \in K} \left| F_n(x) - e^{ikx} \right| = 0. \tag{5.2}$$

In the next corollary, which is a simple consequence of Theorem 4.6, it will be shown that superoscillating initial data $(F_n)_n$ (with a slightly stronger convergence property) leads to solutions $(\Psi(t, x; F_n))_n$ that converge on compact subsets for all times $t > 0$. We mention that the characteristic superoscillatory behaviour of the functions $(F_n)_n$ is on a compact set K in (5.2), but this is not enough to ensure the same convergence for the sequence of solutions $(\Psi(t, x; F_n))_n$. As the functions (5.1) admit entire extensions to the whole complex plane,

$$F_n(z) = \sum_{j=0}^{n} c_j(n) e^{ik_j(n)z}, \qquad z \in \mathbb{C}, \tag{5.3}$$

a fact that is also important for several considerations related with the so-called supershift property, it is meaningful to assume the stronger convergence

$$\lim_{n\to\infty}\sup_{z\in\mathbb{C}}\left|F_n(z)-e^{ikz}\right|e^{-C|z|}=0 \tag{5.4}$$

for some $C \geq 0$. Note, that in our standard example of superoscillating functions in (1.7) one indeed has this kind of uniform convergence; cf. [37, Theorem 2.1] and [8] for more details.

Corollary 5.2 *(Stability of superoscillations). Let the sequence $(F_n)_n$, $n \in \mathbb{N}_0$, be superoscillating in the sense of Definition 5.1 and assume, in addition, that their entire extensions* (5.3) *converge as in* (5.4) *for some $C \geq 0$. Then also the corresponding solutions of* (1.4) *converge as*

$$\lim_{n\to\infty}\Psi(t,x;F_n)=\Psi(t,x;e^{ik\cdot}),$$

uniformly on compact subsets of $(0,\infty)\times\mathbb{R}$.

Proof. In order to apply Theorem 4.6, we first note that (5.3) implies the estimate

$$|F_n(z)| \leq \sum_{j=0}^{n}|c_j(n)|e^{\mathrm{Re}(ik_j(n)z)} \leq \sum_{j=0}^{n}|c_j(n)|e^{|k_j(n)||\mathrm{Im}(z)|}, \qquad z\in\mathbb{C}.$$

Together with the convergence (5.4) this shows that the functions F_n satisfy the assumptions of Theorem 4.6 for any $\alpha \in (0, \frac{\pi}{2})$, and hence the statement follows. □

To analyse the oscillatory behaviour of the functions $\Psi(t,x;F_n)$ and $\Psi(t,x;e^{ik\cdot})$ in Corollary 5.2 it is useful to compute the explicit form of the plane wave solution $\Psi(t,x;e^{ik\cdot})$ and to provide its long time asymptotics.

Proposition 5.3. *For every $k \in \mathbb{R}$ the solution of the Schrödinger equation* (1.4) *with initial condition $F(x) = e^{ikx}$ is given by*

$$\begin{aligned}\Psi(t,x;e^{ik\cdot}) &= \left(\frac{\mu_+^{(x,0^+)}}{\omega_+ + ik}+\frac{\mu_-^{(x,0^+)}}{\omega_- + ik}+\frac{\mu_0^{(x,0^+)}}{2}\right)e^{-\frac{x^2}{4it}}\Lambda\Big(\frac{|x|}{2\sqrt{it}}-ik\sqrt{it}\Big)\\ &+\left(\frac{\mu_+^{(x,0^-)}}{\omega_+ - ik}+\frac{\mu_-^{(x,0^-)}}{\omega_- - ik}+\frac{\mu_0^{(x,0^-)}}{2}\right)e^{-\frac{x^2}{4it}}\Lambda\Big(\frac{|x|}{2\sqrt{it}}+ik\sqrt{it}\Big)\\ &-\sum_{j=\pm}\left(\frac{\mu_j^{(x,0^-)}}{\omega_j - ik}+\frac{\mu_j^{(x,0^+)}}{\omega_j + ik}\right)e^{-\frac{x^2}{4it}}\Lambda\Big(\frac{|x|}{2\sqrt{it}}+\omega_j\sqrt{it}\Big)\\ &+e^{ikx-ik^2t},\end{aligned} \tag{5.5}$$

using the coefficients μ_0, $\mu_\pm$, and $\omega_\pm$ from Theorem 2.4. In the special case $k = 0$ this formula is understood in the sense that $\mu_j^{(x,0^\pm)}/\omega_j = 0$, whenever $\omega_j = 0$.

Proof. We start by calculating the functions $\Psi_j(t,x,e^{ik\cdot})$ for $j \in \{0, 1, \text{free}\}$ from (4.6). Since the holomorphic continuation $F(z) = e^{ikz}$ of the initial condition satisfies the assumption (4.5) for the special choice $\alpha = \frac{\pi}{4}$, we can use the absolutely convergent integral representation (4.8). For the functions Ψ_0 and Ψ_{free} we now use the integral identity (2.7a) to get

$$\Psi_0\big(t, x; e^{\pm ik\cdot}\big) = \frac{1}{2\sqrt{\pi t}} \int_0^\infty e^{-\frac{(|x|+y\sqrt{i})^2}{4it}} e^{\pm iky\sqrt{i}} dy = \frac{1}{2} e^{-\frac{x^2}{4it}} \Lambda\Big(\frac{|x|}{2\sqrt{it}} \mp ik\sqrt{it}\Big),$$

as well as

$$\Psi_{\mathrm{free}}\big(t, x; e^{\pm ik\cdot}\big) = \frac{1}{2\sqrt{\pi t}} \int_0^\infty e^{-\frac{(x-y\sqrt{i})^2}{4it}} e^{\pm iky\sqrt{i}} dy = \frac{1}{2} e^{-\frac{x^2}{4it}} \Lambda\Big(\frac{-x}{2\sqrt{it}} \mp ik\sqrt{it}\Big).$$

For the function Ψ_1 we use the integral (2.7b) to get, at least for ω and k not both vanishing, the explicit solution

$$\begin{aligned}\Psi_1\big(t, x; \omega, e^{\pm ik\cdot}\big) &= \sqrt{i} \int_0^\infty \Lambda\Big(\frac{|x| + y\sqrt{i}}{2\sqrt{it}} + \omega\sqrt{it}\Big) e^{-\frac{(|x|+y\sqrt{i})^2}{4it}} e^{\pm iky\sqrt{i}} dy \\ &= \frac{e^{-\frac{x^2}{4it}}}{\omega \pm ik} \left(\Lambda\Big(\frac{|x|}{2\sqrt{it}} \mp ik\sqrt{it}\Big) - \Lambda\Big(\frac{|x|}{2\sqrt{it}} + \omega\sqrt{it}\Big)\right).\end{aligned}$$

For the special case $\omega = k = 0$ the second integral in (2.7b) gives

$$\Psi_1(t, x; 0, 1) = \sqrt{i} \int_0^\infty \Lambda\Big(\frac{|x| + y\sqrt{i}}{2\sqrt{it}}\Big) e^{-\frac{(|x|+y\sqrt{i})^2}{4it}} dy = -\sqrt{it}\, \Lambda'\left(\frac{|x|}{2\sqrt{it}}\right) e^{-\frac{x^2}{4it}};$$

here, however, the precise value of the integral is not needed since $\mu_j^{(x,y)} = 0$, $j = \pm$, whenever $\omega_j = 0$ in Cases I-III in Theorem 2.4, and thus the corresponding term in the decomposition (4.26) is absent. Assembling now all these terms as in the decomposition (4.26) and using the identity (2.4) for the terms involving Ψ_{free} gives (5.5). □

In the next example we provide an explicit form of the solution $\Psi(t, x; e^{ik\cdot})$ in (5.5) for decoupled systems, that is, separated interface (or boundary) conditions at the origin.

Example 5.4. Observe first that the interface conditions in (1.4b) decouple (separate) if and only if the matrix J is of diagonal form, i.e. $\beta = 0$ in (2.18). Furthermore, since in general $|\alpha|^2 + |\beta|^2 = 1$ it follows that the interaction depends only on ϕ in (2.18) and $\mathrm{Arg}(\alpha)$. In this situation the wave function of the negative half line does not interact with the wave function on the positive half line, and this property is also manifested in the plane wave solution (5.5). In fact, for decoupled systems a technical computation shows that the solution admits the form

$$\Psi(t, x; e^{ik\cdot}) = \begin{cases} \Psi_+(t, x; e^{ik\cdot}), & \text{if } x > 0, \\ \Psi_-(t, x; e^{ik\cdot}), & \text{if } x < 0, \end{cases} \tag{5.6}$$

where $\Psi_\pm$ depend only on the coefficients

$$\gamma_\pm := \tan\Big(\frac{\phi \pm \mathrm{Arg}(\alpha)}{2}\Big).$$

Here the functions $\Psi_\pm$ are explicitely given by

$$\begin{aligned}\Psi_\pm(t,x;e^{ik\cdot}) =& \frac{1}{2}e^{-\frac{x^2}{4it}}\left(\frac{\gamma_\pm \pm ik}{-\gamma_\pm \pm ik}\Lambda\Big(\frac{|x|}{2\sqrt{it}} \mp ik\sqrt{it}\Big) - \Lambda\Big(\frac{|x|}{2\sqrt{it}} \pm ik\sqrt{it}\Big)\right)\\ &+ \frac{\gamma_\pm}{\gamma_\pm \mp ik}e^{-\frac{x^2}{4it}}\Lambda\Big(\frac{|x|}{2\sqrt{it}} - \gamma_\pm\sqrt{it}\Big) + e^{ikx-ik^2t};\end{aligned}$$

in the case $\gamma_+ = \infty$ and/or $\gamma_- = \infty$ (that is, $\phi + \mathrm{Arg}(\alpha) = \pi$ and/or $\phi - \mathrm{Arg}(\alpha) = \pi$) this is understood in the sense that

$$\frac{\infty \pm ik}{-\infty \pm ik} := -1 \qquad \text{and} \qquad \frac{\infty}{\infty \mp ik}\Lambda\Big(\frac{|x|}{2\sqrt{it}} - \infty\sqrt{it}\Big) := 0.$$

In the next theorem the long time asymptotics of the plane wave solution in Proposition 5.3 is found. While the exponentially decaying $e^{\omega_j|x|}$-terms in (5.7) and (5.8) are due to negative bound states (see Remark 5.7), the oscillating terms e^{ikx} and $e^{i|kx|}$ in the first line of (5.7), or their absence in (5.8), show that the solution $\Psi(t,x;e^{ik\cdot})$ oscillates with frequency k. Therefore, roughly speaking, the sequence $(\Psi(t,x;F_n))_n$ shows the characteristic superoscillatory property since the functions $\Psi(t,x;F_n)$ oscillate with the frequencies $k_j(n)$ and the limit function $\Psi(t,x;e^{ik\cdot})$ oscillates with the larger frequency k.

Theorem 5.5. *For every $k \in \mathbb{R}\setminus\{0\}$ the solution of the Schrödinger equation (1.4) with initial condition $F(x) = e^{ikx}$ admits the long time asymptotics*

$$\begin{aligned}\Psi(t,x;e^{ik\cdot}) =& e^{ikx-ik^2t} + 2\left(\frac{\mu_+^{(x,-k)}}{\omega_+ - i|k|} + \frac{\mu_-^{(x,-k)}}{\omega_- - i|k|} + \frac{\mu_0^{(x,-k)}}{2}\right)e^{i|kx|-ik^2t}\\ &- \sum_{j=\pm}\left(\frac{\mu_j^{(x,0^-)}}{\omega_j - ik} + \frac{\mu_j^{(x,0^+)}}{\omega_j + ik}\right)2\Theta(-\omega_j)e^{\omega_j|x|+i\omega_j^2t} + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big),\end{aligned} \tag{5.7}$$

as $t \to \infty$, using the coefficients μ_0, $\mu_\pm$, and $\omega_\pm$ from Theorem 2.4. Moreover, for $k = 0$ we get the similar expansion

$$\begin{aligned}\Psi(t,x;1) =& \frac{\mu_+^{(x,0^+)} + \mu_+^{(x,0^-)}}{\omega_+} + \frac{\mu_-^{(x,0^+)} + \mu_-^{(x,0^-)}}{\omega_-} + \frac{\mu_0^{(x,0^+)} + \mu_0^{(x,0^-)}}{2} + 1\\ &- \sum_{j=\pm}\frac{\mu_j^{(x,0^-)} + \mu_j^{(x,0^+)}}{\omega_j}2\Theta(-\omega_j)e^{\omega_j|x|+i\omega_j^2t} + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big),\end{aligned} \tag{5.8}$$

as $t \to \infty$. The formula (5.8) is understood in the sense that $\mu_j^{(x,0^\pm)}/\omega_j = 0$, whenever $\omega_j = 0$.

Proof. In the explicit solution (5.5) we can use the asymptotic expansion (2.6) of the function Λ, to get for every $k, \omega_j \in \mathbb{R} \setminus \{0\}$

$$\Lambda\Big(\frac{|x|}{2\sqrt{it}} \pm ik\sqrt{it}\Big) = 2\Theta(\pm k) e^{(\frac{|x|}{2\sqrt{it}} \pm ik\sqrt{it})^2} + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big), \quad \text{as } t \to \infty,$$

$$\Lambda\Big(\frac{|x|}{2\sqrt{it}} + \omega_j\sqrt{it}\Big) = 2\Theta(-\omega_j) e^{(\frac{|x|}{2\sqrt{it}} + \omega_j\sqrt{it})^2} + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big), \quad \text{as } t \to \infty.$$

Note, that all the terms in (5.5) with $\omega_j = 0$ vanish since in this case also $\mu_j^{(x,0^\pm)} = 0$ by its definition in Theorem 2.4. Hence we can use the above asymptotics to get the long time behaviour

$$\begin{aligned}\Psi(t,x;e^{ik\cdot}) = &\left(\frac{\mu_+^{(x,0^+)}}{\omega_+ + ik} + \frac{\mu_-^{(x,0^+)}}{\omega_- + ik} + \frac{\mu_0^{(x,0^+)}}{2}\right) 2\Theta(-k) e^{-ik|x| - ik^2 t} \\ &+ \left(\frac{\mu_+^{(x,0^-)}}{\omega_+ - ik} + \frac{\mu_-^{(x,0^-)}}{\omega_- - ik} + \frac{\mu_0^{(x,0^-)}}{2}\right) 2\Theta(k) e^{ik|x| - ik^2 t} \\ &- \sum_{j=\pm} \left(\frac{\mu_j^{(x,0^-)}}{\omega_j - ik} + \frac{\mu_j^{(x,0^+)}}{\omega_j + ik}\right) 2\Theta(-\omega_j) e^{\omega_j |x| + i\omega_j^2 t} \\ &+ e^{ikx - ik^2 t} + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big), \quad \text{as } t \to \infty,\end{aligned}$$

which easily simplifies to (5.7). For $k = 0$ we get from (5.5) the representation

$$\begin{aligned}\Psi(t,x;1) = &\left(\frac{\mu_+^{(x,0^+)} + \mu_+^{(x,0^-)}}{\omega_+} + \frac{\mu_-^{(x,0^+)} + \mu_-^{(x,0^-)}}{\omega_-} + \frac{\mu_0^{(x,0^+)} + \mu_0^{(x,0^-)}}{2}\right) e^{-\frac{x^2}{4it}} \Lambda\Big(\frac{|x|}{2\sqrt{it}}\Big) \\ &- \sum_{j=\pm} \left(\frac{\mu_j^{(x,0^-)}}{\omega_j} + \frac{\mu_j^{(x,0^+)}}{\omega_j}\right) e^{-\frac{x^2}{4it}} \Lambda\Big(\frac{|x|}{2\sqrt{it}} + \omega_j\sqrt{it}\Big) + 1.\end{aligned}$$

Using the Taylor series $\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(2n+1)} z^{2n+1}$ we get the asymptotics

$$e^{-\frac{x^2}{4it}} \Lambda\Big(\frac{|x|}{2\sqrt{it}}\Big) = 1 - \operatorname{erf}\Big(\frac{|x|}{2\sqrt{it}}\Big) = 1 + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big).$$

Hence the wave function $\Psi(t,x;1)$ reduces to (5.8) in the limit $t \to \infty$. □

Example 5.6. In the same setting as in Example 5.4 one can compute the long time asymptotics (5.7) and (5.8) for decoupled systems. For $k \neq 0$ we obtain the wave function

$$\begin{aligned}\Psi(t,x;e^{ik\cdot}) =&\Theta(-kx)\Big(e^{ikx}+\frac{\gamma_{-\,\mathrm{sgn}(k)}-i|k|}{-\gamma_{-\,\mathrm{sgn}(k)}-i|k|}e^{-ikx}\Big)e^{-ik^2t}\\&+\Theta(-\gamma_+)\Theta(x)\frac{2\gamma_+}{\gamma_+-ik}e^{-\gamma_+x+i\gamma_+^2t}\\&+\Theta(-\gamma_-)\Theta(-x)\frac{2\gamma_-}{\gamma_-+ik}e^{\gamma_-x+i\gamma_-^2t}+\mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big)\end{aligned}$$

and for $k=0$ we find the representation

$$\Psi(t,x;1)=2\Theta(-\gamma_+)\Theta(x)e^{-\gamma_+x+i\gamma+^2t}+2\Theta(-\gamma_-)\Theta(-x)e^{\gamma_-x+i\gamma_-^2t}+\mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big).$$

Again, similar as in Example 5.4, if $\gamma_+=\infty$ and/or $\gamma_-=\infty$ are infinite (that is, $\phi+\mathrm{Arg}(\alpha)=\pi$ and/or $\phi-\mathrm{Arg}(\alpha)=\pi$) this is understood in the sense that

$$\frac{\infty-i|k|}{-\infty-i|k|}:=-1\qquad\text{and}\qquad\Theta(-\infty):=0.$$

Remark 5.7. We note that the $e^{\omega_j|x|}$-terms, $j=\pm$, in the asymptotics in (5.7) and (5.8) correspond to negative bound states of the underlying self-adjoint Schrödinger operator. In fact, a bound state corresponding to the eigenvalue (energy) $E\in\mathbb{R}$ is a function $\psi\in L^2(\mathbb{R})$ which satisfies

$$-\frac{\partial^2}{\partial x^2}\psi(x)=E\,\psi(x),\qquad x\in\mathbb{R}\setminus\{0\},\tag{5.9a}$$

$$(I-J)\begin{pmatrix}\psi(0^+)\\ \psi(0^-)\end{pmatrix}=i(I+J)\begin{pmatrix}\frac{\partial}{\partial x}\psi(0^+)\\ -\frac{\partial}{\partial x}\psi(0^-)\end{pmatrix}.\tag{5.9b}$$

In order to get a non-trivial L^2-solution of the differential equation (5.9a) we need $E<0$; in this case the general solution is given by

$$\psi(x)=\begin{cases}A\,e^{-x\sqrt{-E}}, & x>0,\\ B\,e^{x\sqrt{-E}}, & x<0,\end{cases}$$

for some constants $A,B\in\mathbb{C}$. Plugging the limits $\psi(0^\pm)$ and $\frac{\partial}{\partial x}\psi(0^\pm)$ into the jump condition leads to the linear system of equations

$$(I-J)\begin{pmatrix}A\\ B\end{pmatrix}=-i\sqrt{-E}\,(I+J)\begin{pmatrix}A\\ B\end{pmatrix}.\tag{5.10}$$

A direct calculation using the matrix (2.18) and the property $|\alpha|^2+|\beta|^2=1$ of the matrix entries shows

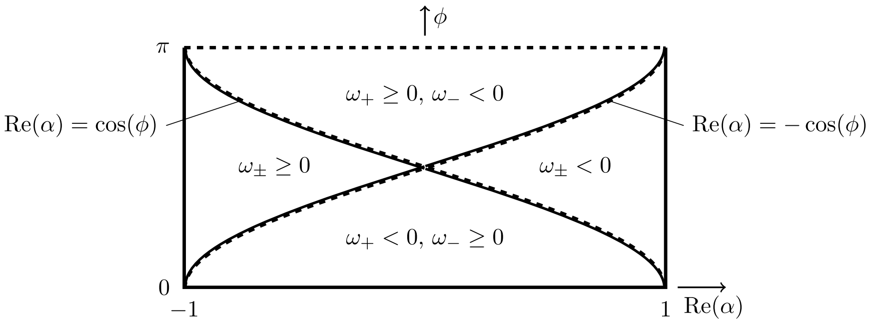


Fig. 1. Possible negative eigenvalues $\omega_\pm < 0$ of the Schrödinger operator depending on the choice of $\phi \in [0, \pi)$ and $\mathrm{Re}(\alpha) \in [-1, 1]$ in the matrix J. The continuous/dashed lines illustrate boundaries that do/don't belong to the parameter regions. Case III in Theorem 2.4 corresponds to the left lower corner $(-1, 0)$, Case II is depicted by the curve $\mathrm{Re}(\alpha) = -\cos(\phi)$, and the remaining points constitute Case I.

$$
\begin{aligned}
&\det\big((I-J) + i\sqrt{-E}(I+J)\big) \\
&\quad = \det\left(\begin{pmatrix} 1-\alpha e^{i\phi} & \bar\beta e^{i\phi} \\ -\beta e^{i\phi} & 1-\bar\alpha e^{i\phi}\end{pmatrix} + i\sqrt{-E}\begin{pmatrix} 1+\alpha e^{i\phi} & -\bar\beta e^{i\phi} \\ \beta e^{i\phi} & 1+\bar\alpha e^{i\phi}\end{pmatrix}\right) \\
&\quad = \big(1 - 2\,\mathrm{Re}(\alpha)e^{i\phi} + e^{2i\phi}\big) + 2i\big(1-e^{2i\phi}\big)\sqrt{-E} - \big(1 + 2\,\mathrm{Re}(\alpha)e^{i\phi} + e^{2i\phi}\big)\big(\sqrt{-E}\big)^2 \\
&\quad = 2e^{i\phi}\Big(\big(\cos(\phi) - \mathrm{Re}(\alpha)\big) + 2\sin(\phi)\sqrt{-E} - \big(\cos(\phi) + \mathrm{Re}(\alpha)\big)\big(\sqrt{-E}\big)^2\Big)
\end{aligned}
$$

and for $E < 0$ this determinant vanishes if and only if

$$
\sqrt{-E} = \begin{cases} \frac{\sin(\phi) \mp \sqrt{1-\mathrm{Re}(\alpha)^2}}{\cos(\phi)+\mathrm{Re}(\alpha)}, & \mathrm{Re}(\alpha) \neq -\cos(\phi), \\ -\cot(\phi), & \mathrm{Re}(\alpha) = -\cos(\phi) \neq -1. \end{cases}
$$

When comparing with the three different cases in Theorem 2.4 we see that $\sqrt{-E} = -\omega_\pm$ with $\omega_\pm < 0$ in Case I and $\sqrt{-E} = -\omega_+$ with $\omega_+ < 0$ in Case II lead to negative eigenvalues. More precisely, if $\omega := \omega_+ = \omega_- < 0$, then $E = -\omega^2$ is an eigenvalue of multiplicity two with linear independent eigenfunctions

$$
\psi_1(x) = e^{\omega|x|} \quad \text{and} \quad \psi_2(x) = \mathrm{sgn}(x)e^{\omega|x|}. \tag{5.11}
$$

If $\omega_+ \neq \omega_-$, then each $\omega_\pm < 0$ leads to an eigenvalue $E_\pm = -\omega_\pm^2$ of multiplicity one with corresponding eigenfunction

$$
\psi(x) = \left(1 \mp \frac{\mathrm{Im}(\beta) + \mathrm{sgn}(x)\big(\mathrm{Im}(\alpha) + i\,\mathrm{Re}(\beta)\big)}{\sqrt{1-\mathrm{Re}(\alpha)^2}}\right) e^{\omega_\pm|x|}; \tag{5.12}
$$

we leave it to the reader to check that the function in (5.11) and (5.12) satisfy the interface condition (5.10).

We conclude this section with an example illustrating Proposition 5.3 and Theorem 5.5 for the important special case of δ and δ'-potentials; cf. [2, Theorem 3.2].

Example 5.8. Using the coefficients μ_0, $\mu_\pm$, and $\omega_\pm$ from Example 3.2 and Example 3.3 it follows that for $k \in \mathbb{R}$ the plane wave solutions for the δ and δ'-interaction are given by

$$\begin{aligned}\Psi_\delta(t,x;e^{ik\cdot}) &= \Big(-\frac{c}{2(c+ik)}\Lambda\Big(\frac{|x|}{2\sqrt{it}} - ik\sqrt{it}\Big) - \frac{c}{2(c-ik)}\Lambda\Big(\frac{|x|}{2\sqrt{it}} + ik\sqrt{it}\Big) \\ &\qquad + \frac{c^2}{c^2+k^2}\Lambda\Big(\frac{|x|}{2\sqrt{it}} + c\sqrt{it}\Big)\Big) e^{-\frac{x^2}{4it}} + e^{ikx-ik^2t}, \\ \Psi_{\delta'}(t,x;e^{ik\cdot}) &= \Big(\frac{ik\,\mathrm{sgn}(x)}{2(c+ik)}\Lambda\Big(\frac{|x|}{2\sqrt{it}} - ik\sqrt{it}\Big) + \frac{ik\,\mathrm{sgn}(x)}{2(c-ik)}\Lambda\Big(\frac{|x|}{2\sqrt{it}} + ik\sqrt{it}\Big) \\ &\qquad - \frac{ikc\,\mathrm{sgn}(x)}{c^2+k^2}\Lambda\Big(\frac{|x|}{2\sqrt{it}} + c\sqrt{it}\Big)\Big) e^{-\frac{x^2}{4it}} + e^{ikx-ik^2t}.\end{aligned} \tag{5.13}$$

For $k \in \mathbb{R} \setminus \{0\}$ in the attractive case $c < 0$ their asymptotics as $t \to \infty$ are

$$\begin{aligned}\Psi_\delta(t,x;e^{ik\cdot}) &= e^{-ik^2t}\left(e^{ikx} - \frac{c}{c-i|k|}e^{i|kx|}\right) + \frac{2c^2}{c^2+k^2}e^{c|x|+ic^2t} + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big), \\ \Psi_{\delta'}(t,x;e^{ik\cdot}) &= e^{-ik^2t}\left(e^{ikx} + \frac{ik\,\mathrm{sgn}(x)}{c-i|k|}e^{i|kx|}\right) - \frac{2ick\,\mathrm{sgn}(x)}{c^2+k^2}e^{c|x|+ic^2t} + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big)\end{aligned} \tag{5.14}$$

and for $k \in \mathbb{R} \setminus \{0\}$ in the repulsive case $c > 0$ the asymptotics of the plane wave solutions as $t \to \infty$ are

$$\begin{aligned}\Psi_\delta(t,x;e^{ik\cdot}) &= e^{-ik^2t}\left(e^{ikx} - \frac{c}{c-i|k|}e^{i|kx|}\right) + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big), \\ \Psi_{\delta'}(t,x;e^{ik\cdot}) &= e^{-ik^2t}\left(e^{ikx} + \frac{ik\,\mathrm{sgn}(x)}{c-i|k|}e^{i|kx|}\right) + \mathcal{O}\Big(\frac{1}{\sqrt{t}}\Big).\end{aligned} \tag{5.15}$$

In the attractive case $c < 0$ the time evolutions

$$\psi_\delta(x) = \frac{2c^2}{c^2+k^2}e^{ic^2t}e^{c|x|} \quad \text{and} \quad \psi_{\delta'}(x) = -\frac{2ick}{c^2+k^2}e^{ic^2t}\,\mathrm{sgn}(x)e^{c|x|}$$

of the eigenfunctions $e^{c|x|}$ and $\mathrm{sgn}(x)e^{c|x|}$ (see also (5.11)) appear in (5.14); this is in accordance with Remark 5.7, see also Example 3.2 and Example 3.3. The function ψ_δ represents the damped wave that interacts with the δ-potential well (and similarly for $\psi_{\delta'}$). In fact, the exponential damping $e^{c|x|}$ in space, as well as the oscillations e^{ic^2t} in time, depend on c. In the repulsive case $c > 0$ equation (5.15) shows that for large times the wave keeps oscillating as e^{-ik^2t}, as the free wave does, but with a different complex prefactor, which means a different amplitude as well as a phase shift. Moreover, in the formulas (5.13) also the resonance frequencies $k = \pm ic$ appear, where the plane wave solutions have singularities. These observations are in accordance with the spectral theory results for the corresponding self-adjoint Schrödinger operators in [16, Chapter I.3.1, Theorem 3.1.4 and below].

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