International Journal of Theoretical Physics, Vol. 35, No. 6, 1996

Point Interactions from Flux Conservation

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Received August 30, 1995

We show that the physical requirement of flux conservation can substitute for the usual matching conditions in point interactions. The study covers an arbitrary superposition of δ and δ' potentials on the real line and can be easily applied to higher dimensions. Our procedure can be seen as a physical interpretation of the deficiency index of some symmetric, but not self-adjoint operators.

1. Point interactions of the delta type have a long history in quantum physics (Albeverio *et al.*, 1988). In this note we show that the conventional matching conditions for these potentials can be obtained easily by enforcing the conservation of the flux across the discontinuity.

For a one-dimensional quantum system with a point interaction at $x = 0$, the continuity equation for the current $\mathbf{j}$ and the density ρ, namely $\dot{\rho} + \operatorname{div} \mathbf{j} = 0$, becomes

$$j_- \equiv j(x < 0) = j_+ \equiv j(x > 0) \tag{1}$$

in a stationary state; the current is ($\hbar = 2m = 1$)

$$\mathbf{j} = \frac{\hbar}{2im}(\psi^* \nabla \psi - \psi \nabla \psi^*) \rightarrow \frac{i}{2}\begin{vmatrix} \psi & \psi^* \\ \psi' & \psi'^* \end{vmatrix} \tag{2}$$

There are essentially *four types* of solutions to (1) and (2). If the flux is zero, we can consider the point $x = 0$ as an infinite wall, and we have

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two families of total-reflection solutions, labeled by a (constant) phase shift, namely

$$\begin{aligned} \psi_\alpha^{\mathrm{I}}(x) &= \begin{cases} e^{ikx} + e^{i\alpha}e^{-ikx}, & x < 0 \\ 0, & x > 0 \end{cases} \\ \psi_\beta^{\mathrm{II}}(x) &= \begin{cases} 0, & x < 0 \\ e^{-ikx} + e^{i\beta}e^{ikx}, & x > 0 \end{cases} \end{aligned} \tag{3}$$

Notice that for generic α, β, neither $\psi(x)$ nor $\psi'(x)$ vanishes at $x = 0$, but the flux does.

2. For nonzero flux, we have another two-parameter family. Let us *assume* first

$$\psi(0-) = \psi(0+) \tag{4}$$

with perhaps discontinuous ψ'; from (1) and (2)

$$\psi(0) \text{ disc } \psi^{*\prime}(0) = \psi^*(0) \text{ disc } \psi'(0) \Rightarrow \frac{\text{disc } \psi'(0)}{\psi(0)} = \text{real const} = g \tag{5}$$

where disc $f(0) \equiv f(0+) - f(0-)$.

Equation (5) characterizes the $\delta(x)$-potential of strength g. In fact, for the scattering situation

$$\begin{aligned} &\psi(x < 0) = e^{ikx} + b(k)e^{-ikx}, \qquad \psi(x > 0) = (1 + f(k))e^{ikx} \\ &\hat{\psi}(x < 0) = (1 + \hat{f}(k))e^{-ikx}, \qquad \hat{\psi}(x > 0) = e^{-ikx} + \hat{b}(k)e^{ikx} \end{aligned} \tag{6}$$

we obtain from (4) and (5) the well known S-matrix (e.g., Gottfried, 1966, p. 50)

$$S(k) \equiv \begin{pmatrix} 1 + f(k) & \hat{b}(k) \\ b(k) & 1 + \hat{f}(k) \end{pmatrix} = \begin{pmatrix} 2ik & g \\ g & 2ik \end{pmatrix} \frac{1}{2ik - g} \tag{7}$$

The pole at $k = -ig/2$ represents a *bound state* (for $g < 0$) or an antibound state (for $g > 0$).

3. The *fourth* family of solutions is obtained by imposing the alternative conditions

$$\text{disc } \psi(0) = g_1\psi'(0), \qquad \text{disc } \psi'(0) = 0 \tag{8}$$

in which case the S-matrix becomes

$$S(k) = \begin{pmatrix} 2 & -g_1 ik \\ -g_1 ik & 2 \end{pmatrix} \frac{1}{2 - ig_1 k} \tag{9}$$

which is the scattering conventionally ascribed to the $\delta'(x)$-potential (Seba, 1986); it also supports a single *bound* state (for $g_1 < 0$) or antibound state (for $g_1 > 0$).

Notice that the $\delta(x)$-potential is blind to the odd wave, $f(k) = b(k) \Rightarrow \delta_-(k) = 0$, and that the $\delta'(x)$-potential proceeds exclusively in the odd wave, $f(k) = -b(k) \Rightarrow \delta_+(k) = 0$. Here, $\delta_\pm(k)$ are the even/odd-phase shifts of the one-dimensional partial waves (Eberly, 1965).

4. Our analysis allows logically for a superposition of $\delta(x)$- and $\delta'(x)$-potentials which seem to have been so far overlooked in the literature. Namely, define $\Phi(x)$ and $\Psi(x)$ by

$$\begin{aligned} \Phi(x) &= \cos\alpha\psi(x) + \frac{1}{m}\sin\alpha\psi'(x) \\ \Psi(x) &= -m\sin\alpha\psi(x) + \cos\alpha\psi'(x) \end{aligned} \tag{10}$$

where m is a quantity with the dimensions of an inverse length. Then Φ and Ψ can substitute by ψ and ψ' in (2) provided m is real since

$$\det\begin{pmatrix} \cos\alpha & +\sin\alpha/m \\ -m\sin\alpha & \cos\alpha \end{pmatrix} = 1 \tag{11}$$

Now we define the general problem by

$$\operatorname{disc}\Phi(0) = 0, \qquad \operatorname{disc}\Psi(0) = g\Phi(0) \tag{12}$$

and solve for b, f, $\hat{b}$, and $\hat{f}$ of equation (6); the calculation is straightforward, yielding

$$\begin{aligned} S(k) &= \begin{pmatrix} 2ik & g(\cos\alpha - (ik/m)\sin\alpha)^2 \\ g(\cos\alpha + (ik/m)\sin\alpha)^2 & 2ik \end{pmatrix} \\ &\quad \times \frac{1}{2ik - g(\cos^2\alpha + (k^2/m^2)\sin^2\alpha)} \end{aligned} \tag{13}$$

which interpolates naturally between the $\delta(x)$-potential, $\cos\alpha = 1$, $\sin\alpha = 0$, equation (7); and the $\delta'(x)$-potential, $\cos\alpha = 0$, $\sin\alpha = 1$, equation (9) with $g/m^2 = -g_1$.

5. Some features of formula (13) are worth noting.

a. $f(k) = \hat{f}(k)$, as demanded by time-reversal invariance (Faddeev, 1964); however, $b(k) \neq \hat{b}(k)$ except in the extreme cases δ or δ'.

b. $\psi_{k=0}(x) = 0$ except in the $\delta'(x)$ case, when $\psi_{k=0}(x) = 1$.

c. S is, of course, unitary; its spectrum determines the eigenphase shifts

$$\exp 2i\delta_1 = \frac{2ik + g(\cos\alpha + (k^2/m^2)\sin^2\alpha)}{2ik - g(\cos^2\alpha + (k^2/m^2)\sin^2\alpha)}, \qquad \exp 2i\delta_2 = 1 \quad (14)$$

This result is worth stressing: *our family of interactions proceeds in a single partial wave, the "orthogonal" one is not affected by the potential.* This is in consonance with the simplicity of the S-matrix, equation (13): potentials which produce a single-mode interaction have a particularly simple pole structure in the S-matrix. This includes the delta potential (only even waves), the delta prime (only odd waves), the "solitonic" potential $V(x) = -l(l+1)\,\mathrm{sech}^2 x$, $l = 0, 1, 2, \ldots$ (only forward scattering), and the one-dimensional Coulomb potential (only odd-wave interaction).

d. For $\sin\alpha \neq 0$ [i.e., excluding the $\delta(x)$ case], the two poles of S are given by

$$k = im^2\left\{1 \pm \left[1 + \left(\frac{g^2}{m^2}\right)\cos^2\alpha\,\sin^2\alpha\right]^{1/2}\right\}/g\sin^2\alpha \qquad (15)$$

so there is always a bound state *and* an antibound state, for any sign of g, in the mixed case $0 \neq \alpha \neq \pi/2$. We already remarked that in the pure cases ($\alpha = 0$ or $\alpha = \pi/2$) there is only one pole, implying either a single bound or antibound state.

e. The eigenvector of the zero-phase shift is readily seen to be

$$V = \begin{pmatrix} i(k/m)\sin\alpha + \cos\alpha \\ ik\sin\alpha - m\cos\alpha \end{pmatrix} \qquad (16)$$

and depends only on $\tan\alpha$, say, not on g; in particular, at low energies $V \simeq \binom{1}{-1}$, that is, the *odd* wave is not affected, corresponding to the pure δ case; at high energies $V \simeq \binom{1}{1}$, characteristic of the δ'-potential, with no force in the even channel. This is a sensible result, because the scale dimension of the $\delta(x)$ is 1, but that of our δ' is 3 (when dim [momentum] $= +1$). Note that the naive dimension of the δ' would be 2, not 3!

f. The reasons to call the matching conditions (8) a $\delta'(x)$-potential are obscure; in fact, for the δ case one can *derive* conditions (4) and (5) by integrating the Schrödinger equation across the discontinuity; this is not so for the $\delta'(x)$.

Also, it is easy to show that a "regularized" $\delta'(x)$-potential

$$g \lim_{a\to 0} \frac{1}{a}\{\delta(x+a) - \delta(x)\} \qquad (17)$$

with renormalized coupling g leads to the conventional $\delta(x)$ [not $\delta'(x)$!] potential (Seba, 1987).

The rationale to call conditions (8) a $\delta'(x)$-potential is that, writing the Schrödinger equation $\psi'' + \epsilon\psi = g\delta'(x)\psi$, ψ'' is proportional to δ', hence ψ' to δ, and ψ to the step function. Hence, heuristically, ψ'' and ψ' are "continuous" at the singularity, but ψ makes a jump, i.e., conditions (8). Notice that the naive $\delta'(x)$ would have dimension $+2$, so it would be potentially scale invariant, whereas the δ' we are using has dimension three; in fact, no trace of scale invariance remains in the δ' S-matrix, equation (9).

g. It is not difficult to extend these results to higher dimensions; we state only the $d = 3$ result (Albeverio *et al.*, 1988). The analogue of equation (5) is now

$$u'/u|_0 = \text{const} \equiv -1/a \tag{18}$$

where $\psi(r) = u(r)/r$. Since $u = A \sin(r + \delta_0)$, the "coupling constant" determines the phase shift by

$$k \cot \delta_0 = -1/a \tag{19}$$

In this case, a is called the scattering length. The $d = 2$ case has been the subject of some recent papers and we refer the reader to them (Holstein, 1993; Mead and Godines, 1991; Gosdzinsky and Tarrach, 1991).

6. The rigorous treatment of the contact potentials entails the theory of extensions of symmetric, non-self-adjoint operators, which started with a paper of Berezin and Faddeev (1961). But self-adjointness of the Hamiltonian implies unitarity of the evolution operators, and also of the S-matrix, which in turn is guaranteed by flux conservation; so there is not much surprise that the families of extensions of the kinetic energy operator $D = \Sigma\ -d^2/dx^2$ acting on $R^n - \{0\}$ would coincide with the families of matching conditions, which we have worked out in detail for the $d = 1$ case (Carreau, 1993).

ACKNOWLEDGMENTS

L.J.B. thanks Prof. George Sudarshan and the Theory Group of the University of Texas for their hospitality and partial support. He is also grateful to the Spanish CAICYT for a travel grant. This work was supported by the Robert A. Welch Foundation and NSF Grant PHY 9009850.

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