

Distribution theory for Schrödinger's integral equation

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Much of the literature on point interactions in quantum mechanics has focused on the differential form of Schrödinger's equation. This paper, in contrast, investigates the integral form of Schrödinger's equation. While both forms are known to be equivalent for smooth potentials, this is not true for distributional potentials. Here, we assume that the potential is given by a distribution defined on the space of discontinuous test functions.

First, by using Schrödinger's integral equation, we confirm a seminal result by Kurasov, which was originally obtained in the context of Schrödinger's differential equation. This hints at a possible deeper connection between both forms of the equation. We also sketch a generalisation of Kurasov's result to hypersurfaces.

Second, we derive a new closed-form solution to Schrödinger's integral equation with a delta prime potential. This potential has attracted considerable attention, including some controversy. Interestingly, the derived propagator satisfies boundary conditions that were previously derived using Schrödinger's differential equation.

Third, we derive boundary conditions for 'super-singular' potentials given by higher-order derivatives of the delta potential. These boundary conditions cannot be incorporated into the normal framework of self-adjoint extensions. We show that the boundary conditions depend on the energy of the solution, and that probability is conserved.

This paper thereby confirms several seminal results and derives some new ones. In sum, it shows that Schrödinger's integral equation is a viable tool for studying singular interactions in quantum mechanics.

Keywords: point interaction, self-adjoint extension (SAE), singular potential, delta potential, delta prime potential, surface delta function, surface delta prime function, distribution theory, discontinuous test function

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I. INTRODUCTION

It has long been known that the Dirac delta potential allows for an exact solution to the time-dependent Schrödinger equation. Equally well known are the corresponding boundary conditions. It may be surprising, therefore, that the Dirac delta *prime* potential has caused headaches, and the corresponding boundary conditions have been subject to debate for much of the last three decades (see e.g.^{1,2,4-6,8,9,11,13,15-17,19,21-23,25-27,32,34,36-42,45-49,51-53,55-62}). It is worth discussing some of the ambiguities surrounding the delta prime potential in more detail (see also Table I):

- **Ambiguous Schrödinger equation:** It has been assumed (correctly) that the wave function ψ is discontinuous in the presence of a delta prime potential. However, the Schrödinger equation is then ambiguous (see e.g.⁴³). For many constructions of the delta prime, e.g. methods 2-4 in Table 1, the integral $\int \delta' \psi$ blows up, since the ‘slope’ of ψ is infinite at the origin.
- **Arbitrary boundary conditions:** To resolve this issue, many authors have decided that the delta prime potential is not to be taken literally. Instead, they define the delta prime *interaction* (as opposed to the delta prime potential) by some self-adjoint boundary condition. A jump in the value but not in the derivative is often assumed^{3,5,12,34,35,52,62}. However, this assumption is arbitrary at best and misleading at worst^{19,21,29,30}. (Indeed, we will show that a different operator, namely $\partial_x (\delta(x) \partial_x \cdot)$, which involves *two* derivatives, produces this particular boundary condition.)
- **Ambiguous limits:** Several authors have explicitly solved Schrödinger’s differential equation for potentials which, in the limit, are equal to the delta prime function. The boundary conditions can then be read off. The transition and reflection properties, however, depend crucially on ‘hidden parameters’ that determine how the potential approaches the limit (see e.g.^{19,36,53,57,58}). Further, this approach does not in general resolve the ambiguity of the Schrödinger equation, in the sense that $\int \delta' \psi$ does not generally exist if ψ is discontinuous.

Our approach is different in that we investigate the *integral form* of Schrödinger’s equation. We assume that the potential is equal to some distribution defined on the space of discontinuous test functions.

First, we replicate a seminal result by Kurasov⁴³, which is based on distribution theory for the *differential form* of Schrödinger’s equation. This is both reassuring and somewhat surprising, since the equivalence of both approaches is guaranteed only for smooth potentials. Our result thus hints at a deeper connection between the integral and differential forms of Schrödinger’s equation.

Second, we consider Schrödinger’s integral equation with a delta prime potential. As pointed out above, this potential has attracted considerable interest in the literature. We derive a new and exact solution for the time-dependent propagator. This solution satisfies boundary conditions previously derived by some authors in the context of distribution theory for Schrödinger’s differential equation, thereby further emphasizing the apparent equivalence of both approaches.

Third, we use Schrödinger’s integral equation to derive boundary conditions for higher-order derivatives of the delta potential. Such ‘super-singular’ potentials are of interest as they cannot be incorporated into the usual framework of self-adjoint extensions. We find that the associated boundary conditions are of the self-adjoint form — but with the crucial difference that the constants in the boundary conditions depend on the *energy* of the solution. We show that probability is conserved for these energy-dependent point interactions.

Method	Literature	Definition	Drawback
1. ‘Label’ for some BCs	1,4,5,34,51 2,6,21-23	$\psi'(0^+) = \psi'(0^-)$ $\psi(0^+) - \psi(0^-) \propto \psi'(0)$	ABC
2. Dipole interaction	26,48,52	$\lim_{\epsilon \searrow 0} \frac{1}{\epsilon^\nu} [\delta(x + \epsilon) + \delta(x - \epsilon)]$	ASE
3. Rectangular approximation	19,56,60	$\lim_{\epsilon, l \searrow 0} \frac{1}{\epsilon l} \left[\mathbb{1}_{[-\frac{l-\epsilon}{2} < x < -\frac{l+\epsilon}{2}]} \dots \right.$ $\left. \dots - \mathbb{1}_{[\frac{l-\epsilon}{2} < x < \frac{l+\epsilon}{2}]} \right]$	ASE, AL
4. Short-range potentials	36,39 37,38	$\lim_{\epsilon \searrow 0} \frac{1}{\epsilon^2} V(x/\epsilon)$ s.t. $\int V = 0, \int xV = -1$	ASE

Table I. Overview of common definitions of the delta prime potential in the literature. Possible drawbacks are an ambiguous Schrödinger equation (ASE), arbitrary boundary conditions (ABC), and ambiguous limits (AL).

This paper is structured as follows. Section II re-derives Kurasov’s potential based purely on a symmetry argument. Section III re-writes the corresponding boundary conditions concisely in the *jump-average* form. Section IV extends Kurasov’s result by showing that these boundary conditions follow directly from Schrödinger’s *integral* equation. Section V proposes to further extend this result to hypersurfaces. Section VI presents the scattering matrix in one dimension. Sections VII and VIII show that the jump-average boundary conditions form a subset of all possible self-adjoint extensions. Section IX derives a new, exact result for the propagator in the presence of a delta prime potential. Section X show that super-singular potentials, given by higher-order derivatives of the delta function, lead to energy-dependent boundary conditions that conserve probability. Section XI, finally, sums up our findings and points to future research.

II. KURASOV’S POTENTIAL REVISITED

Suppose we seek a Hermitian operator that connects the Dirac delta function with a maximum of two differential operators. We quickly see that we can construct *three* fundamental point interactions, namely

$$V(x) = c_1 \delta(x) + c_2 \frac{d}{dx} \delta(x) - \bar{c}_2 \delta(x) \frac{d}{dx} + c_3 \frac{d}{dx} \delta(x) \frac{d}{dx}. \quad (1)$$

It is understood that differential operators differentiate everything to their right. Complex conjugation is denoted by $\bar{\cdot}$. The requirement that V is Hermitian implies $c_1, c_3 \in \mathbb{R}$, while $c_2 \in \mathbb{C}$ is allowed. The action of the Dirac delta function on possibly discontinuous test functions has not yet been defined. The maximal domain of this operator is the Sobolev space $W_2^2(\mathbb{R} \setminus 0)$.

Assume the Dirac delta function is even under parity. Then it holds that the first and third point interactions, defined by c_1 and c_3 , are also even, since they contain an even number of derivatives. The second point interaction, defined by c_2 and \bar{c}_2 , on the other hand, is odd. If c_2 is real, the potential simplifies to

$$V = c_1 \delta(x) + c_2 \delta'(x) + c_3 \frac{d}{dx} \delta(x) \frac{d}{dx}.$$

The operator (1) was originally discovered by an entirely different route by Kurasov⁴³. We can make the correspondence explicit by taking

$$c_1 = X_1, \quad c_2 = X_2 + \mathfrak{i}X_3, \quad c_3 = -X_4,$$

with $X_1, X_2, X_3, X_4 \in \mathbb{R}$. In that notation, $L = -d^2/dx^2 + V$ can be written as

$$L = -\frac{d^2}{dx^2} + X_1 \delta(x) + \mathbf{i} \frac{d}{dx} \left(2X_3 \delta(x) - \mathbf{i} X_4 \delta'(x) \right) + \left(X_2 - \mathbf{i} X_3 \right) \delta'(x) - X_4 \frac{d^2}{dx^2} \delta(x), \quad (2)$$

which corresponds exactly to Kurasov p. 307. Our representation, which is different only in form, further underpins Kurasov's famous operator by showing that it follows directly from symmetry considerations.

Other authors^{7,14,20} have also considered operators of the form (1). For example, four independent complex numbers have been allowed in place of our c_1, c_2, \bar{c}_2 and c_3 ^{7,20}. The form (1) was subsequently derived using symmetry considerations⁷. It follows that there are four degrees of freedom, since only the second point interaction can be imaginary.

The historical labels associated with these point interactions have been summarised¹⁴, although it must be said that they can be somewhat misleading. Instead, we will simply refer to interactions defined by c_1, c_2 and c_3 as the first, second and third fundamental point interactions.

Of course, the above analysis could be extended to situations where a maximum of $n > 2$ differential operators are allowed. It would then be interesting to investigate whether the resulting boundary conditions are a self-adjoint extension of the operator $(-\mathbf{i} d/dx)^n$.

III. JUMP-AVERAGE BOUNDARY CONDITIONS

The boundary conditions corresponding to the operator (2) have been derived in the context of Schrödinger's differential equation⁴³ (p. 307-308). As it turns out, however, the resulting boundary conditions can be expressed differently, and quite naturally, using the average and discontinuity of the solution. To this end, we define $\{u\}$ and $[u]$ as follows:

$$\{u(0)\} = \frac{u(0^+) + u(0^-)}{2}, \quad [u(0)] = u(0^+) - u(0^-).$$

In line with Kurasov⁴³, we suppose that the action of the Dirac delta function on the space of discontinuous functions $u \in W_2^{(n+1)}(\mathbb{R} \setminus 0)$ is defined by

$$\int_{-\infty}^{\infty} \delta^{(n)}(x) u(x) dx = (-1)^n \{u^{(n)}(0)\}. \quad (3)$$

The boundary conditions associated with the operator (2), can now be written in compact form as

$$\begin{pmatrix} [u'(0)] \\ [u(0)] \end{pmatrix} = \begin{pmatrix} c_1 & -\bar{c}_2 \\ c_2 & c_3 \end{pmatrix} \begin{pmatrix} \{u(0)\} \\ \{u'(0)\} \end{pmatrix}, \quad c_1, c_3 \in \mathbb{R}, c_2 \in \mathbb{C}. \quad (4)$$

We will refer to these boundary conditions as the *jump-average boundary conditions*. In appearance they are quite different to the boundary conditions originally derived by Kurasov⁴³ (p. 307-308), but they are identical in content. In the next section, we will re-derive this important result — but in the context of the *integral* form of Schrödinger’s equation.

Boundary conditions of the jump-average form were first explored in the nineties by Exner and Grosse³⁰. They argue that the jump-average boundary conditions are “natural for the problem under consideration”. More recently, other authors^{10,14,20} have supposed that an *arbitrary* complex matrix connects the jumps to the averages — thus allowing eight degrees of freedom. A different set of papers has considered jump-average boundary conditions with the additional (but unnecessary) requirement that c_2 is real (see^{24,25,27,54}).

Interestingly, it is the *third* point interaction, given by $c_3 \partial_x(\delta(x) \partial_x \cdot)$, that generates a boundary condition labelled the ‘delta prime interaction’ by some authors. Since the third point interaction in fact contains two derivatives, this label can lead to confusion.

An attractive property of the jump-average representation, which seems to have been overlooked in the literature, is its behaviour under parity. As $x \rightarrow -x$, we get

$$\begin{pmatrix} [u'(0)] \\ [u(0)] \end{pmatrix} \rightarrow P \begin{pmatrix} [u'(0)] \\ [u(0)] \end{pmatrix}, \quad \begin{pmatrix} \{u(0)\} \\ \{u'(0)\} \end{pmatrix} \rightarrow P \begin{pmatrix} \{u(0)\} \\ \{u'(0)\} \end{pmatrix}, \quad \text{where } P = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

As a result, the connection matrix changes to

$$\begin{pmatrix} c_1 & -\bar{c}_2 \\ c_2 & c_3 \end{pmatrix} \rightarrow P \begin{pmatrix} c_1 & -\bar{c}_2 \\ c_2 & c_3 \end{pmatrix} P^{-1} = \begin{pmatrix} c_1 & \bar{c}_2 \\ -c_2 & c_3 \end{pmatrix}.$$

Thus c_1 and c_3 are even under parity, while c_2 is odd. Indeed, this was to be expected from the heuristic reasoning which led to the potential (1). For future reference, we note that the determinant $D = c_1 c_3 + |c_2|^2$ is real and even under parity.

IV. INTEGRAL EQUATION WITH KURASOV’S POTENTIAL

This section considers Schrödinger’s *integral* equation with the potential (1), which reads (see e.g.^{31,33,47,50}):

$$\psi(y, t|x, s) = \psi_0(y, t|x, s) - \mathfrak{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) V(\alpha) \psi(\alpha, \tau|x, s). \quad (5)$$

As in Kurasov⁴³, we take $\hbar = 1$ and $m = 1/2$. In these units, the free propagator ψ_0 reads

$$\psi_0(y, t|x, s) = \frac{1}{\sqrt{4\pi \text{i} (t-s)}} \exp \left[\frac{-(y-x)^2}{4 \text{i} (t-s)} \right], \quad t > s. \quad (6)$$

If the potential is singular, then ψ is not generally continuous. It is crucial, therefore, to define the potential as a distribution acting on the space of discontinuous test functions; otherwise the integral equation (5) goes undefined. For example, it is tempting to define the delta function as the limit of a Gaussian, and the delta prime as the limit of the derivative of a Gaussian. But then the integral equation (5) with the potential (1) has no solution. In that case, $\int \delta' \psi$ blows up for discontinuous ψ . Since the integral equation does not *allow* continuous solutions, and does not *exist* for discontinuous solutions, it has no solutions at all. In fact, only for a definition of the delta function (and its derivatives) that allows discontinuous test functions is there a solution to Schrödinger's integral equation.

The smoothness assumptions required on $\psi(\cdot, t|x, s)$ depend on the singularity of the potential. For the potential (1), it is sufficient to assume $\psi(\cdot, t|x, s) \in W_2^2(\mathbb{R} \setminus \{0\})$. Then Schrödinger's integral equation reads:

$$\begin{aligned} \psi(y, t|x, s) = & \psi_0(y, t|x, s) - c_1 \text{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta(\alpha) \psi(\alpha, \tau|x, s) \\ & - c_2 \text{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \frac{d}{d\alpha} \left(\delta(\alpha) \psi(\alpha, \tau|x, s) \right) \\ & + \bar{c}_2 \text{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta(\alpha) \frac{d}{d\alpha} \psi(\alpha, \tau|x, s) \\ & - c_3 \text{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \frac{d}{d\alpha} \left(\delta(\alpha) \frac{d}{d\alpha} \psi(\alpha, \tau|x, s) \right). \end{aligned}$$

The manipulations that follow are relatively straightforward. First, by writing out all dif-

ferentiations, we obtain

$$\begin{aligned}
\psi(y, t|x, s) = & \psi_0(y, t|x, s) - c_1 \mathbb{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta(\alpha) \psi(\alpha, \tau|x, s) \\
& - c_2 \mathbb{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta'(\alpha) \psi(\alpha, \tau|x, s) \\
& - c_2 \mathbb{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta(\alpha) \psi'(\alpha, \tau|x, s) \\
& + \bar{c}_2 \mathbb{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta(\alpha) \psi'(\alpha, \tau|x, s) \\
& - c_3 \mathbb{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta'(\alpha) \psi'(\alpha, \tau|x, s) \\
& - c_3 \mathbb{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta(\alpha) \psi''(\alpha, \tau|x, s).
\end{aligned}$$

Primes denote differentiation with respect to α . Second, using the definition of the Dirac delta function in (3), we get

$$\begin{aligned}
\psi(y, t|x, s) = & \psi_0(y, t|x, s) - c_1 \mathbb{i} \int_s^t d\tau \psi_0(y, t|0, \tau) \{\psi(0, \tau|x, s)\} \\
& + c_2 \mathbb{i} \int_s^t d\tau \left\{ \psi'_0(y, t|0, \tau) \psi(0, \tau|x, s) + \psi_0(y, t|0, \tau) \psi'(0, \tau|x, s) \right\} \\
& - c_2 \mathbb{i} \int_s^t d\tau \psi_0(y, t|0, \tau) \{\psi'(0, \tau|x, s)\} \\
& + \bar{c}_2 \mathbb{i} \int_s^t d\tau \psi_0(y, t|0, \tau) \{\psi'(0, \tau|x, s)\} \\
& + c_3 \mathbb{i} \int_s^t d\tau \left\{ \psi'_0(y, t|0, \tau) \psi'(0, \tau|x, s) + \psi_0(y, t|0, \tau) \psi''(0, \tau|x, s) \right\} \\
& - c_3 \mathbb{i} \int_s^t d\tau \psi_0(y, t|0, \tau) \{\psi''(0, \tau|x, s)\}.
\end{aligned}$$

Since the free propagator ψ_0 is smooth, it can be pulled out of the averaging operator. Four terms (two pairs) cancel, and we obtain

$$\begin{aligned}
\psi(y, t|x, s) = & \psi_0(y, t|x, s) - c_1 \mathbb{i} \int_s^t d\tau \psi_0(y, t|0, \tau) \{\psi(0, \tau|x, s)\} \\
& + c_2 \mathbb{i} \int_s^t d\tau \psi'_0(y, t|0, \tau) \{\psi(0, \tau|x, s)\} \\
& + \bar{c}_2 \mathbb{i} \int_s^t d\tau \psi_0(y, t|0, \tau) \{\psi'(0, \tau|x, s)\} \\
& + c_3 \mathbb{i} \int_s^t d\tau \psi'_0(y, t|0, \tau) \{\psi'(0, \tau|x, s)\}.
\end{aligned}$$

Finally, the free propagator $\psi_0(y, t|\alpha, \tau)$ satisfies $\partial_\alpha \psi_0 = -\partial_y \psi_0$. Therefore

$$\begin{aligned}
\psi(y, t|x, s) &= \psi_0(y, t|x, s) - c_1 \mathfrak{i} \int_s^t \psi_0(y, t|0, \tau) \{\psi(0, \tau|x, s)\} d\tau \\
&\quad - c_2 \mathfrak{i} \frac{d}{dy} \int_s^t \psi_0(y, t|0, \tau) \{\psi(0, \tau|x, s)\} d\tau \\
&\quad + \bar{c}_2 \mathfrak{i} \int_s^t \psi_0(y, t|0, \tau) \{\psi'(0, \tau|x, s)\} d\tau \\
&\quad - c_3 \mathfrak{i} \frac{d}{dy} \int_s^t \psi_0(y, t|0, \tau) \{\psi'(0, \tau|x, s)\} d\tau.
\end{aligned} \tag{7}$$

The derivatives with respect to y have been pulled to the outside of the integrals. This is allowed for all $y \neq 0$, where $\psi(\cdot, t|x, s)$ is smooth. As a result, we can meaningfully speak of $\{\psi(0, t|x, s)\}$ and $[\psi(0, t|x, s)]$. Of course, the quantities $\psi(0, t|x, s)$ and $\psi'(0, t|x, s)$ have no meaning.

The jump-average boundary conditions follow directly from the integral equation (7). To see why, consider the auxiliary function f , defined as

$$f(y, t|x, s) := -\mathfrak{i} \int_s^t \psi_0(y, t|0, \tau) g(\tau|x, s) d\tau, \tag{8}$$

where g is some other function. Note that all integral terms on the right-hand side of (7) can be written as either f or as $\partial_y f$ for some g . It can be shown that $f(\cdot, t|x, s)$ is discontinuous only for odd derivatives. Specifically,

$$\begin{aligned}
[f(0, t|x, s)] &= 0, \\
[f^{(1)}(0, t|x, s)] &= g(t|x, s), \\
[f^{(2)}(0, t|x, s)] &= 0.
\end{aligned} \tag{9}$$

This implies that $[\psi(0, t|x, s)]$ is determined purely by the second and fourth integrals in (7), which have the derivative d/dy in front of them. Similarly, $[\psi'(0, t|x, s)]$ is determined purely by the first and third integrals in (7), which have no derivative. The solution ψ , which appears on the left-hand side, inherits the discontinuities of all terms on the right-hand side. Thus, by (9), the integral equation (7) implies

$$\begin{pmatrix} [\psi'(0, t|x, s)] \\ [\psi(0, t|x, s)] \end{pmatrix} = \begin{pmatrix} c_1 & -\bar{c}_2 \\ c_2 & c_3 \end{pmatrix} \begin{pmatrix} \{\psi(0, t|x, s)\} \\ \{\psi'(0, t|x, s)\} \end{pmatrix}. \tag{10}$$

Thus Schrödinger's integral equation with the potential (1) implies the jump-average boundary conditions (4). While our conclusion is consistent with that of Kurasov⁴³ this was not a priori obvious, given that the differential and integral forms of Schrödinger's equation are known to be equivalent only for smooth potentials. Our result thus hints at a possible deeper connection between both forms of Schrödinger's equation. A further advantage of our method is that it can be extended relatively easily to hypersurfaces (see the next section) and to super-singular potentials (see section X).

V. EXTENSION TO HYPERSURFACES

This section sketches informally how Kurasov's result, as extended in the previous section to Schrödinger's integral equation, may be generalised further to surfaces of co-dimension one. A rigorous treatment would define self-adjoint operators acting on Sobolev spaces, and show resolvent convergence of operators used to approximate singular potentials. For the sake of brevity, however, we will confine ourselves to a heuristic treatment only. It is hoped that the reader will permit this brief digression, which demonstrates, albeit not overly rigorously, a neat link with classical potential theory.

As is well known, Dirac's delta function can be defined (purely formally) as the derivative of the Heaviside step function. In other words: as the inward-pointing derivative of the indicator function of the positive halfline. In higher dimensions, we argue, it is natural to consider the inward normal derivative of the indicator function of some domain D .

Let S be a smooth hypersurface enclosing some domain D in d dimensions, where the *inside* of S is defined to be the side where D is located. As in previous work⁴⁵, we define the surface delta function as $\delta_S(x) = n_x \cdot \nabla_x \mathbb{1}_{x \in D}$, where n_x is the inward normal, ∇_x is the gradient operator, and $\mathbb{1}_{x \in D}$ is the indicator function of the domain D . Similarly, again as in⁴⁵, we define the surface delta prime function as $\delta'_S(x) = n_x \cdot \nabla_x \delta_S(x) = \nabla_x^2 \mathbb{1}_{x \in D}$, i.e. as the Laplacian of the indicator function. Then, we extend these definitions to allow for discontinuous test functions as follows:

$$\begin{aligned} \int_{\mathbb{R}^d} \delta_S(x) u(x) dx &= \int_S \{u(\beta)\} d\beta, \\ \int_{\mathbb{R}^d} \delta'_S(x) u(x) dx &= - \int_S \{u'(\beta)\} d\beta. \end{aligned} \tag{11}$$

In analogy with one dimension, we use $\{\cdot\}$ and $[\cdot]$ to denote the average and discontinuity across the surface S in the inward normal direction, while a prime denotes the normal derivative, also in the inward direction. By taking D to be the positive real line, the one dimensional formulas are recovered. With these definitions, we propose the following hypersurface generalisation of (1):

$$V(x) = c_1 \delta_S(x) + c_2 (n_x \cdot \nabla_x) \delta_S(x) - \bar{c}_2 \delta_S(x) (n_x \cdot \nabla_x) + c_3 (n_x \cdot \nabla_x) \delta_S(x) (n_x \cdot \nabla_x). \quad (12)$$

In (1), we have simply replaced $\delta(x)$ by $\delta_S(x)$ and d/dx by $n_x \cdot \nabla_x$. As in one dimension, we have $c_1, c_3 \in \mathbb{R}$ and $c_2 \in \mathbb{C}$. If c_2 is real, the potential simplifies to

$$V(x) = c_1 \delta_S(x) + c_2 \delta'_S(x) + c_3 (n_x \cdot \nabla_x) \delta_S(x) (n_x \cdot \nabla_x).$$

To complete our problem set-up, we consider a wave-function $\psi(\cdot, \cdot | x, s)$ that satisfies Schrödinger's integral equation in \mathbb{R}^d , i.e.

$$\psi(y, t | x, s) = \psi_0(y, t | x, s) - \mathbf{i} \int_s^t d\tau \int_{\mathbb{R}^d} d\alpha \psi_0(y, t | \alpha, \tau) V(\alpha) \psi(\alpha, \tau | x, s), \quad (13)$$

where the potential V is given by (12), and ψ_0 now equals the free propagator in d dimensions, with the usual conventions that $\hbar = 1$ and $m = 1/2$.

By the same approach as in one dimension, Schrödinger's integral equation (13) with the potential V as in (12) implies that $\psi(\cdot, t | x, s)$ must satisfy the following *surface jump-average* boundary conditions:

$$\begin{pmatrix} [\psi'(\beta, t | x, s)] \\ [\psi(\beta, t | x, s)] \end{pmatrix} = \begin{pmatrix} c_1 & -\bar{c}_2 \\ c_2 & c_3 \end{pmatrix} \begin{pmatrix} \{\psi(\beta, t | x, s)\} \\ \{\psi'(\beta, t | x, s)\} \end{pmatrix}, \quad \forall \beta \in S. \quad (14)$$

These boundary conditions form a self-adjoint extension of the Laplacian, and probability is conserved locally, i.e. for each point on the surface.

These surface boundary conditions have some interesting implications. It can be verified directly that $c_2 = 2$ with $c_1 = c_3 = 0$ leads to Neumann boundary conditions on the *inside* of S , and Dirichlet boundary conditions on the *outside* of S . Conversely, $c_2 = -2$ (again with $c_1 = c_3 = 0$) leads to Dirichlet boundary conditions on the *inside* of S , and Neumann boundary conditions on the *outside* of S .

By a rotation to imaginary time, i.e $t \rightarrow -\mathbf{i}t$, the free propagator ψ_0 turns into the propagation density of a d -dimensional Brownian motion. The propagator of a Brownian

motion started in the interior of D and absorbed (reflected) on the surface S satisfies Dirichlet (Neumann) boundary conditions there. Focusing on the inside of S , it turns out that these boundary conditions are generated by $c_2 = -2$ ($c_2 = +2$), i.e. by the surface delta prime potential $V(x) = \mp 2\delta'_S(x)$. Intriguingly, as has been previously noted⁴⁵, the only difference between the classical Dirichlet/Neumann boundary value problems for the Brownian propagator resides in the *sign* of the potential!

Finally, Robin boundary conditions on the inside of S are generated by $c_2 = 2$, $c_3 = 0$ and c_1 being real and non-zero. As noted, these results are not overly rigorous; however, this section has demonstrated that interactions on surfaces of co-dimension one are a natural generalisation of point interactions in one dimension.

VI. SCATTERING MATRIX IN ONE DIMENSION

This section presents the scattering coefficients for the three fundamental point interactions in one dimension. Although the result is straightforward to obtain, it is quite insightful. Consider a stationary wave ψ_+ incoming from the left and moving towards the right, i.e.

$$\psi_+(x) = \begin{cases} e^{ikx} + R_+ e^{-ikx}, & x < 0, \\ T_+ e^{ikx}, & x > 0, \end{cases} \quad (15)$$

where k is related to the energy by $k^2 = E$. Similarly, we denote by ψ_- a stationary wave that is moving towards the left with transmission and reflection coefficients T_- and R_- . Imposing the jump-average boundary conditions (4) on the wave-function (15), it is simple to work out that T and R are as follows:

$$T_{\pm} = \frac{(1 - \frac{D}{4}) \pm i \operatorname{Im}(c_2)}{(1 + \frac{D}{4}) + \frac{1}{2} i (\frac{c_1}{k} - k c_3)}, \quad R_{\pm} = \frac{\mp \operatorname{Re}(c_2) - \frac{1}{2} i (\frac{c_1}{k} + k c_3)}{(1 + \frac{D}{4}) + \frac{1}{2} i (\frac{c_1}{k} - k c_3)}. \quad (16)$$

As a result, the probability of transmission is

$$|T_+|^2 = |T_-|^2 = \frac{(1 - \frac{D}{4})^2 + \operatorname{Im}(c_2)^2}{(1 - \frac{D}{4})^2 + |c_2|^2 + \frac{1}{4} (\frac{c_1}{k} + k c_3)^2}. \quad (17)$$

Recall that D is the determinant of the connection matrix, i.e. $D = c_1 c_3 + |c_2|^2$, such that D is real and even under parity. The scattering coefficients for waves travelling towards the right and left are related by a parity operation (i.e. by $c_2 \rightarrow -c_2$). Clearly, the probability of transmission is unaffected by parity. If c_2 is real and $D = 4$, no transmission takes place.

Contrary to some claims in the literature, $\text{Im}(c_2)$ generally does affect the transmission and reflection probabilities.

The scattering matrix S is unitary for all $c_1, c_3 \in \mathbb{R}$ and $c_2 \in \mathbb{C}$, i.e.

$$S := \begin{pmatrix} T_+ & R_- \\ R_+ & T_- \end{pmatrix} \quad \text{satisfies } S S^\dagger = \mathbb{1}, \quad \forall c_1, c_3 \in \mathbb{R}, c_2 \in \mathbb{C}.$$

Thus probability is conserved for jump-average boundary conditions of the form (4).

The three fundamental point interactions are quite distinct when it comes to their scattering behaviour. The transition probabilities for each of the three fundamental point interactions are as follows:

$$|T_\pm|^2 = \frac{1}{1 + \frac{1}{4}c_1^2/k^2}, \quad |T_\pm|^2 = \frac{(c_2^2 - 4)(\bar{c}_2^2 - 4)}{(|c_2|^2 + 4)^2}, \quad |T_\pm|^2 = \frac{1}{1 + \frac{1}{4}c_3^2 k^2}.$$

For the first, second and third fundamental point interactions, high-energy waves are more, equally and less likely to be transmitted, respectively. If $c_1 = c_3 = 0$ and c_2 is purely imaginary, the probability of transmission is one. If $c_1 = c_3 = 0$ and $c_2 = \pm 2$, the probability of transmission is zero. As $c_1 \rightarrow \infty$ or $c_3 \rightarrow \infty$, the first and third point interactions become fully reflecting. If c_2 is real and $c_2 \rightarrow \infty$, however, the second point interaction disappears.

VII. RELATION TO CONNECTED SELF-ADJOINT EXTENSIONS

Traditionally, the literature has classified the full set of self-adjoint extensions (SAEs) as *connected* or *separated*. Depending on the numerical values of c_i , the jump-average boundary conditions are either connected or separated. However, the converse is not true: the jump-average boundary conditions only form a *subset* of all possible SAEs. This section and the next make these claims explicit.

Connected boundary conditions can be written in several ways, for example as (see e.g. ^{2,18,21,34,35,52}):

$$\begin{pmatrix} u'(0^+) \\ u(0^+) \end{pmatrix} = e^{i\theta} \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix} \begin{pmatrix} u'(0^-) \\ u(0^-) \end{pmatrix}, \quad \theta, a_i \in \mathbb{R}, \quad a_1 a_4 - a_2 a_3 = 1. \quad (18)$$

First, assume the jump-average boundary conditions (4) hold. Then the connected param-

eters a_i and θ can be written as a function of the jump-average parameters c_i as follows:

$$\begin{aligned} \theta &= \text{Tan}^{-1}[1 - D/4, \text{Im}(c_2)], \\ a_1 &= \frac{D/4 + 1 - \text{Re}(c_2)}{\sqrt{(D/4 - 1)^2 + \text{Im}(c_2)^2}}, \quad a_2 = \frac{c_1}{\sqrt{(D/4 - 1)^2 + \text{Im}(c_2)^2}}, \\ a_3 &= \frac{c_3}{\sqrt{(D/4 - 1)^2 + \text{Im}(c_2)^2}}, \quad a_4 = \frac{D/4 + 1 + \text{Re}(c_2)}{\sqrt{(D/4 - 1)^2 + \text{Im}(c_2)^2}}. \end{aligned} \quad (19)$$

These expressions are valid as long as $(D/4 - 1)^2 + \text{Im}(c_2)^2 > 0$. Here, $\text{Tan}^{-1}(x, y)$ is defined so as to give the arc tangent of y/x , taking into account which quadrant the point (x, y) is in. If c_2 is real, we get $\theta = 0$ or $\theta = \pi$. Similar expressions can be found elsewhere¹⁴ (p. 8), although the angle θ is not explicitly given there. The correspondence with that paper can be made clear by writing

$$\frac{\exp(i\theta)}{\sqrt{(D/4 - 1)^2 + \text{Im}(c_2)^2}} = \frac{-1}{D/4 - 1 + i \text{Im}(c_2)}$$

where θ is given by (19).

From the parity behaviour of the c_i , it follows that a_2, a_3 and $a_1 + a_4$ are even under parity, while $a_1 - a_4$ is odd. The angle θ , when visualized in the complex plane, is reflected in the horizontal axis under a parity operation. This implies $\theta \rightarrow -\theta$, such that $\cos(\theta) \rightarrow \cos(\theta)$ and $\sin(\theta) \rightarrow -\sin(\theta)$.

Suppose instead that some connected boundary conditions in terms of the a_i are given. The jump-average parameters c_i may then be written as

$$c_1 = \frac{4 a_2}{a_1 + a_4 + 2 \cos(\theta)}, \quad c_2 = \frac{2(-a_1 + a_4 + 2 i \sin(\theta))}{a_1 + a_4 + 2 \cos(\theta)}, \quad c_3 = \frac{4 a_3}{a_1 + a_4 + 2 \cos(\theta)}. \quad (20)$$

These expressions seem to be new and are valid as long as $a_1 + a_4 + 2 \cos(\theta) \neq 0$. We conclude that some connected self-adjoint extensions, namely those for which with $a_1 + a_4 + 2 \cos(\theta) = 0$, cannot be generated by the potential (1).

VIII. RELATION TO SEPARATED SELF-ADJOINT EXTENSIONS

Suppose that $(D/4 - 1)^2 + \text{Im}(c_2)^2 = 0$. Then the jump-average boundary conditions cannot be re-written as connected boundary conditions. In this case, the jump-average boundary conditions are equivalent to boundary conditions that are traditionally known as *separated*, and which can be written as

$$\begin{pmatrix} u'(0^+) \\ u'(0^-) \end{pmatrix} = \begin{pmatrix} b^+ & 0 \\ 0 & b^- \end{pmatrix} \begin{pmatrix} u(0^+) \\ u(0^-) \end{pmatrix}, \quad b^+, b^- \in \mathbb{R} \cup \infty, \quad (21)$$

or as

$$\begin{pmatrix} u(0^+) \\ u(0^-) \end{pmatrix} = \begin{pmatrix} \tilde{b}^+ & 0 \\ 0 & \tilde{b}^- \end{pmatrix} \begin{pmatrix} u'(0^+) \\ u'(0^-) \end{pmatrix}, \quad \tilde{b}^+, \tilde{b}^- \in \mathbb{R} \cup \infty. \quad (22)$$

In this section, we assume $D = 4$ and $c_2 \in \mathbb{R}$. This implies $c_1 c_3 + c_2^2 = 4$, such that three real parameters remain, with only two degrees of freedom. It will be convenient to distinguish between three collectively exhaustive cases: c_1 is not zero, c_3 is not zero, or both c_1 and c_3 are zero:

- **Case 1:** $D = 4$, $c_2 \in \mathbb{R}$, and $c_1 \neq 0$. The constant c_3 can be eliminated since it must satisfy $c_3 = (4 - c_2^2)/c_1$. Then the separated parameters can be written as a function of c_1 and c_2 as follows:

$$\tilde{b}^+ = \frac{c_2 + 2}{c_1}, \quad \tilde{b}^- = \frac{c_2 - 2}{c_1}. \quad (23)$$

If, additionally, $c_2 = 2$ (and thus $c_3 = 0$), we get a Dirichlet boundary condition to the left of the origin. To the right, we get a Robin boundary condition governed by the remaining free parameter c_1 . For $c_2 = -2$, the opposite is true (Dirichlet on the right, Robin on the left). As $c_1 \rightarrow \infty$, Dirichlet boundary conditions on both sides of zero are obtained. Equivalently, the c_i may be written as

$$c_1 = \frac{4}{\tilde{b}^+ - \tilde{b}^-}, \quad c_2 = \frac{2(\tilde{b}^+ + \tilde{b}^-)}{\tilde{b}^+ - \tilde{b}^-}, \quad c_3 = \frac{-4\tilde{b}^+\tilde{b}^-}{\tilde{b}^+ - \tilde{b}^-} \quad (24)$$

It follows that SAEs for which $\tilde{b}^+ = \tilde{b}^-$ cannot be obtained using the potential (1).

- **Case 2:** $D = 4$, $c_2 \in \mathbb{R}$, and $c_3 \neq 0$. The constant c_1 can be eliminated, as we must have $c_1 = (4 - c_2^2)/c_3$. Then the separated parameters can be written as a function of c_2 and c_3 as follows:

$$b^+ = \frac{2 - c_2}{c_3}, \quad b^- = \frac{-2 - c_2}{c_3}. \quad (25)$$

If, additionally, $c_2 = 2$ (and thus $c_1 = 0$), we get a Neumann boundary condition on the right of the origin. On the left, we get a Robin boundary condition, governed by the remaining free parameter c_3 . For $c_2 = -2$, the opposite is true (Neumann on the left, Robin on the right). For $c_3 \rightarrow \infty$, Neumann conditions on both sides of zero are obtained. Equivalently, the c_i may be written as

$$c_1 = \frac{-4b^+b^-}{b^+ - b^-}, \quad c_2 = \frac{-2(b^+ + b^-)}{b^+ - b^-}, \quad c_3 = \frac{4}{b^+ - b^-}, \quad (26)$$

As above, we find that SAEs with $b^+ = b^-$ cannot be generated by the potential (1).

- **Case 3:** $D = 4$, $c_2 \in \mathbb{R}$, and $c_1 = c_3 = 0$. This implies $c_2 = \pm 2$. If $c_2 = 2$, we obtain Neumann (Dirichlet) boundary conditions to the right (left) of zero. If $c_2 = -2$, we obtain Dirichlet (Neumann) conditions to the right (left) of zero.

While the jump-average boundary conditions (4) do not cover *all* self-adjoint extensions, they do describe those which can be generated by the potential (1). Having considered, in this section and the previous section, all cases using the traditional framework of connected and separated boundary conditions, the reader may appreciate the conciseness of the jump-average boundary conditions. One unanswered question, as far as we know, is whether there is a singular potential that can generate all self-adjoint extensions.

IX. PROPAGATOR FOR THE DELTA PRIME POTENTIAL

Suppose we write down Schrödinger's integral equation (see e.g.^{31,33,47,50}) with a delta prime potential:

$$\psi(y, t|x, s) = \psi_0(y, t|x, s) - c \mathfrak{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta'(\alpha) \psi(\alpha, \tau|x, s), \quad (27)$$

where $c \in \mathbb{R}$, the delta function was defined in (3), ψ_0 was defined in (6), and it is assumed that $\psi(\cdot, t|x, s) \in W_2^2(\mathbb{R} \setminus \{0\})$. As highlighted in section IV, the integral equation allows no solutions if the definition of the delta prime is such that $\int \delta' \psi$ blows up for discontinuous ψ . With our distributional definition (3), however, the integral equation can be solved in closed form as follows:

$$\psi(y, t|x, s) = \psi_0(y, t|x, s) + \begin{cases} + \frac{4c}{4+c^2} \psi_0(y, t|-x, s), & x > 0, y > 0, \\ - \frac{2c^2}{4+c^2} \psi_0(y, t|x, s), & x > 0, y < 0, \\ - \frac{2c^2}{4+c^2} \psi_0(y, t|x, s), & x < 0, y > 0, \\ - \frac{4c}{4+c^2} \psi_0(y, t|-x, s), & x < 0, y < 0. \end{cases} \quad (28)$$

As far as we are aware, this exact solution to Schrödinger's equation is new. What's more, it is remarkably simple; much simpler, in fact, than the well-known propagator for the delta potential. The calculation is carried out below. From the explicit solution, we can verify

that the propagator ψ satisfies the following boundary conditions:

$$\begin{pmatrix} [\psi'(0, t|x, s)] \\ [\psi(0, t|x, s)] \end{pmatrix} = \begin{pmatrix} 0 & -c \\ c & 0 \end{pmatrix} \begin{pmatrix} \{\psi(0, t|x, s)\} \\ \{\psi'(0, t|x, s)\} \end{pmatrix}. \quad (29)$$

These boundary conditions are of the jump-average form (4), with $c_2 = c \in \mathbb{R}$ and $c_1 = c_3 = 0$. The derived boundary conditions are consistent with the independently derived boundary conditions in previous work^{2,28,32,44}. Interestingly, those derivations were based on Schrödinger's differential (rather than integral) equation.

As can be seen from the solution, $c = \pm 2$ implies that the propagator is zero for x and y on opposite sides of the origin. For $c = 2$, the propagator satisfies Neumann boundary conditions at 0^+ and Dirichlet boundary conditions at 0^- . The opposite is true for $c = -2$. If we focus on 0^+ , we have Dirichlet (Neumann) boundary conditions for $c = -2$ ($c = +2$). As in section V, the only difference between Dirichlet and Neumann boundary conditions on a given side of the boundary resides in the *sign* of the delta prime potential (see also⁴⁵).

For $c \neq \pm 2$, the potential is partially transparent with the scattering matrix given in section VI. Recently, several authors have found the delta prime potential to be transparent only for particular values of c ^{19,21,25,53,57,60,61}. The difference is attributable to the construction of the delta prime function. Here it is expressly defined so as to be compatible with discontinuous test functions. For methods 2-4 in Table I, the integral equation (27) would not exist for discontinuous ψ .

The solution to Schrödinger's integral equation was obtained as follows. By repeatedly substituting the integral equation (27) into itself, the solution may be written as:

$$\psi(y, t|x, s) = \psi_0(y, t|x, s) + \sum_{i=1}^{\infty} (-1)^i \psi_i(y, t|x, s),$$

where the correction terms ψ_i are defined recursively as

$$\psi_i(y, t|x, s) = \text{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) V(\alpha) \psi_{i-1}(\alpha, \tau|x, s),$$

and $V(x) = c \delta'(x)$. For singular potentials, the recursive structure of the correction terms should be carefully observed, i.e.

$$\psi_2 = \int \int \psi_0 V \int \int \psi_0 V \psi_0 \neq \int \int \int \int \psi_0 V \psi_0 V \psi_0.$$

In other words, the interchange of integrals and distributions is not generally allowed, i.e. integrals cannot be pulled to the front.

The first correction term is $\psi_1 = c\text{i} \int \int \psi_0 \delta' \psi_0$. Since ψ_0 is continuously differentiable across zero, no ambiguities whatsoever arise regarding the interpretation of the δ' -function. Performing the integration, we obtain the following expression:

$$\psi_1(y, t|x, s) = \begin{cases} -c \psi_0(y, t| -x, s) & x > 0, y > 0, \\ 0 & x > 0, y < 0, \\ 0 & x < 0, y > 0, \\ c \psi_0(y, t| -x, s) & x < 0, y < 0. \end{cases}$$

Since ψ_1 is discontinuous, the exact distributional definition of the delta prime is crucial for the calculation of $\psi_2 = c\text{i} \int \int \psi_0 \delta' \psi_1$. Using our definition of the delta function, all correction terms are finite and can be calculated explicitly. For e.g. ψ_2, ψ_3, ψ_4 and ψ_5 , we obtain the following expressions:

$$\psi_2(y, t|x, s) = \begin{cases} 0 & x > 0, y > 0, \\ -\frac{1}{2}c^2 \psi_0(y, t|x, s) & x > 0, y < 0, \\ -\frac{1}{2}c^2 \psi_0(y, t|x, s) & x < 0, y > 0, \\ 0 & x < 0, y < 0. \end{cases}$$

$$\psi_3(y, t|x, s) = \begin{cases} \frac{1}{4}c^3 \psi_0(y, t| -x, s) & x > 0, y > 0, \\ 0 & x > 0, y < 0, \\ 0 & x < 0, y > 0, \\ -\frac{1}{4}c^3 \psi_0(y, t| -x, s) & x < 0, y < 0. \end{cases}$$

$$\psi_4(y, t|x, s) = \begin{cases} 0 & x > 0, y > 0, \\ \frac{1}{2^3}c^4 \psi_0(y, t|x, s) & x > 0, y < 0, \\ \frac{1}{2^3}c^4 \psi_0(y, t|x, s) & x < 0, y > 0, \\ 0 & x < 0, y < 0. \end{cases}$$

$$\psi_5(y, t|x, s) = \begin{cases} -\frac{1}{2^4}c^5 \psi_0(y, t| -x, s) & x > 0, y > 0, \\ 0 & x > 0, y < 0, \\ 0 & x < 0, y > 0, \\ \frac{1}{2^4}c^5 \psi_0(y, t| -x, s) & x < 0, y < 0. \end{cases}$$

It becomes clear that the following series solution arises:

$$\psi(y, t|x, s) = \begin{cases} \psi_0(y, t, x, s) + 2\left(\frac{c}{2} - \frac{c^3}{2^3} + \frac{c^5}{2^5} - \frac{c^7}{2^7} + \dots\right) \psi_0(y, t|-x, s) & x > 0, y > 0, \\ \psi_0(y, t, x, s) - 2\left(\frac{c^2}{2^2} - \frac{c^4}{2^4} + \frac{c^6}{2^6} - \frac{c^8}{2^8} + \dots\right) \psi_0(y, t|x, s) & x > 0, y < 0, \\ \psi_0(y, t, x, s) - 2\left(\frac{c^2}{2^2} - \frac{c^4}{2^4} + \frac{c^6}{2^6} - \frac{c^8}{2^8} + \dots\right) \psi_0(y, t|x, s) & x < 0, y > 0, \\ \psi_0(y, t, x, s) - 2\left(\frac{c}{2} - \frac{c^3}{2^3} + \frac{c^5}{2^5} - \frac{c^7}{2^7} + \dots\right) \psi_0(y, t|-x, s) & x < 0, y < 0. \end{cases}$$

These expressions may be recognised as the Taylor series expansions of the exact solution (28). Although the solution was derived using the series expansion, it can be verified directly that the proposed solution satisfies the integral equation.

X. SUPER-SINGULAR POTENTIALS

This section considers Schrödinger's integral equation with the potential $V(x) = c\delta^{(n)}(x)$ with $c \in \mathbb{R}$ for $n \geq 1$. These super-singular potentials are interesting as they cannot be incorporated into the normal framework of self-adjoint extensions. We show that the resulting boundary conditions are of the jump-average form (4), with the crucial difference that the constants c_i depend on the energy $E = k^2$. Specifically, we show that

$$V(x) = c\delta^{(n)}(x) \Rightarrow \begin{cases} \text{For even } n, \text{ BCs (4) with:} & \text{For odd } n, \text{ BCs (4) with:} \\ c_1(k) = c2^{n-1}(\mathbf{i}k)^n, & c_1(k) = 0 \\ c_2(k) = 0, & c_2(k) = c(2\mathbf{i}k)^{n-1}, \\ c_3(k) = -c2^{n-1}(\mathbf{i}k)^{n-2}, & c_3(k) = 0. \end{cases} \quad (30)$$

For even n , only even constants c_i are non-zero (i.e. c_1 and c_3). For odd n , only the odd constant c_2 is non-zero. We also note that all c_i are real. Setting n equal to 1 yields the boundary conditions of section IX. For $n > 1$, however, we obtain boundary conditions that are *energy-dependent* in the sense that the c_i 's depend on k . For $n = 2$, for example, only c_1 depends on the energy E . These boundary conditions seem to be new.

The transmission and reflection coefficients are given by (16) with the c_i as above. Probability is conserved for all boundary conditions of the jump-average form, even if the constants c_i depend on k . Crucially, therefore, probability is conserved.

Jump-average boundary conditions of the form (4) are self-adjoint when the parameters

c_i are constant, but not when they depend on the energy through k . Thus it appears that these super-singular interactions conserve probability without being self-adjoint.

The proof of (30) consists of two steps. First, we show that $\psi(\cdot, t|x, s)$ must satisfy

$$\begin{aligned} [\psi^{(1)}(0, t|x, s)] &= c 2^{n-1} (-1)^n \{\psi^{(n)}(0, t|x, s)\}, \\ [\psi(0, t|x, s)] &= c 2^{n-1} (-1)^{(n-1)} \{\psi^{(n-1)}(0, t|x, s)\}. \end{aligned} \quad (31)$$

These boundary conditions are slightly different from Griffiths' boundary conditions⁴¹, as the numerical prefactors on the right-hand side are different. While the original derivation of Griffiths' boundary conditions is known to be erroneous^{21,24,25,30}, the resulting boundary conditions have generated interest in their own right (see e.g.²⁷). The second step of the proof shows that the boundary conditions (31) are equivalent to (30).

We now turn to the first step of the proof. We begin by extending lemma (9) to state that all *odd* derivatives of the auxiliary function f , defined as

$$f(y, t|x, s) := -\mathbf{i} \int_s^t \psi_0(y, t|0, \tau) g(\tau|x, s) d\tau, \quad (32)$$

are discontinuous as follows:

$$[f^{(k)}(0, t|x, s)] = \begin{cases} 0 & k \in 0, \text{ even,} \\ \left(-\mathbf{i} \frac{d}{dt}\right)^{\frac{k-1}{2}} g(t|x, s) & k \in \text{odd.} \end{cases} \quad (33)$$

This will be useful in the context of Schrödinger's integral equation, which can be re-written for $V(x) = c \delta^{(n)}(x)$ as follows:

$$\begin{aligned} \psi(y, t|x, s) &= \psi_0(y, t|x, s) - c \mathbf{i} \int_s^t d\tau \int_{-\infty}^{\infty} d\alpha \psi_0(y, t|\alpha, \tau) \delta^{(n)}(\alpha) \psi(\alpha, \tau|x, s), \\ &= \psi_0(y, t|x, s) - c \mathbf{i} (-1)^n \sum_{i=0}^n \binom{n}{i} \int_s^t \psi_0^{(i)}(y, t|0, \tau) \{\psi^{(n-i)}(0, \tau|x, s)\} d\tau, \\ &= \psi_0(y, t|x, s) - c \mathbf{i} (-1)^n \sum_{i=0}^n \binom{n}{i} (-1)^i \frac{d^i}{dy^i} \int_s^t \psi_0(y, t|0, \tau) \{\psi^{(n-i)}(0, \tau|x, s)\} d\tau. \end{aligned}$$

The second line used the definition of the delta function (3), as well as the fact that the free propagator can be pulled out of the averaging operator. The third line used the fact that $d/d\alpha \psi_0(y, t|\alpha, \tau) = -d/dy \psi_0(y, t|\alpha, \tau)$. Further, derivatives d/dy can be pulled out of the integral sign for all $y \neq 0$, since $\psi(\cdot, t|x, s)$ is smooth away from the origin.

Referring to (33), we realise that integral terms with an *odd* number of derivatives $(d/dy)^i$ are discontinuous. Equally, integral terms with an *even* number of derivatives $(d/dy)^i$ are continuous, but then the first derivative with respect to y is discontinuous. Thus the discontinuity in the value of $\psi(\cdot, t|x, s)$ is determined by the sum over all odd i , while the discontinuity in the derivative is determined by the sum over all even i . Using (33), we get

$$\begin{aligned} [\psi^{(1)}(0, t|x, s)] &= c(-1)^n \sum_{i=0,2,4,\dots \leq n} \binom{n}{i} \left(-\mathfrak{i} \frac{d}{dt}\right)^{\frac{i}{2}} \{\psi^{(n-i)}(0, t|x, s)\}, \\ [\psi(0, t|x, s)] &= -c(-1)^n \sum_{i=1,3,5,\dots \leq n} \binom{n}{i} \left(-\mathfrak{i} \frac{d}{dt}\right)^{\frac{i-1}{2}} \{\psi^{(n-i)}(0, t|x, s)\}. \end{aligned}$$

Above and below zero, $\psi(\cdot, \cdot|x, s)$ satisfies the free Schrödinger equation. As a result, we have $-\mathfrak{i}\partial_t\{\psi^{(n)}(0, t|x, s)\} = \{\psi^{(n+2)}(0, t|x, s)\}$ and thus

$$\begin{aligned} [\psi^{(1)}(0, t|x, s)] &= c(-1)^n \sum_{i=0,2,4,\dots \leq n} \binom{n}{i} \{\psi^{(n)}(0, t|x, s)\}, \\ [\psi(0, t|x, s)] &= -c(-1)^n \sum_{i=1,3,5,\dots \leq n} \binom{n}{i} \{\psi^{(n-1)}(0, t|x, s)\}. \end{aligned}$$

As claimed, this implies

$$\begin{aligned} [\psi^{(1)}(0, t|x, s)] &= c 2^{n-1} (-1)^n \{\psi^{(n)}(0, t|x, s)\}, \\ [\psi(0, t|x, s)] &= c 2^{n-1} (-1)^{(n-1)} \{\psi^{(n-1)}(0, t|x, s)\}, \end{aligned} \tag{34}$$

where the combinatorial factors on the right-hand side arise from the summation over half of all the binomial coefficients, i.e. $2^n/2 = 2^{n-1}$.

Moving on to the second step, we will consider separately even and odd n . Suppose n is even and consider a stationary state ψ of the form (15). Then $\{\psi^{(n)}(0)\} = (\mathfrak{i}k)^n\{\psi(0)\}$ and $\{\psi^{(n-1)}(0)\} = (\mathfrak{i}k)^{n-2}\{\psi^{(1)}(0)\}$, such that the boundary conditions (34) can be written as follows:

$$\begin{pmatrix} [\psi'(0)] \\ [\psi(0)] \end{pmatrix} = c 2^{n-1} \begin{pmatrix} (\mathfrak{i}k)^n & 0 \\ 0 & -(\mathfrak{i}k)^{n-2} \end{pmatrix} \begin{pmatrix} \{\psi(0)\} \\ \{\psi'(0)\} \end{pmatrix}. \tag{35}$$

These boundary conditions are of the jump-average form (4), with c_1 and c_3 as in (30). The scattering matrix is unitary for all boundary conditions of the jump-average form, and thus probability is conserved.

Now suppose n is odd, such that $\{\psi^{(n)}(0)\} = (\mathbf{i}k)^{n-1}\{\psi^{(1)}(0)\}$ and $\{\psi^{(n-1)}(0)\} = (\mathbf{i}k)^{n-1}\{\psi(0)\}$. Then the boundary conditions (34) can be written as follows:

$$\begin{pmatrix} [\psi'(0)] \\ [\psi(0)] \end{pmatrix} = c 2^{n-1} \begin{pmatrix} 0 & -(\mathbf{i}k)^{n-1} \\ (\mathbf{i}k)^{n-1} & 0 \end{pmatrix} \begin{pmatrix} \{\psi(0)\} \\ \{\psi'(0)\} \end{pmatrix}. \quad (36)$$

Again, these boundary conditions are of the jump-average form (4), with c_2 as in (30).

We conclude that the potential $\delta^{(n)}$ is permissible if probability conservation is imposed. Despite being of self-adjoint *form*, however, the boundary conditions are not self-adjoint since the parameters depend on the energy k^2 . We leave open the question whether the derived boundary conditions can be made self-adjoint by considering, in addition to the real line, some internal space at the origin.

XI. CONCLUSION

This paper considered the integral form of Schrödinger's equation, where the potential is given by a distribution that is defined on the space of discontinuous functions. Broadly, it has shown that Schrödinger's integral equation is a viable tool for studying singular interactions in quantum mechanics.

Section II re-derived Kurasov's potential based purely on symmetry considerations. Section III showed that the associated boundary conditions can be expressed quite naturally using the jump-average representation.

Section IV showed that the same result can be obtained relatively simply in the context of Schrödinger's integral equation. This result hints at a deeper equivalence between both approaches, which are normally thought to be equivalent only for smooth potentials.

Section V proposed an extension of Kurasov's result to hypersurfaces. Our result is based on an informal treatment only, but points at an interesting connection with classical potential theory. It turns out that the surface delta prime potential can generate solutions to the Dirichlet and Neumann boundary value problems, where the only difference between these two classical problems resides in the sign of the potential.

Section VI derived the scattering matrix in one dimension, and showed that for the first, second and third fundamental point interactions, high-energy waves are more, equally and less likely to be transmitted, respectively.

Sections VII and VIII showed that the jump-average boundary conditions form a *subset* of all possible connected and separated self-adjoint extensions. Whether a singular potential exists that can generate all SAEs remains an open question.

Section IX solved Schrödinger's integral equation for the delta prime potential. While the propagator for the delta potential has long been known, the propagator for the delta prime potential derived here is new. Our solution suffers from none of the drawbacks often found in the literature, such as an ambiguous Schrödinger equation, arbitrary boundary conditions or ambiguous limits. By confronting the issue of a discontinuous solution head on, all ambiguities disappear. In contrast with some recent findings, the delta prime potential turns out to be partially transparent for almost all values of the coupling constant.

Section X used the same method to derive boundary conditions for higher-order derivatives of the delta potential. It turns out that the boundary conditions associated with these super-singular potentials are of the jump-average form — but with the crucial difference that the parameters depend on the energy of the solution. While probability is conserved, these energy-dependent boundary conditions are not self-adjoint when considering only the real line. If we consider a larger space, containing some internal space at the origin, then it is possible that the derived boundary conditions are, in fact, self-adjoint. This may be an interesting avenue for further research.

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