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POINT INTERACTIONS FROM FLUX CONSERVATION

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Abstract

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 [1]. 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 one-dimensional quantum system with a point interaction at $x = 0$, the continuity equation for the current $\vec{\jmath}$ and the density ρ, namely $\dot{\rho} + div\vec{\jmath} = 0$ becomes

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

in a stationary state; the current is

$$\vec{\jmath} = \frac{\hbar}{2im}\left(\psi^* \vec{\bigtriangledown}\psi - \psi\vec{\bigtriangledown}\psi^*\right) \to \frac{i}{2}\begin{vmatrix} \psi & \psi^* \\ \psi' & \psi'^* \end{vmatrix} . \tag{2}$$

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 two families of total-reflection solutions,

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labeled by a (constant) phase shift, namely

$$\psi^I_\alpha(x) = \begin{cases} e^{ikx} + e^{i\alpha}e^{-ikx} & x < 0 \\ 0 & x > 0 \end{cases} \qquad \psi^{II}_\beta(x) = \begin{cases} 0 & x < 0 \\ e^{-ikx} + e^{i\beta}e^{ikx} & x > 0 \end{cases} \tag{3}$$

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

(2.) For non-zero 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)

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

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

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

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

we obtain from (4) and (5) the well known [2] S-matrix

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

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

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

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 a $\delta'(x)-$ potential [3]; 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 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 [4].

(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

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

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 they are 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

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

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

$$S(k) = \begin{pmatrix} 2ik & g(\cos\alpha - \frac{ik}{m}\sin\alpha) \\ g(m\cos\alpha - ik\sin\alpha)^2 & 2ik \end{pmatrix} \frac{1}{2ik - g\left(\cos^2\alpha + \frac{k^2}{m^2}\right)\sin^2\alpha}. \tag{13}$$

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

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

1. $f(k) = \hat{f}(k)$, as demanded by time-reversal invariance[5]; however, $b(k) \neq \hat{b}(k)$ except in the extreme cases δ or δ'.

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

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

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

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, eq. (13): potentials which produce single-mode interaction have particularly simple pole structure in the S-matrix[6]. This includes the delta potential (only even wave), the delta prime (only odd waves), the "solitonic" potential $V(x) = -\ell(\ell+1)\,\mathrm{sech}^2 x$, $\ell = 0, 1, 2, \dots$ (only forward scattering) and the one-dimensional Coulomb potential (only odd-wave interaction).

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

$$k = im^2 \left(1 \pm \sqrt{1 + \left(\frac{g^2}{m^2}\right) \cos^2\alpha \sin^2\alpha} \right) \Big/ b \sin^2\alpha \tag{15}$$

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, meaning either a bound or antibound state.

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

$$V = \begin{pmatrix} i\frac{k}{m} \sin\alpha + \cos\alpha \\ ik \sin\alpha - m\cos\alpha \end{pmatrix} \tag{16}$$

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!

6. 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

$$g \lim_{a\to\theta} \frac{1}{a} \{\delta(x+a) = \delta(x)\} \tag{17}$$

with renormalized coupling g, leads to the conventional $\delta(x)$ (not $\delta'(x)$!) potential.[7]

The rationale to call conditions (8) a $\delta'(x)$ 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 potentially be scale invariant, whereas the δ' we are using has dimension three; in fact, no trace of scale invariance remains in the δ' S-matrix, eq. (9).

7. It is not difficult to extend these results to higher dimensions; we state only the $d = 3$ result.[1] The analogue of eq. (5) is now

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

where $\psi(r) = u(r)/r$ and $u_0(0) = 0$; as

$$\psi(r) = \frac{1}{r}\, u(r); \tag{19}$$

Since $u = A\sin(r + \delta_0)$, the “coupling constant” determines the phase shift by

$$k \cot\, \delta_\theta = -1/a\,. \tag{20}$$

In this case, a is called the scattering length. The $d = 2$ case has been the subject of some recent papers[8] and we refer the reader to them.

8. The rigorous treatment of the contact potentials entails the theory of extensions of symmetric, non-self-adjoint operators, which started with a paper of Fadeev and Berezin.[9] 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 $D = -d^2/dx^2$ acting on $\mathbb{R}^n - \{0\}$ would coincide with the families of matching conditions, which we have worked out in detail for the $d = 1$ case.[10]

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