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LETTER TO THE EDITOR

Time-reversal aspect of the point interactions in one-dimensional quantum mechanics

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Abstract. It is known that there is a four-parameter family of point interactions in one-dimensional quantum mechanics. We point out that, as far as physics is concerned, it is sufficient to use three of the four parameters. The fourth parameter is redundant. The apparent violation of time-reversal invariance in the presence of the fourth parameter is an artifact.

Including the familiar δ-function potential, there is a four-parameter family of point interactions in one-dimensional quantum mechanics [1–10]. It is said that, if time-reversal invariance is imposed, the number of the parameters that specify the interactions is reduced to three [8–10]. The purpose of this letter is to point out that the three-parameter family actually exhausts all physics of the point interactions in one dimension. The fourth parameter introduces no new physics beyond that of the three-parameter family. This implies that the *apparent* violation of time-reversal invariance in the presence of the fourth parameter is an artifact. Indeed, the transformation of the wavefunction under time-reversal can be redefined such that the point interaction with the fourth parameter also conforms to time-reversal invariance.

Let us consider a particle interacting with a point interaction at $x = 0$. It is understood that the particle has no spin. The point interaction is such that it is zero everywhere except at $x = 0$. The point interaction can be interpreted in terms of self-adjoint extension of the nonrelativistic kinetic energy operator $-(\hbar^2/2m)\,\mathrm{d}^2/\mathrm{d}x^2$ where m is the mass of the particle concerned†. In the following we use units in which $\hbar^2/2m = 1$. The point interaction can be expressed in terms of the boundary condition on the wavefunction at $x = 0$. The condition in its most general form can be written as

$$\begin{pmatrix} \psi'(+0) \\ \psi(+0) \end{pmatrix} = U \begin{pmatrix} \psi'(-0) \\ \psi(-0) \end{pmatrix} \tag{1}$$

$$U = \mathrm{e}^{\mathrm{i}\theta} \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} \qquad \alpha\gamma - \beta\delta = 1 \tag{2}$$

where $\psi'(x) = \mathrm{d}\psi(x)/\mathrm{d}x$ and α, β, γ, δ and θ are all real constants. Among α, β, γ and δ, three are independent. Thus we have a four-parameter family of point interactions.

† To be more precise, we are referring to an extension of the kinetic energy operator that is restricted to the domain of $C_0^\infty(R\backslash\{0\})$ [2]. We focus on a self-adjoint extension that links the two half-axes of $x > 0$ and $x < 0$. We do not consider the case in which the two half-axes are completely disjoint.

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It would be useful to relate the parameters that we are using to other sets of parameters that have appeared in the literature. Carreau *et al* [5] and Carreau [6] used four real parameters α, β, ρ and θ. Their α, β and θ are different from ours. In terms of their notation, U is expressed as

$$U = \mathrm{e}^{-\mathrm{i}\theta} \begin{pmatrix} 1 + \frac{\beta}{\rho} & \alpha + \beta + \frac{\alpha\beta}{\rho} \\ \frac{1}{\rho} & 1 + \frac{\alpha}{\rho} \end{pmatrix}. \tag{3}$$

Albeverio *et al* [9] recently used a, b, c and θ, in terms of which U becomes

$$U = \mathrm{e}^{\mathrm{i}\theta} \begin{pmatrix} d & c \\ b & a \end{pmatrix} \qquad ad - bc = 1 \tag{4}$$

In this letter we use the notation of (1) and (2) throughout.

Let us require that the system is invariant under time reversal. According to the standard interpretation, if the wavefunction $\psi(x, t)$ is an admissible solution of the time-dependent Schrödinger equation of the system, then its complex conjugate with t replaced by $-t$, $\psi^*(x, -t)$, is also admissible; see, e.g., [11]. The latter describes the motion backward in time. Alternatively, if we consider a stationary state, we should be able to choose the wavefunction to be real. It then follows that the factor $\mathrm{e}^{\mathrm{i}\theta}$ of the boundary condition has to be real, i.e. $\theta = 0$ (modulo π). Thus we are left with three independent parameters.

In [8], we worked out the transmission and bound state problems for the three-parameter family of the point interactions that conform to time-reversal invariance. Following [2, 3], we chose parameter θ such that $\mathrm{e}^{\mathrm{i}\theta} = -1$ in [8]. Let us now re-examine the transmission and bound state problems with the four-parameter family (with arbitrary θ) and see if we can find anything new beyond what is known with the three-parameter family. If the wave is incident from the left, the wavefunction can be written as

$$\psi_{\mathrm{L}}(x) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + R_{\mathrm{L}}\mathrm{e}^{-\mathrm{i}kx} & \text{for} \quad x < 0 \\ T_{\mathrm{L}}\mathrm{e}^{\mathrm{i}kx} & \text{for} \quad x > 0 \end{cases} \tag{5}$$

where $k = \sqrt{E}$ and $E > 0$ is the energy. The subscript L refers to the situation when the wave is incident from the left. The $\psi_{\mathrm{R}}(x)$ can be written down similarly.

Imposing the boundary condition (1) on ψ_{L} and ψ_{R}, we obtain

$$T_{\mathrm{L}} = 2\mathrm{i}k\mathrm{e}^{\mathrm{i}\theta}/D \qquad T_{\mathrm{R}} = 2\mathrm{i}k\mathrm{e}^{-\mathrm{i}\theta}/D \tag{6}$$

$$R_{\mathrm{L}} = [\beta + \delta k^2 + \mathrm{i}k(\alpha - \gamma)]/D \tag{7}$$

$$R_{\mathrm{R}} = [\beta + \delta k^2 - \mathrm{i}k(\alpha - \gamma)]/D \tag{8}$$

$$D = -\beta + \delta k^2 + \mathrm{i}k(\alpha + \gamma). \tag{9}$$

As expected, $T_{\mathrm{L}} \neq T_{\mathrm{R}}$ when time-reversal invariance (in its usual interpretation) does not hold [12, 13]. Note, however, that $|T_{\mathrm{L}}|$, $|T_{\mathrm{R}}|$, R_{L} and R_{R} are all independent of θ.

Next let us examine the bound state. If $D = 0$ for $k = \mathrm{i}\kappa$ ($\kappa > 0$), there is a bound state of energy $-\kappa^2$. The wavefunction of the bound state takes the form

$$\psi(x) = \begin{cases} \psi(+0)\mathrm{e}^{-\kappa x} & \text{for} \quad x > 0 \\ \psi(-0)\mathrm{e}^{\kappa x} & \text{for} \quad x < 0 \end{cases} \tag{10}$$

where

$$\frac{\psi(+0)}{\psi(-0)} = -\mathrm{e}^{\mathrm{i}\theta}\left(\alpha + \frac{\beta}{\kappa}\right) = \mathrm{e}^{\mathrm{i}\theta}(\gamma + \kappa\delta). \tag{11}$$

It can be shown that $|\psi(+0)/\psi(-0)| = 1$ if and only if $\alpha = \gamma$.

If we put $\mathrm{e}^{\mathrm{i}\theta} = -1$, we recover the results that were given in [8]. If we compare the results that we have just derived with the corresponding ones of [8], it is clear that no new physics has emerged. For a given set of values of the three parameters α, β and γ, the transmission and reflection probabilities are the same as before. They are independent of the fourth parameter θ. For the bound state, the energy and the probability density $|\psi(x)|^2$ are also independent of θ. All that has changed, when the complex factor $e^{i\theta}$ was introduced into the boundary condition, is essentially the following. If we let the wavefunction in the region of $x < 0$ remain the same, the wavefunction for $x > 0$ is multiplied by $e^{i\theta}$. The factor $e^{i\theta}$ of T_L and $\psi(+0)/\psi(-0)$ can be understood in this way. For T_R, one can keep the wavefunction for $x > 0$ the same and multiply that for $x < 0$ with $e^{-i\theta}$. This constant phase factor $e^{\pm i\theta}$ does not add any new physics. In evaluating matrix elements of any physical quantities, this phase factor disappears. In no way does the wavefunction for $x > 0$ interfere with that for $x < 0$.

A time-dependent nonstationary state can be expressed as a superposition of stationary states. For example, let us consider a situation such that a wavepacket is incident from the left. The wavefunction, which is time dependent, can be constructed as a superposition of $\psi_L(x)$ times e^{-ik^2t} with an appropriate weight function of k. In such a linear combination of stationary states, however, the wavefunctions for $x > 0$ and those for $x < 0$ are separately superposed. Hence the phase factor $e^{i\theta}$ has no interesting effect.

If the parameter θ is as unimportant as we have indicated above, it must be redundant. We can show that the apparent violation of time-reversal invariance that is caused by the complex factor $e^{i\theta}$ of the boundary condition is actually an artifact. Under time-reversal transformation $t \to -t$, we usually replace the wavefunction $\psi(x, t)$ with $\psi^*(x, -t)$ so that the time-dependent Schrödinger equation remains the same in form. It is clear that this prescription as such does not work in the presence of the complex boundary condition. However, if we transform the wavefunction as

$$\psi(x, t) \to \chi(x, -t) = f(x)\psi^*(x, -t) \tag{12}$$

where

$$f(x) = \begin{cases} 1 & \text{for} \quad x < 0 \\ e^{2i\theta} & \text{for} \quad x > 0 \end{cases} \tag{13}$$

the Schrödinger equation does remain the same in form and $\chi(x, -t)$ satisfies the boundary condition (1). This transformation is anti-unitary [11]. The wavefunction $\chi(x, -t)$ describes the development of the system, backward in time. For the wavefunctions of stationary states like $\psi_L(x)$ of (5) and $\psi(x)$ of (10), the transformation reads

$$\psi(x) \to \chi(x) = f(x)\psi^*(x) \tag{14}$$

while the time-dependent factor of the wavefunction remains the same: $e^{-iEt} \to e^{iE(-t)}$.

With this new prescription the system that is subject to the complex boundary condition (1) is invariant under time-reversal transformation. This situation reminds us of the case of a particle with spin interacting with a magnetic field. If we simply transform the wavefunction as $\psi(x, t) \to \psi^*(x, -t)$, the Schödinger equation is not invariant. One has to appropriately rearrange the spin components of the wavefunction [11].

Let us quote the remark that we made earlier regarding the time-reversal invariance of the point interactions in one dimension and the unitarity of the S matrix that appears in the transmission-reflection problem: see the last paragraph of section 3 of [8]. It was essentially the following:

> If $e^{i\theta}$ is not real, then $T_L \neq T_R$ which implies that time-reversal invariance does not hold. Unitarity however holds even when $e^{i\theta}$ is not real. We find this feature very interesting in the following sense. Suppose $V(x)$ of the Hamiltonian is an ordinary finite potential. Time-reversal invariance requires that $V(x)$ is real. Then unitarity

> holds. On the other hand, unitarity requires that $V(x)$ is real. Then time-reversal invariance ensues. Thus time-reversal invariance and unitarity are inseparable for a finite potential. For generalized point interactions, however, we can have a situation such that time-reversal invariance is violated, yet unitarity is valid.

We withdraw the last sentence. Within the extended scheme of time-reversal transformation that we have proposed above, all point interactions conform to time-reversal invaiance. We can have $T_L \neq T_R$ within the extended time-reversal invariance. Unitarity and time-reversal invariance remain inseparable.

In this letter we focused on the nonrelativistic case with the Schrödinger equation. Let us add that exactly the same situation holds for the relativistic case with the Dirac equation in one dimension. In this connection, see section 5 of [8]. There is a four-parameter family of point interactions for the Dirac equation. As far as physics is concerned, however, the fourth parameter of the point interactions is again redundant. The three-parameter family represents all of the physically interesting features of the point interations in one dimension. The apparent violation of time-reversal invariance in the presence of the complex boundary condition with the fourth parameter is an artifact. The time-reversal transformation of the wavefunction can be extended such that, in the presence of the fourth parameter, the Dirac equation remains invariant.

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Note added in proof. Equations (6)–(9) were derived earlier by Chernoff and Hughes: Chernoff P R and Hughes R J 1993 *J. Func. Anal.* **111** 97.

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