Realization of a Four Parameter Family of Generalized One-Dimensional Contact Interactions by Three Nearby Delta Potentials with Renormalized Strengths

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SUMMARY We propose a new method to construct a four parameter family of quantum-mechanical point interactions in one dimension, which is known as all possible self-adjoint extensions of the symmetric operator $T = -\Delta [C^\infty_0(\mathbb{R}\setminus\{0\})]$. It is achieved in the small distance limit of equally spaced three neighboring Dirac’s $\delta$ potentials. The strength for each $\delta$ is appropriately renormalized according to the distance and it diverges, in general, in the small distance limit. The validity of our method is ensured by numerical calculations. In general cases except for usual $\delta$, the wave function discontinuity appears around the interaction and one can observe such a tendency even at a finite distance level.

key words: quantum mechanics, one dimension, generalized point interaction, wave function discontinuity, functional analysis

1. Introduction

Point interaction is a simple but useful object for examining the effect of small impurities on low-energy dynamics in quantum mechanics. It serves as a minimal perturbation which gives light on the influence of more complicated perturbations on dynamical nature of the system. It has been first observed [1], [2] that wave chaos (chaotic nature in quantum spectrum) is induced by point perturbation in two-dimensional integrable billiards and a general condition for its emergence has been clarified in [3]–[5]. In [6], the dependence of the “degree” of chaos on the number of point impurities has been examined in details.

Historically, the first influential paper on point interactions was given by Kronig and Penney [7]. The Kronig-Penney model (potential consisting of a periodic array of $\delta$ functions) has been widely considered as a standard reference model in solid state physics for more than six decades. In two and three dimensions, the point interaction is nothing but an extended object of the usual $\delta$ potential. However the phenomena are much richer in one dimension. This is due to the fact that whereas the symmetric operator $T = -\Delta [C^\infty_0(\mathbb{R}\setminus\{0\})]$ has deficiency indices (1, 1) in spatial dimension $d = 2, 3$, it has deficiency indices (2, 2) in dimension $d = 1$ [8]. As a result, the operator $T$ has in one dimension a four-parameter family of self-adjoint extensions [9]. The general connection condition is characterized by

\[
\begin{pmatrix}
\varphi'(+0) \\
\varphi(+0)
\end{pmatrix} = V \begin{pmatrix}
\varphi(-0) \\
\varphi(-0)
\end{pmatrix},
\]

where $V$ takes a form

\[
V = e^{i\theta}U
\]

with $\theta \in \mathbb{R}$ and

\[
U = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \in SL(2, \mathbb{R}),
\]

namely, $\alpha \delta - \beta \gamma = 1$ [10]. Here we assume that the point interaction is placed at the origin on $x$-axis. The condition (1) covers the usual $\delta$ potential, the connection matrix of which is given by

\[
V = V_\delta(u) = \begin{pmatrix} 1 & v \\ 0 & 1 \end{pmatrix}.
\]

Here $v$ is the potential strength. Another interesting example is a so-called (historically ill-called) $\delta'$ potential, which induces such a boundary condition that the wave function has continuous first derivative on the right and left, but it has a jump proportional to the first derivative [11]:

\[
V = V_{\delta'}(u) = \begin{pmatrix} 1 & 0 \\ u & 1 \end{pmatrix},
\]

where $u$ is regarded as the strength of the interaction. It has been shown [12] that the connection condition (5) has little to do with the derivative of $\delta$ potential. In this paper, we denote the contact interaction with the transfer matrix (5) by $\varepsilon(x)$.

Except for $\delta$, the connection condition (1) appears at first sight to be unnatural for quantum mechanics, and some efforts have been made in order to seek the physical Hamiltonians which embody the condition (1). Seba has observed [13] that a certain two-parameter family is obtained by non-local pseudopotentials with $\varepsilon$ potential. Chernoff and Hughes have shown [14] that a
three-parameter family disjoint from Šeba’s class corresponds to local pseudopotentials involving the so-called δ². Carreau has succeeded in realizing a general class in the small-size limit of non-symmetric operators [15]. A local realization has been given by Román and Tar-rach by using a potential consisting of a step-like barrier sandwiched in two δ potentials [16]. Their model requires, however, a subtle limiting procedure and indeed the height of the middle barrier as well as the strengths of the two side δ’s are necessary to be renormalized with a doubly logarithmic dependence on the distance between the two δ’s. In spite of considerable works, existing approximations do not seem to have much relevance to the experimentally realizable systems. Our main purpose is to rectify this situation. In [17], [18], we have constructed the ε potential in the small distance limit of three nearby δ potentials and realized in terms of usual δ and ε potentials a three-parameter family of self-adjoint extensions under the assumption of time reversal symmetry. In this paper, we generalize the previous formalism and give in a direct manner within the three δ’s model a complete solution for the four-parameter extensions covering the cases without the time reversal symmetry.

In Sect.2, we start by solving the one-dimensional Schrödinger equation with a constant vector potential within the framework of the transfer matrix formalism. Considering the potential which consists of equally spaced three δ’s with a constant vector potential between the two side δ’s, we show that all possible extensions are attained in the short range limit of the assumed potential if the strengths of the δ’s as well as that of vector potential are renormalized according to the distance in a simple manner. In Sect.3, We give numerical examples which justify the method in the small-size limit of non-symmetric operators [15]. Carreau has succeeded in realizing a general class of self-adjoint extensions under the assumption δ’s with a constant vector potential be-

\[ H = (p - A)^2, \]  

where \( p = -i\hbar \frac{d}{dx} \) is the momentum operator and constant \( A \) is the strength of the vector potential. The Schrödinger equation for the Hamiltonian (6) reads

\[ -\frac{d^2 \varphi(x)}{dx^2} + 2iA \frac{d\varphi(x)}{dx} + A^2 \varphi(x) = k^2 \varphi(x). \]  

Here \( k \) is the wave number of the particle. For later convenience, we rewrite the equation (7) within the transfer matrix formalism. For this purpose, let us introduce a vector notation for the wave function and its space derivative;

\[ \Psi(x) = \begin{pmatrix} \varphi'(x) \\ \varphi(x) \end{pmatrix}. \]  

In this notation, the equation (7) is rewritten by the first-order coupled equation

\[ \Psi'(x) = \mathcal{H}(A,k)\Psi(x) \]  

with

\[ \mathcal{H}(A,k) = \begin{pmatrix} 2iA & -k^2 + A^2 \\ 1 & 0 \end{pmatrix}. \]  

The solution of Eq.(9) is given by

\[ \Psi(x) = \mathcal{G}(A,k;x-x_0)\Psi(x_0), \]  

where \( \mathcal{G}(A,k;x) \) is the exponential function of \( \mathcal{H}(A,k)x \);

\[ \mathcal{G}(A,k;x) = e^{\mathcal{H}(A,k)x} = e^{iAx} \begin{pmatrix} \cos(kx) & 0 \\ 0 & 1 \end{pmatrix} + \frac{\sin(kx)}{k} \begin{pmatrix} iA & -k^2 + A^2 \\ 1 & -iA \end{pmatrix}. \]  

Since

\[ Tr\mathcal{H}(A,k) = 2iA, \]  

the matrix \( \mathcal{G}(A,k;x) \) satisfies

\[ \det \mathcal{G}(A,k;x) = e^{2iAx}, \]  

indicating that the matrix on the RHS of Eq.(12) has determinant one.

In order to realize the general condition (1) in the small-size limit of a realistic finite-range potential, we consider three neighboring usual δ’s as well as

\[ A_a(x) = A\theta(a - x)\theta(x + a), \]  

where \( \theta \) is a usual step function. The Hamiltonian is hence given by

\[ H_a = (p - A_a(x))^2 + v_-\delta(x + a) + v_0\delta(x) + v_+\delta(x - a), \]  

where the strengths of the three delta’s at \( x = \pm a \) and \( 0 \) are set to \( v_\pm \) and \( v_0 \), respectively. The assumed potential \( V_a(x) \) is shown in Fig.1. Inserting Eq.(15) into Eq.(16), one obtains

\[ H_a = -\frac{d^2}{dx^2} + 2iA_a(x) \frac{d}{dx} + A_a(x)^2 \]

\[ + (v_- + iA)\delta(x + a) + v_0\delta(x) \]

\[ + (v_+ - iA)\delta(x - a). \]
The appearance of the complex $\delta$'s at $x = \pm a$ are inevitable for ensuring the Hamiltonian to be symmetric and they indeed describe a sudden change of the vector potential at the location of the two side $\delta$'s. With the Hamiltonian (17), the connection of $\Psi$ between $x = -a - 0$ and $x = a + 0$ is given by

$$\Psi(a + 0) = V_a(A, k)\Psi(-a - 0),$$

where

$$V_a(A, k) = V_0(v_+ - iA)G(A, k; a)\Psi_0(v_0)\times G(A, k; a)\Psi_0(v_-),$$

Inserting Eqs.(4) and (12) into Eq.(19), we obtain

$$V_a(A, k) = e^{2iAa}U_a(k),$$

where the (2, 1) component of $U_a(k)$ is given by

$$[U_a(k)]_{21} = \frac{\sin(2ka)}{k} + \frac{\sin^2(ka)}{k^2}v_0$$

and the other elements are written as

$$[U_a(k)]_{11} = \cos(2ka) + \frac{\sin(2ka)}{2k}v_0 + [U_a(k)]_{21}v_+,$$

$$[U_a(k)]_{22} = \cos(2ka) + \frac{\sin(2ka)}{2k}v_0 + [U_a(k)]_{21}v_-,$$

$$[U_a(k)]_{12} = \cos^2(ka)\cdot (v_+ + v_0) - \sin^2(ka)\cdot (v_+ + v_-)$$

$$+ \frac{\sin(2ka)}{2k}\left\{-2k^2 + v_0(v_+ + v_-)\right\}$$

$$+[U_a(k)]_{21}v_+v_-\]$$

in terms of $[U_a(A, k)]_{21}$, respectively. Note that the effect of the magnetic field is absorbed in the phase factor in front of the matrix $U_a(k)$ in Eq.(20). Since

$$\det V_a(A, k) = e^{4iAa}$$

from Eqs.(14) and (19), the real matrix $U_a(k)$ satisfies

$$\det U_a(k) = 1,$$

namely, $U_a(k) \in SL(2, \mathbb{R})$.

The phase factor of the matrix (20) shows that in order to realize the general connection condition (1), one has to take a small-size limit under the condition

$$2Aa = \theta$$

with a fixed $\theta \in \mathbb{R}$. Accordingly, the strength of the vector potential increases as $a \to +0$;

$$A(a) = \frac{\theta}{2a}$$

As shown just below, a singular behavior for small $a$ is demanded for the strengths of the three $\delta$'s potentials in order to attain the condition (1). This enforces a careful analysis of each matrix element of $U_a(k)$ in the small distance limit. Indeed, it requires the expansions of triangular functions appeared in Eqs.(21) – (24) up to the orders shown below;

$$\cos(2ka) = 1 + O(a^2),$$

$$\sin(2ka) = 2ka - \frac{4}{3}k^3a^3 + O(a^5),$$

$$\cos^2(ka) = 1 - k^2a^2 + O(a^4),$$

$$\sin^2(ka) = k^2a^2 - \frac{1}{3}k^4a^4 + O(a^6).$$

Inserting Eqs.(30) and (32) into Eq.(21), one observes

$$[U_a(k)]_{21} = 2a + v_0a^2 + O(a^3).$$

This indicates that the strength $v_0$ of the middle $\delta$ is required to diverge with the order of $1/a^2$ in the small distance limit in order to make $[U_a(k)]_{21}$ have a nonzero limit. Indeed, if $v_0$ is changed according to the distance $a$ as

$$v_0(a) = \frac{\gamma}{a^2}$$

with an arbitrary real constant $\gamma \neq 0$, one obtains

$$[U_a(k)]_{21} = \gamma + 2a - 3k^2a^2 + O(a^3),$$

leading to

$$\lim_{a \to +0} [U_a(k)]_{21} = \gamma.$$ 

Using Eq.(35), one has the estimates

$$[U_a(k)]_{11} = \gamma + 1 + (\gamma + 2a + O(a^2))v_+ + O(a),$$

$$[U_a(k)]_{22} = \gamma + 1 + (\gamma + 2a + O(a^2))v_- + O(a).$$
for small $a$. The RHS of Eqs.(37) and (38) diverge in the small $a$ limit if one keeps $v_+$ and $v_-$ constant. The strengths $v_+$, $v_-$ of the side $\delta$'s are demanded to diverge with the order of $1/a$ to make $[U_a(k)]_{11}$ and $[U_a(k)]_{22}$ converge in the small $a$ limit; If

$$v_+(a) = -\frac{1}{a} + \frac{\alpha + 1}{\gamma},$$  \hspace{1cm} (39)\]

$$v_-(a) = -\frac{1}{a} + \frac{\delta + 1}{\gamma},$$  \hspace{1cm} (40)

with real constants $\alpha$ and $\delta$, the diagonal elements converge into

$$\lim_{a \to +0} [U_a(k)]_{11} = \alpha,$$  \hspace{1cm} (41)

$$\lim_{a \to +0} [U_a(k)]_{22} = \delta,$$  \hspace{1cm} (42)

respectively. Note that the divergent term in $v_+$ and $v_-$ is dependent only on the distance $a$ between neighboring $\delta$'s and the regular part determines the boundary condition around the generalized point interaction. Since $U_a(k) \in SL(2, \mathbb{R})$, one obtains under the constraints (34), (39) and (40)

$$\lim_{a \to +0} [U_a(k)]_{12} = \frac{\alpha \delta - 1}{\gamma} = \beta,$$  \hspace{1cm} (43)

which can be shown in a direct manner by noticing Eqs.(30)–(32) and (35). Since $v_0 = O(1/a^2)$, $v_+ = O(1/a)$ and $v_- = O(1/a)$ respectively, a close examination of the higher order terms in each equation is required to observe the cancellation among the terms of $O(1/a^2), O(1/a)$ and $O(a^0)$.

For the $\varepsilon$ potential of strength $u$, we have

$$v_0(a) = \frac{u}{a^2},$$  \hspace{1cm} (44)

$$v_+(a) = v_-(a) = -\frac{1}{a} + \frac{2}{u},$$  \hspace{1cm} (45)

which is exactly what we have shown in [18].

Up to now, we have excluded the case of $\gamma = 0$. For this case, we start by assuming $v_0$ to be constant (independent of the distance $a$), which is appropriately determined later. With this assumption, we see from Eq.(21)

$$\gamma = \lim_{a \to +0} [U_a(k)]_{21} = 0.$$  \hspace{1cm} (46)

Moreover, Eqs.(22) and (23) are reduced to

$$[U_a(k)]_{11} = 1 + (2a + O(a^2))v_+ + O(a),$$  \hspace{1cm} (47)

$$[U_a(k)]_{22} = 1 + (2a + O(a^2))v_- + O(a),$$  \hspace{1cm} (48)

respectively. Eqs.(47) and (48) indicate that if

$$v_+(a) = \alpha - \frac{1}{2a},$$  \hspace{1cm} (49)

$$v_-(a) = \delta - \frac{1}{2a},$$  \hspace{1cm} (50)

for small $a$, we attain

$$\lim_{a \to +0} [U_a(k)]_{11} = \alpha,$$  \hspace{1cm} (51)

$$\lim_{a \to +0} [U_a(k)]_{22} = \delta = 1/a.$$  \hspace{1cm} (52)

Here $\alpha \delta = 1$ is imposed since $\det U_a(k) = 1$ and $\gamma = 0$. It is easy to see from Eqs.(49) and (50) that the condition $\alpha \delta = 1$ is equivalent to

$$v_+ + v_- + 2v_+v_- = 0.$$  \hspace{1cm} (53)

Using Eqs.(33), (49), (50) and (53), we have

$$v_+ + v_- + [U_a(k)]_{21}v_+v_- = \frac{v_0(\alpha - 1)(\delta - 1)}{4} + O(a).$$  \hspace{1cm} (54)

We thus obtain the estimate of Eq.(24) for small $a$:

$$[U_a(k)]_{12} = v_+ + v_- + v_0(v_+ + v_-)a$$

$$+ [U_a(k)]_{21}v_+v_- + O(a)$$

$$= \frac{\alpha + \delta + 2}{4}v_0 + O(a).$$  \hspace{1cm} (55)

Eq.(55) shows that if the constant $v_0$ is taken as

$$v_0 = \frac{4\beta}{\alpha + \delta + 2},$$  \hspace{1cm} (56)

with an arbitrary real $\beta$, one obtains the limit

$$\lim_{a \to +0} [U_a(k)]_{12} = \beta.$$  \hspace{1cm} (57)

This completes the case of $\gamma = 0$. In a particular case of $\alpha = \delta = 1$ and $\beta = v$, Eqs.(49), (50) and (56) are reduced to $v_+ = v_- = 0$ and $v_0 = v$, namely a single $\delta$ potential of strength $v$ as expected. [Strictly speaking, Eq.(56) excludes the case of $\alpha = \delta = -1$; $U = -V\delta(-\beta)$. However, this is easily realized by using a single $\delta$ ($v_0 = -\beta, v_+ = v_- = 0$) together with the phase replacement from $\theta$ to $\theta + \pi$.]

Our findings in this section are summarized as follows. The Hamiltonian $H_a$ in Eq.(17) produces all possible connection conditions in Eq.(1) in the small $a$ limit together with suitably renormalized strengths; In case of $\gamma \neq 0$, Eqs.(39), (40), (34) and (28) for $v_+, v_-$, $v_0$ and $A$ respectively, whereas in the case $\gamma = 0$, Eqs.(49), (50) and (56) for $v_+, v_-$ and $v_0$ together with Eq.(28) for $A$.

3. Numerical Examples

In order to show the validity of the three $\delta$’s approximation, we perform numerical tests in this section. For simplicity, we consider the bounded region $X_1, X_2$ ($X_1 < 0 < X_2$) together with the Dirichlet boundary condition $\varphi(X_1) = \varphi(X_2) = 0$. The eigenvalues $k_n$ for the generalized point interaction are determined by

$$[G(0, k_n; X_2)VG(0, k_n; -X_1)]_{21} = 0.$$  \hspace{1cm} (58)
Following, we set the vector potential \( \mathbf{A} \) take the endpoints \( \gamma \) in Eqs. (34), (39), (40) for \( \gamma \). In Eq. (19), the strengths of three \( \delta \)'s are determined by \( \alpha \). The eigenvalues for the three \( \delta \)'s potential with the distance \( a = 0.2 \) is exhibited by the broken line. In this case, the wave number is \( k_{10} = 0.905264 \) and \( k_{13} = 1.142775 \), respectively.

with Eqs. (2) and (12). The associated (not necessarily normalized) eigenfunction is calculated by

\[
\varphi_n(x) = \begin{cases} 
\left[ G(0, k_n; x - X_1) \right]_{21}, & x < 0, \\
\left[ G(0, k_n; x) \right]_{21}, & x > 0.
\end{cases}
\]  

The eigenvalues for the three \( \delta \)'s approximation are determined by

\[
\left[ G(0, k_n; X_2 - a) \right]_{21} = 0 \quad (60)
\]

with Eq. (19), where \( A = \theta/(2a) \) according to Eq. (28). In Eq. (19), the strengths of three \( \delta \)'s are determined by Eqs. (34), (39), (40) for \( \gamma = 0 \) and Eqs. (49), (50), (56) for \( \gamma = 0 \) respectively. The associated wave function is calculated in a similar manner to in Eq. (59). In the following, we set the vector potential \( A = 0 \) \( (\theta = 0) \) since its effect is trivial. In the numerical calculations, we take the endpoints \( X_2 = -X_1 = 15.0 \) and the distance \( a = 0.2 \).

Figure 2 shows the eigenfunction of two low-energy (tenth in upper and thirteenth in lower) eigenstates for the case of \( \alpha = 3, \beta = -2, \gamma = -7 \) and \( \delta = 5 \). The solid line is a calculation for the point interaction, whereas the broken line is the wave function approximated by three nearby \( \delta \)'s. Figure 3 shows a typical example for the case of \( \gamma = 0 \). We take \( \alpha = 5, \beta = 3, \delta = 0.2 \). In all cases, one can observe the wave function discontinuity around the point interaction, which is successfully reproduced in the corresponding eigenfunction approximated by three \( \delta \)'s potential with appropriately renormalized strengths. However, it is worthy to mention that the approximated \( \varphi_n \) always has \( n - 1 \) nodes on the intervals as long as the distance \( a \) is kept finite, whereas this is not necessarily the case in the limit of \( a \to +0 \), namely for the case of the generalized point interaction. Indeed, the lower part in Fig. 2 shows that \( \varphi_{13} \) for the exactly point case loses two nodes in the vicinity of the interaction and as a result it has only ten nodes on the interval \( (X_1, X_2) \). On the other hand, the approximated (continuous) wave function behaves around the three \( \delta \)'s in a somewhat complicated manner to ensure the relation between the number of nodes and the quantum number \( n \) mentioned above. Clearly, the convergence of the wave function in the small \( a \) limit is not uniform on the interval including the origin in general.

### 4. Conclusion

We have constructed one-dimensional generalized point interactions characterized by four parameters in the small distance limit of equally spaced three \( \delta \)'s potentials. A constant vector field added on the interval be-
between the two side $\delta$’s has no effect except for changing the phase of wave function. The remaining part, the transfer matrix $U_0(k)$ can be made converge into an arbitrarily fixed special linear matrix by adjusting the strengths of the three $\delta$’s according to the distance in an appropriate manner. Though a divergent term is inevitable for each strength in the small distance limit, it takes a remarkably simple and experimentally realizable form. Numerical examples support our model and show a satisfactory coincidence with the corresponding zero-range case even at a finite distance level.

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