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1993 J. Phys. A: Math. Gen. 26 427

(http://iopscience.iop.org/0305-4470/26/2/025)

J. Phys. A: Math. Gen. 26 (1993) 427–432. Printed in the UK

Four-parameter point-interaction in 1D quantum systems

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Received 30 March 1992, in final form 28 August 1992

Abstract. We construct a four-parameter point-interaction for a non-relativistic particle moving on a line as the limit of a short-range interaction with a range tending toward zero. For particular choices of the parameters, we can obtain a δ-interaction or the so-called δ'-interaction. The Hamiltonian corresponding to the four-parameter point-interaction is shown to correspond to the four-parameter self-adjoint Hamiltonian of the free particle moving on the line with the origin excluded.

1. Introduction

Point-interactions in non-relativistic quantum mechanics have been studied extensively in recent years [1]. The interest in this subject is twofold. First there is the hope that a point-interaction can be a good approximation of a very localized interaction. Second, it is possible to obtain exact solutions for quantum systems with point-interactions. Physically, a very localized interaction can be due to the interaction of a particle with an impurity or a local defect in a solid for example. It could also be due to the region of contact (point-contact) between two conducting materials, etc.

In two or three dimensions a point-interaction can be thought of as the interaction of a particle with a δ-potential with a renormalized coupling constant [2]. However, it is also possible to describe the point-interaction in terms of boundary conditions on the wavefunctions at the interaction point which is excluded from the configuration space [1]. In this case the different strengths of the interaction are characterized by different boundary conditions.

In one dimension, the situation is different. Before our paper, the most general point-interaction in one dimension could only be expressed in terms of boundary conditions which we review later. The object of our paper is to construct a short-range interaction which, in the zero-range limit, gives a physical realization of the point-interaction in one dimension.

The general point-interaction in one dimension is obtained by considering the self-adjoint extensions of the Hamiltonian of a free particle moving on a line with the origin excluded (see figure 1). It is found that there is a four-parameter family of self-adjoint Hamiltonians that can be characterized by a four-parameter family of boundary condition imposed on the wavefunctions [3, 4]. Let us recall this boundary condition, following the notation of [4]. For the wavefunction $\psi(x)$, defined everywhere except at $x = 0$, we require

$$\begin{bmatrix} -\psi'_{\mathrm{L}} \\ \psi'_{\mathrm{R}} \end{bmatrix} = M \begin{bmatrix} \psi_{\mathrm{L}} \\ \psi_{\mathrm{R}} \end{bmatrix} \tag{1.1}$$

where

$$\psi_R \equiv \lim_{\epsilon\to 0+} \psi(\epsilon) \qquad \psi_R' \equiv \lim_{\epsilon\to 0+} \frac{d\psi}{dx}(\epsilon)$$
$$\psi_L \equiv \lim_{\epsilon\to 0-} \psi(\epsilon) \qquad \psi_L' \equiv \lim_{\epsilon\to 0-} \frac{d\psi}{dx}(\epsilon) \tag{1.2}$$

and M is an arbitrary 2×2 Hermitian matrix which can be parametrized in terms of four real parameters

$$M = \begin{pmatrix} \rho+\alpha & -\rho e^{i\theta} \\ -\rho e^{-i\theta} & \rho+\beta \end{pmatrix} \tag{1.3}$$

with $\rho \geqslant 0$ and $0 \leqslant \theta < 2\pi$. If the domain of the Hamiltonian consists of wavefunctions obeying (1.1) for a fixed M, then the Hamiltonian will be self-adjoint and will be denoted H_M. This boundary condition ensures the conservation of probability at the origin or, equivalently, that the current of probability is continuous through the origin.

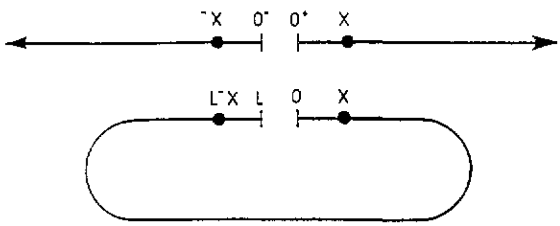

Figure 1. The upper diagram shows the line with a hole. The lower diagram shows the box distorted to indicate the similarity between the boundary conditions at the walls of the box and the two sides of the hole.

Note that, for the quantum system consisting of a free particle restricted to move inside an interval of length L, we have a similar story. We can imagine bringing the extremities of the interval close to each other, making it look like a circle with a hole, see figure 1. The result of our paper applies to this system as well.

An interpretation of the parameters $\rho, \alpha, \beta, \theta$ in the context of functional integrals was given in [4]. It was found that the measure on paths in the functional integral is controlled by these parameters. Let us recall, also from [4], that the current of probability at the origin is proportional to ρ. For $\rho = 0$, the boundary condition reduces to $-\psi_L' = \alpha\psi_L$ and $\psi_R' = \beta\psi_R$ which describes the physics of two separate half-lines. For ρ infinite, $\theta = 0$, and, α and β finite, the wavefunction is continuous, and $\psi_R' - \psi_L' = (\alpha+\beta)\psi_L$ which is the δ-interaction. For ρ finite and $\theta = \alpha = \beta = 0$, the derivative of the wavefunction is continuous and $\psi_R - \psi_L = (1/\rho)\psi_L'$ which is the so-called δ'-interaction (see, eg., [1]).

In this paper, we construct a Hamiltonian defined on the whole line which described a four-parameter family point-interaction. The interacting terms in the Hamiltonian provides a physical understanding of the four parameters.

The organization of the paper is as follows: in section 2, we construct a four-parameter point-interaction. We show that the effect of adding this point-interaction to the free Hamiltonian on the whole line leads to a system that is identical to the free particle on the line with a hole with the boundary condition (1.1). In section 3, we study the scaling properties of the point-interaction.

2. Point-interaction

In this section, we construct a four-parameter point-interaction for a non-relativistic particle moving on the whole line. We define the point-interaction as the limit of a local interaction of range of order ϵ with ϵ going to zero. We construct the local interaction in such a way that, in the limit where ϵ goes to zero, it forces the wavefunction to satisfy the boundary condition (1.1). In particular, we will see that the so-called δ'-interaction is obtained as the zero-range limit of an operator that is non-self-adjoint for finite range (see [5] for an alternative representation of the δ'-interaction).

We would like to mention that progress in this direction by P Šeba [3] led to a two-parameter point-interaction expressed formally as a sum of terms involving $\delta(x)$ and $\delta'(x)$. However, the physical interpretation of this formal expression seems unclear to us.

Let us consider the following Hamiltonian for the local interaction depending upon the parameters $\rho, \theta, \alpha, \beta$

$$H^{\epsilon} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + I^{\epsilon} \tag{2.1}$$

where

$$I^{\epsilon} = \begin{cases} K^{\epsilon}(\rho\,\mathrm{e}^{\mathrm{i}\theta})\left(\dfrac{\mathrm{d}}{\mathrm{d}x} + \alpha + \rho - \rho\,\mathrm{e}^{\mathrm{i}\theta}\right) & -\epsilon < x < 0 \\ -K^{\epsilon}(\rho\,\mathrm{e}^{-\mathrm{i}\theta})\left(\dfrac{\mathrm{d}}{\mathrm{d}x} + \beta + \rho - \rho\,\mathrm{e}^{-\mathrm{i}\theta}\right) & 0 < x < \epsilon \\ 0 & \text{elsewhere} \end{cases} \tag{2.2}$$

is a local interaction. Also, $K^{\epsilon}(\eta)$ is the solution of the transcendental equation

$$K^{\epsilon}(\eta)\mathrm{e}^{-2K^{\epsilon}(\eta)\epsilon} = \eta \tag{2.3}$$

for which $K^{\epsilon}(\eta)$ goes to infinity as ϵ goes to zero. The solution can be written as an expansion for small ϵ, that is

$$K^{\epsilon}(\eta) = \frac{1}{2\epsilon}\{-\ln(2\eta\epsilon) + \ln[-\ln(2\eta\epsilon) + \ln[\ldots]]\}. \tag{2.4}$$

This Hamiltonian describes the motion of a particle which moves under the influence of the interaction I^{ϵ} only whenever it is inside the interval $[-\epsilon, \epsilon]$, otherwise it moves freely.

We observe that the Hamiltonian H^{ϵ} is not self-adjoint (not even Hermitian) since the coefficient of $\mathrm{d}/\mathrm{d}x$ is not purely imaginary. However, we will show that, in the limit where ϵ goes to zero, H^{ϵ} becomes self-adjoint. Specifically, we will show that, given a particular value of the parameters ρ, α, β and θ, H^{ϵ} converges toward the self-adjoint Hamiltonian H_M described in the previous section for the particle on the line with the origin excluded.

To show that, we simply demonstrate that in the limit where ϵ goes to zero, the energy eigenvalues of H^{ϵ} and the corresponding energy eigenstates are identical to those of H_M. Let us solve the eigenvalue equation for the Hamiltonian H^{ϵ}

$$H^{\epsilon}\psi_{\mathrm{E}} = E\psi_{\mathrm{E}}. \tag{2.5}$$

This is easy; we just solve this equation for each interval for which it is a constant-coefficient differential equation, and match the solutions at the junctions of the different intervals so that the wavefunction and its derivative are continuous for all x. Once this is done, we simply let ϵ tends toward zero. In the limit of small ϵ, we find

$$\psi_E(x) \approx \begin{cases} \psi_L \cos[k(x+\epsilon)] + (\psi_L'/k)\sin[k(x+\epsilon)] \\ \qquad x \leqslant -\epsilon \\ \psi_L \mathrm{e}^{-D_\alpha x} + (\mathrm{e}^{-\mathrm{i}\theta}/2\rho)[\psi_L' + D_\alpha \psi_L] \exp([2K^\epsilon(\rho \mathrm{e}^{\mathrm{i}\theta}) + D_\alpha]x) \\ \qquad -\epsilon < x < 0 \\ \psi_R \mathrm{e}^{\tilde{D}_\beta x} - (\mathrm{e}^{\mathrm{i}\theta}/2\rho)[\psi_R' - \tilde{D}_\beta \psi_R] \exp([-2K^\epsilon(\rho \mathrm{e}^{-\mathrm{i}\theta}) - \tilde{D}_\beta]x) \\ \qquad 0 < x < \epsilon \\ \psi_R \cos[k(x-\epsilon)] + (\psi_R'/k)\sin[k(x-\epsilon)] \\ \qquad x \geqslant \epsilon \end{cases} \tag{2.6}$$

where

$$D_\alpha = \alpha + \rho - \rho \mathrm{e}^{\mathrm{i}\theta} \tag{2.7a}$$

$$\tilde{D}_\beta = \beta + \rho - \rho \mathrm{e}^{-\mathrm{i}\theta} \tag{2.7b}$$

$$K^\epsilon(\rho \mathrm{e}^{\pm \mathrm{i}\theta}) = \frac{1}{2\epsilon}\{-\ln(2\rho\epsilon) \mp \mathrm{i}\theta\} + \cdots. \tag{2.7c}$$

We have also set $\psi_L \equiv \psi_E(-\epsilon)$, $\psi_L' \equiv (\mathrm{d}/\mathrm{d}x)\psi_E(x)|_{x=-\epsilon}$, $\psi_R \equiv \psi_E(\epsilon)$, $\psi_R' \equiv (\mathrm{d}/\mathrm{d}x)\psi_E(x)|_{x=\epsilon}$, $E \equiv k^2/2$ and

$$\begin{bmatrix} \psi_R' \\ \psi_R \end{bmatrix} = \mathrm{e}^{-\mathrm{i}\theta} \begin{bmatrix} 1+\beta/\rho & \alpha+\beta+\alpha\beta/\rho \\ 1/\rho & 1+\alpha/\rho \end{bmatrix} \begin{bmatrix} \psi_L' \\ \psi_L \end{bmatrix}. \tag{2.8}$$

We can now easily check that $\psi_E(x)$ is continuously differentiable and that it satisfies equation (2.5) to leading orders, in the limit of small ϵ. Since (2.8) is actually identical to the boundary condition (1.1), we immediately see that the energy eigenstate, $\psi_E(x)$, in the limit where ϵ goes to zero, satisfies the boundary condition (1.1), for all $E \equiv k^2/2$. Moreover, the energy, E, must be real in order to have finite energy eigenstates at x equal plus or minus infinity. Therefore, the energy eigenstates, ψ_E, with energy $E = k^2/2$, of H^ϵ, in the limit of zero ϵ, are identical to those of the Hamiltonian H_M, as we wanted to show. (A more delicate technique, which is more abstract, to show the convergence of a sequence of operators which become singular in the limit can be found in the paper of Albeverio and Šeba [2, 3], and I urge the interested readers to read these papers.)

Let us make a few comments about the short-range interaction I^ϵ. The parameter θ is responsible for the phase discontinuity of the wavefunction as can be seen from (2.8). The parameter ρ controls the size of the discontinuity of the wavefunction. This can be seen explicitly by setting $\theta = \beta = \alpha = 0$ in (2.7). The boundary condition becomes $\psi_R - \psi_L = (1/\rho)\psi_L'$ and $\psi_R' = \psi_L'$ which is the so-called δ'-interaction. We observe that, in (2.6), the derivative of the wavefunction at the origin, $\psi_E'(x)|_{x=0}$, is proportional to $K^\epsilon(\rho \mathrm{e}^{\mathrm{i}\theta})$ and becomes infinite in the limit where ϵ goes to zero which forces the discontinuity of the wavefunction.

3. Scaling

In this section, we study the scaling properties of the point-interaction described in the previous section.

Consider the following transformation

$$x \to \lambda x \qquad (\alpha,\beta,\rho) \to (1/\lambda)(\alpha,\beta,\rho) \qquad \theta \to \theta. \tag{3.1}$$

We can readily see that, for the quantum system consisting of a free particle moving on a line with the origin excluded, discussed in the first section, the four-parameter boundary condition, (1.1), is invariant under these transformations. Since, in the previous section, we have shown that the point-interaction has the effect of dynamically forcing the boundary condition (1.1) on the wavefunction, we expect that the Schrödinger equation, at the location of the point-interaction, will be invariant under the this transformation.

To see that, we recall that in the previous section, we have defined the point-interaction as the limit of the local interaction (2.2) for which ϵ goes to zero. We can readily see that, under the above transformation, with

$$\begin{aligned} \epsilon &\to \lambda\epsilon \\ t &\to \lambda^2 t \\ \psi &\to \frac{1}{\sqrt{\lambda}}\psi\,. \end{aligned} \tag{3.2}$$

also the Schrödinger equation

$$H^{\epsilon}\psi(x,t) = \frac{1}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}\psi(x,t) \tag{3.3}$$

is invariant in the limit where ϵ goes to zero. Which is what we expected.

4. Conclusions

We have constructed a quantum system for a particle moving on the whole line, subject to a local interaction, and have shown that in the limit where the range of the interaction tends to zero (point-interaction) our quantum system tends toward the quantum system of a free moving particle on the line with the origin excluded. The main point in the demonstration of this result was the observation that the point-interaction dynamically forces the wavefunction to satisfy a boundary condition which ensures conservation of probability at the origin. We also observed that, at the location of the point-interaction, the physics is invariant under a certain scale transformation.

Acknowledgments

I thank Edward Farhi, Sam Gutmann and the referees for many valuable comments. This work is supported in part by funds provided by the US Department of Energy (DOE) under contract no DE-AC02-89ER40509, and by the Natural Science and Engineering Research Council of Canada.

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