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Energy-dependent point interactions in one dimension

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Abstract

We consider a new type of point interaction in one-dimensional quantum mechanics. It is characterized by a boundary condition at the origin that involves the second and/or higher order derivatives of the wavefunction. The interaction is effectively energy dependent. It leads to a unitary S-matrix for the transmission–reflection problem. The energy dependence of the interaction can be chosen such that any given unitary S-matrix (or the transmission and reflection coefficients) can be reproduced at all energies. Generalization of the results to coupled-channel cases is discussed.

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1. Introduction

In one-dimensional quantum mechanics there are point interactions that can be interpreted as self-adjoint extensions (SAEs) of the nonrelativistic kinetic energy operator $p^2/(2m)$ where $p = -\mathrm{i}\hbar\,(\mathrm{d}/\mathrm{d}x)$ and m is the mass of the particle of the system under consideration. We use units such that $\hbar = 1$ and $2m = 1$ in the following. Each of the SAEs can be characterized by the following boundary condition that applies to any wavefunction $\psi(x)$ at $x = 0$ [1–4]:

$$\begin{pmatrix}\psi'_+\\ \psi_+\end{pmatrix} = U\begin{pmatrix}\psi'_-\\ \psi_-\end{pmatrix}, \qquad U = \mathrm{e}^{\mathrm{i}\theta}\begin{pmatrix}\alpha & \beta\\ \delta & \gamma\end{pmatrix}, \tag{1}$$

where $\psi' = \mathrm{d}\psi/\mathrm{d}x$, $\psi_\pm = \psi(\pm 0)$ and $\psi'_\pm = \psi'(\pm 0)$. (We do not consider cases in which the two half-spaces of $x > 0$ and $x < 0$ are disjoint.) It is understood that $\psi(x)$ and $\psi'(x)$ are discontinuous at $x = 0$ in general but, at $x \neq 0$, $\psi(x)$ is twice differentiable. The matrix elements α, β, γ and δ are all real parameters (independent of x), which are subject to the condition

$$\alpha\gamma - \beta\delta = 1. \tag{2}$$

Only three of α, β, γ and δ are independent. The phase θ, another real parameter of U, is unimportant in stationary one-body and two-body problems [4]. In many-body problems θ may have subtle implications; see, e.g., [5]. Albeverio *et al* pointed out that θ can play a significant role in non-stationary systems [6]. We do not consider such situations. Let us set θ as

$$e^{i\theta} = -1, \tag{3}$$

throughout this paper as was done in [1–3]. The point interaction described above is energy independent in the sense that the parameters of U are all independent of energy.

The purpose of this paper is first to generalize boundary condition (1) such that the matrix elements of U become energy dependent. Then we explore the implications of such a generalization. In section 2 we set up energy-dependent boundary conditions. In section 3 we examine the transmission–reflection problem. In section 4 we examine the relation between the energy-dependent boundary condition and those derived by Griffiths [7]. In sections 2–4, we focus on stationary states with definite energies. The boundary condition however can be used for non-stationary states, which we examine in the appendix. The results are summarized and discussed in section 5.

2. Energy-dependent boundary condition

In this section we construct energy-dependent boundary conditions. Let us begin with a simple illustration. Assume that

$$U = -\begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} = \begin{pmatrix} 1 & 2c_0 \\ 0 & 1 \end{pmatrix}, \tag{4}$$

where c_0 is a real constant. Then we have

$$\psi'_+ - \psi'_- = c_0(\psi_+ + \psi_-), \tag{5}$$

$$\psi_+ - \psi_- = 0. \tag{6}$$

The point interaction that is specified by (5) and (6) is the δ-function potential $2c_0\delta(x)$. Now let us replace (5) with

$$\psi'_+ - \psi'_- = -c_1(\psi''_+ + \psi''_-), \tag{7}$$

where $\psi'' = d^2\psi/dx^2$ and c_1 is a real constant. Assume that there is no interaction at $x \neq 0$. For a stationary state with energy E we obtain

$$\psi'' = -E\psi \qquad (x \neq 0), \tag{8}$$

where E can be positive or negative. Equations (7) and (8) together with (6) lead to

$$U = \begin{pmatrix} 1 & 2c_1E \\ 0 & 1 \end{pmatrix}, \tag{9}$$

which depends on E. This U represents an energy-dependent δ-function potential.

We assumed above that there is no interaction except at $x = 0$. This restriction is not essential. Suppose there is a finite range potential $V(x)$ other than the point interaction at $x = 0$. Assume for simplicity that $V(x)$ is continuous at $x = 0$. Then E of (8) and (9) has to be replaced with $E - V(0)$. In the following we assume that $V(0) = 0$ for simplicity but there is no difficulty in incorporating nonzero $V(0)$.

The example given above can be extended as follows. Assume that $c(E)$ is a function of E such that

$$c(E) = \sum_{\nu=0}^{\infty} c_\nu E^\nu, \tag{10}$$

where c_ν is a real constant. Replace (5) with

$$\psi'_+ - \psi'_- = \sum_{\nu=0}^{\infty}(-1)^\nu c_\nu\big[\psi_+^{(2\nu)} + \psi_-^{(2\nu)}\big], \tag{11}$$

where $\psi^{(2\nu)} = \mathrm{d}^{2\nu}\psi/\mathrm{d}x^{2\nu}$. Here it is understood that $\psi^{(2\nu)}$ is well-defined except at $x = 0$. We then obtain

$$U = \begin{pmatrix} 1 & 2c(E) \\ 0 & 1 \end{pmatrix}. \tag{12}$$

We now turn to a more general situation. Boundary condition (1) together with (2) can be recast into the following form:

$$\psi'_+ - \psi'_- = \lambda_1(\psi_+ + \psi_-) - \lambda_2(\psi'_+ + \psi'_-), \tag{13}$$

$$\psi_+ - \psi_- = \lambda_2(\psi_+ + \psi_-) - \lambda_3(\psi'_+ + \psi'_-), \tag{14}$$

where λ_1, λ_2 and λ_3 are real parameters. Then U turns out to be

$$U = -\begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} = -\begin{pmatrix} 1 - 2(1-\lambda_2)/\Delta & -2\lambda_1/\Delta \\ 2\lambda_3/\Delta & 1 - 2(1+\lambda_2)/\Delta \end{pmatrix}, \tag{15}$$

where

$$\Delta = (1+\lambda_2)(1-\lambda_2) + \lambda_1\lambda_3. \tag{16}$$

It is understood that $\Delta \neq 0$. The three parameters λ_1, λ_2 and λ_3 are independent of one another. They are related to α, β, γ and δ by

$$2\lambda_1 = -\beta\Delta, \qquad 2\lambda_2 = \frac{1}{2}(\alpha - \gamma)\Delta, \qquad 2\lambda_3 = \delta\Delta, \qquad \Delta = \frac{4}{2 - \alpha - \gamma}. \tag{17}$$

Boundary condition (4) is a special case in which $\lambda_1 = c_0$ and $\lambda_2 = \lambda_3 = 0$. Apart from $\mathrm{e}^{\mathrm{i}\theta}$ which is unimportant in the context of this paper, the boundary condition consisting of (13) and (14) is completely equivalent to (1) and (2). Boundary conditions in the form of (13) and (14) have recently been used in relation to the Fermi pseudo-potential in one dimension [8]. Parameters λ_1, λ_2 and λ_3 respectively, correspond to $g_1/2$, $g_2/2$ and $g_3/2$ of [8, 9].

Any of λ_1, λ_2 and λ_3 can be made energy dependent in the way we illustrated with (10)–(12). For example, assume that

$$\lambda_2(E) = \sum_{\nu=0}^{\infty} d_\nu E^\nu, \tag{18}$$

where d_ν is a real constant. Then we make the following substitutions in (13) and (14):

$$\lambda_2(\psi'_+ + \psi'_-) \to \sum_{\nu=0}^{\infty}(-1)^\nu d_\nu\big[\psi_+^{(2\nu+1)} + \psi_-^{(2\nu+1)}\big], \tag{19}$$

$$\lambda_2(\psi_+ + \psi_-) \to \sum_{\nu=0}^{\infty}(-1)^\nu d_\nu\big[\psi_+^{(2\nu)} + \psi_-^{(2\nu)}\big]. \tag{20}$$

The λ_1 and λ_3 can be dealt with similarly. In the following it is understood that α, etc, and λ_1, etc, are in general energy dependent.

3. Transmission and reflection problem

Let us consider the transmission–reflection problem assuming that the point interaction that we examined in section 2 is the only interaction in the system. If a wave of a given wavelength is incident from the left, the wavefunction can be written as [10]

$$\psi(x) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + R_{\mathrm{L}}\,\mathrm{e}^{-\mathrm{i}kx} & \text{for} \quad x < 0 \\ T_{\mathrm{L}}\,\mathrm{e}^{\mathrm{i}kx} & \text{for} \quad x > 0 \end{cases}, \tag{21}$$

where $k > 0$ is related to the energy by $E = k^2$. The wavefunction of the case in which the wave is incident from the right can be written in a similar manner, with coefficients T_R and R_R. The S-matrix is a 2×2 matrix, which is related to T and R by [10],

$$S = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix} = \begin{pmatrix} T_L & R_R \\ R_L & T_R \end{pmatrix}. \tag{22}$$

The suffix $\pm$ of S_{++}, etc, refers to the direction of the wave propagation. By using the U of (15) we can determine the T and R and then the S-matrix explicitly as [3]

$$S = [-\beta + k^2\delta + \mathrm{i}k(\alpha+\gamma)]^{-1} \begin{pmatrix} -2\mathrm{i}k & \beta + k^2\delta - \mathrm{i}k(\alpha-\gamma) \\ \beta + k^2\delta + \mathrm{i}k(\alpha-\gamma) & -2\mathrm{i}k \end{pmatrix} \tag{23}$$

$$= \left[k^2\lambda_3 - \mathrm{i}k\left(1 - \lambda_1\lambda_3 + \lambda_2^2\right) + \lambda_1\right]^{-1} \begin{pmatrix} -\mathrm{i}k\left(1 + \lambda_1\lambda_3 - \lambda_2^2\right) & k^2\lambda_3 - 2\mathrm{i}k\lambda_2 - \lambda_1 \\ k^2\lambda_3 + 2\mathrm{i}k\lambda_2 - \lambda_1 & -\mathrm{i}k\left(1 + \lambda_1\lambda_3 - \lambda_2^2\right) \end{pmatrix}. \tag{24}$$

This is a unitary matrix. Note that $T_L = T_R$, which means that the boundary condition conforms to time-reversal invariance [4, 10]. In the following we suppress suffices L and R of T.

If parameters α, etc, and λ_1, etc, are independent of energy, the point interaction can support one or two bound states. Let the wavefunction of a bound state be

$$\psi_{\pm}(x) = C_{\pm}\,\mathrm{e}^{-\kappa|x|}, \tag{25}$$

where $\kappa > 0$ and $C_{\pm}$ is a constant coefficient. The suffix $\pm$ refers to the sign of x. The energy of the bound state is given by $E = -\kappa^2$. The κ is determined by

$$\delta\kappa^2 + (\alpha+\gamma)\kappa + \beta = 0, \tag{26}$$

which leads to $S(k = \mathrm{i}\kappa) = \infty$. If α, etc, are functions of $E = -\kappa^2$, then the number of bound states can be different from that of the case of energy-independent α, etc. Let us add that the N-body problem with the same point interaction can be solved exactly in the same way as was done in [11]. The number of bound states does not depend on N. The energy of the bound state is again given by (26) of [11], i.e., $E = -\frac{1}{6}N(N^2-1)\kappa^2$, where κ is the same as that of (25) and (26).

When time-reversal invariance holds, which is the case throughout this paper, the S-matrix elements can be expressed in terms of three energy-dependent parameters. For example, they can be written as

$$T = \tfrac{1}{2}(\mathrm{e}^{2\mathrm{i}\eta_0} + \mathrm{e}^{2\mathrm{i}\eta_1}), \tag{27}$$

$$R_L = \tfrac{1}{2}(\mathrm{e}^{2\mathrm{i}\eta_0} - \mathrm{e}^{2\mathrm{i}\eta_1})\,\mathrm{e}^{2\mathrm{i}\epsilon}, \qquad R_R = R_L\,\mathrm{e}^{-4\mathrm{i}\epsilon}. \tag{28}$$

Here $\eta_0(E)$ and $\eta_1(E)$ are the phase shifts in two partial waves with even and odd parity respectively, and $\epsilon(E)$ is the mixing parameter. For the definitions of these quantities, see [10]. Note that the number of parameters of the S-matrix is the same as the number of parameters of the SAEs. This fact has an important implication as we discuss towards the end of section 5.

Suppose the S-matrix is given at all energies. Then one can determine an energy-dependent point interaction that reproduces the given S-matrix. To be explicit, α, etc, of the point interaction can be determined by the following:

$$\alpha = -\frac{1}{2}\left(\frac{1}{T} + \frac{1}{T^*} + \frac{R_L - R_R}{T}\right), \tag{29}$$

$$\beta = \frac{\mathrm{i}k}{2}\left(\frac{1}{T} - \frac{1}{T^*} - \frac{R_L + R_R}{T}\right), \tag{30}$$

$$\gamma = -\frac{1}{2}\left(\frac{1}{T} + \frac{1}{T^*} - \frac{R_L - R_R}{T}\right), \tag{31}$$

$$\delta = -\frac{\mathrm{i}}{2k}\left(\frac{1}{T} - \frac{1}{T^*} + \frac{R_L + R_R}{T}\right). \tag{32}$$

Parameters α, etc, so determined are real and satisfy (2). Once α, etc, are determined, λ_1, etc, can be found through (17). It is obvious that the number of independent parameters of the SAEs cannot exceed the number of independent parameters of the S-matrix.

Consider the following two models, A and B. Model A is defined by means of the Hamiltonian

$$H = p^2 + V(x), \tag{33}$$

where p^2 is the kinetic energy operator and potential $V(x)$ is real and of a finite range. Model B is specified by means of an energy-dependent point interaction that we have introduced. Start with model A and determine its S-matrix for all energies by solving the Schrödinger equation with H of (33). (This S-matrix can be imagined as a set of 'experimental data' of the model system.) Next set up model B such that it is equivalent to model A as far as the S-matrix is concerned. Bound states, if any, have the same energies. Models A and B, however, are not completely equivalent. The wavefunctions of the two models agree with each other in the asymptotic region but are different within the range of potential $V(x)$. If we solve a many-body problem with the interactions of models A and B, we will find different results such as different binding energies. A question that would naturally arise here is: if one starts with model B that has been arbitrarily specified in terms of the phase shifts and mixing parameter, can one find $V(x)$ of model A such that the two models share the same S-matrix? This is not always possible. For example, if the given phase shifts of model B do not conform to the Levinson theorem [12, 13], we cannot find $V(x)$ that reproduces such phase shifts.

The energy-dependent point interaction that we have introduced above has a similarity to the pseudo-potential in three dimensions that Huang and Yang constructed a long time ago [14]. Their pseudo-potential can exactly reproduce any given partial-wave phase shifts at all energies. It has many interesting applications. Huang and Yang pointed out that their pseudo-potential is not a Hermitian operator. As they remarked, the non-Hermiticity of the pseudo-potential requires that some care be exercised when one applies the usual perturbation formulae in an actual calculation (for a many-body system). Essentially the same remark applies to our energy-dependent point interaction. We should however mention the following difference. Huang and Yang's pseudo-potential, which is an extension of Fermi's pseudo-potential [15, 16], is an effective potential that is meant to be used in the Born approximation. In contrast, our point interaction is a 'true' potential that is meant to be treated exactly.

Returning to the one-dimensional case, consider two arbitrary normalizable wavefunctions $\psi(x)$ and $\phi(x)$ that are both subject to boundary condition (1) at the origin with energy-dependent parameters. In order for the kinetic-energy operator $-\mathrm{d}^2/\mathrm{d}x^2$ combined with the boundary to be self-adjoint, we require [3, 17]

$$-\int_{-\infty}^{\infty}(\phi^*\psi'' - \phi''^*\psi)\,\mathrm{d}x = [(\phi^*\psi' - \phi'^*\psi)]_{-0}^{+0} = 0. \tag{34}$$

By using (1) we can reduce (34) to

$$(\phi_-^*, -\phi_-'^*)\big(U_\phi^{-1}U_\psi - 1\big)\begin{pmatrix}\psi_-'\\ \psi_-\end{pmatrix} = 0, \tag{35}$$

where matrix $U_{\phi(\psi)}$ is associated with the boundary condition for ϕ (ψ). Equation (35) requires that $U_\phi = U_\psi$ and hence the boundary condition be independent of energy. If boundary condition (1) is energy dependent, the point interaction represented by (1) is not self-adjoint. Interestingly enough, however, it leads to a unitary S-matrix. The energy-dependent boundary condition guarantees the continuity of the probability current across the boundary and the conservation of probability.

4. Griffiths' boundary condition

Assuming the potential

$$V(x) = 2c\delta^{(n)}(x) = 2c\frac{\mathrm{d}^n\delta(x)}{\mathrm{d}x^n}, \tag{36}$$

where c is a real constant, Griffiths [7] derived the boundary conditions

$$\psi_+' - \psi_-' = (-1)^n c\big[\psi_+^{(n)} + \psi_-^{(n)}\big], \tag{37}$$

$$\psi_+ - \psi_- = (-1)^{(n-1)} nc\big[\psi_+^{(n-1)} + \psi_-^{(n-1)}\big]. \tag{38}$$

Here we have replaced Griffiths' c with $2c$. The derivation of the above conditions involves integrals such as $\int \delta^{(n)}(x)\psi(x)\,\mathrm{d}x$. In dealing with these integrals, integration by parts is liberally done disregarding possible discontinuities of $\psi(x)$ and its derivatives. As remarked in [3, 8] the derivation as such is questionable. Nevertheless (37) and (38) are interesting conditions. It is straightforward to work out the transmission–reflection problem with boundary conditions (37) and (38). The resulting S-matrix, however, turns out to be unitary only if $n = 0$, 1 or a positive even integer.

If $n = 0$ (37) and (38) are trivially reduced to those for the δ-function potential, i.e., (5) and (6). Let us examine the cases with even $n = 2\nu$ and odd $n = 2\nu + 1$ separately. When $n = 2\nu$ with $\nu > 0$, (37) and (38) respectively, become

$$\psi_+' - \psi_-' = c\big[\psi_+^{(2\nu)} + \psi_-^{(2\nu)}\big], \tag{39}$$

$$\psi_+ - \psi_- = -2\nu c\big[\psi_+^{(2\nu-1)} + \psi_-^{(2\nu-1)}\big]. \tag{40}$$

These two equations can be reduced to (13) and (14) with $\lambda_1 = (-E)^\nu c$, $\lambda_2 = 0$ and $\lambda_3 = (-E)^{\nu-1}(2\nu c)$. Al-Jaber examined the case of $n = 2$ in detail [18]. He calculated the transmission and reflection coefficients and confirmed that unitarity holds, i.e., $|T|^2 + |R|^2 = 1$. We can reproduce Al-Jaber's transmission and reflection coefficients by substituting $\lambda_1 = -Ec$, $\lambda_2 = 0$ and $\lambda_3 = 2Ec$ into (24).

In passing let us comment on some of Al-Jaber's results. In examining the transmission–reflection problem he assumed that $c > 0$ but the transmission and reflection coefficients that

he obtained are valid irrespective of the sign of c. He claimed that there are two bound states but actually only one of them (with $k > 0$ in his notation) is a bound state. The wavefunction of the other state (with $k < 0$) is not normalizable. It is interesting that the bound state exists irrespectively of the sign of c. Al-Jaber stated, below his equation (16), that 'This (unitarity of the S-matrix) implies that the Hamiltonian under investigation is a self-adjoint operator'. This statement is incorrect. If n is a positive even integer, condition (35) for the self-adjointness is not satisfied unless ϕ and ψ represent stationary states of the same energy.

If $n = 2\nu + 1$, (37) and (38) respectively become

$$\psi'_+ - \psi'_- = -c\big[\psi_+^{(2\nu+1)} + \psi_-^{(2\nu+1)}\big], \tag{41}$$

$$\psi_+ - \psi_- = (2\nu + 1)c\big[\psi_+^{(2\nu)} + \psi_-^{(2\nu)}\big]. \tag{42}$$

Equation (41) leads to $\lambda_1 = 0$ and $\lambda_2 = (-E)^\nu c$. On the other hand (42) requires $\lambda_2 = (2\nu + 1)(-E)^\nu c$ and $\lambda_3 = 0$. Therefore (41) and (42) can be reduced to (13) and (14) only if $\nu = 0$, i.e., $n = 1$. It is crucial that the terms with λ_2 appear in (13) and (14) in a specific manner. When the boundary conditions cannot be reduced to (13) and (14), the interaction represented by the boundary conditions fails to satisfy unitarity. The probability current of this case is discontinuous across the origin.

Let us add that the point interaction that is associated with Griffiths' condition with $n = 1$ is self-adjoint. Note that the parameters in the boundary condition of this case are actually all independent of energy. The associated point interaction is different from the so-called δ'-interaction. This aspect was already discussed in detail in [3].

5. Summary and discussion

We have shown how an energy-dependent point interaction in one dimension can be constructed in a systematic way by means of a boundary condition on the wavefunction at the origin. The interaction so constructed is not self-adjoint. Nevertheless, when the transmission–reflection problem is worked out with the potential, the probability current is continuous across the boundary and unitarity is satisfied. Suppose a set of 'experimental data' regarding the transmission and reflection coefficients of a one-dimensional system at all energies and the energies of bound states, if any, is given. (It is understood that the data conform to unitarity.) Then we can construct an energy-dependent point interaction that exactly reproduces the given data.

We have also shown that Griffiths' boundary conditions (37) and (38) can be related to our energy-dependent point interaction if and only if $n = 0$, 1 or a positive even integer. If $n = 0$ or 1 the point interaction represented by Griffiths' boundary conditions is actually independent of energy and is self-adjoint. If n is a positive even integer, the interaction is not self-adjoint but is still compatible with unitarity in the transmission and reflection problem. For any other values of n, i.e., positive odd integers exceeding 1, the interaction is not compatible with unitarity.

We have focussed on stationary states. The boundary conditions of the form of (11), (19) and (20) do not contain E explicitly. They can actually be used for nonstationary states as well. In the appendix we show that the conservation of probability and the continuity of the probability current across the boundary hold in any non-stationary state that can be represented as a linear combination of stationary states. We are however concerned about the following possibility. When the interaction involved is not self-adjoint, the stationary states associated with it may not form a complete set.

We have confined ourselves to the one-channel case in this paper but we foresee no difficulty in extending the results to coupled-channel cases. We pointed out in the one-channel case that the number of independent parameters of SAEs of the kinetic energy operator cannot exceed the number of independent parameters of the S-matrix. This statement is valid irrespectively of the number of coupled channels. Recently the SAEs of the two-channel case have been examined [8, 19]. It was found that there can be ten-independent real parameters in the SAEs in the two-channel case [8]. On the other hand, when time-reversal invariance holds, the S-matrix of the two-channel case can be expressed in terms of a 4×4 real symmetric K-matrix that has ten real (energy-dependent) parameters. This situation regarding the number of parameters involved is exactly similar to that of the one-channel case (with three parameters). This convinces us that the ten-parameter family of SAEs that was found in [8] is the most general one of the two-channel case. This naturally leads to the following generalization: in the case of N coupled channels, we can have a family of SAEs with $N(2N+1)$ parameters. Let us add that the relationship between the number of parameters of SAEs of the kinetic-energy operator and the number of parameters of the S-matrix is also valid in the relativistic case with the one-dimensional Dirac equation. In this connection, see section 5 of [3].

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Appendix. Non-stationary states

We start with a set of stationary solutions of the Schrödinger equation, $\phi(k,x)\,\mathrm{e}^{-\mathrm{i}E_k t}$ and $\phi_i(x)\,\mathrm{e}^{-\mathrm{i}E_i t}$, where $E_k = k^2$ and E_i represent continuum and discrete energy spectra, respectively. We normalize them such that

$$\int_{-\infty}^{\infty} \phi^*(k,x)\phi(k',x)\,\mathrm{d}x = 2\pi\delta(k-k'), \tag{43}$$

$$\int_{-\infty}^{\infty} \phi_i^*(x)\phi_{i'}(x)\,\mathrm{d}x = \delta_{i,i'}. \tag{44}$$

It is understood that there are a potential in a finite region around the origin and/or a point interaction that is represented by a boundary condition at the origin. Consider a non-stationary state described by

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k)\phi(k,x)\,\mathrm{e}^{-\mathrm{i}E_k t}\,\mathrm{d}k + \sum_i c_i \phi_i(x)\,\mathrm{e}^{-\mathrm{i}E_i t}, \tag{45}$$

where function $f(k)$ and coefficient c_i are independent of t. This $\psi(x,t)$ satisfies the time-dependent Schrödinger equation. Its normalization is given by

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2\,\mathrm{d}x = \int_{-\infty}^{\infty} |f(k)|^2\,\mathrm{d}k + \sum_i |c_i|^2, \tag{46}$$

which is independent of t and hence the probability is conserved. The $\psi(x,t)$ and $\psi(x,0)$ are related by a unitary transformation. With $\psi(x,t)$ it can be shown that the probability current is continuous at any x and t. Note that, because of (43) and (44), the first integral

of (46) only involves pairs of stationary wavefunctions ϕ^* and ϕ of the same energy. The non-selfadjointness of the energy-dependent boundary condition that we pointed out below (35) does no harm regarding the probability conservation.

In order to gain more insight into the probability conservation, let us examine transmission and reflection of a wavepacket. For stationary solutions we assume that $\phi(k, x)$ has the asymptotic form of (21) and left–right symmetry for simplicity. For $\psi(x, t)$ we assume the initial condition at $t = 0$,

$$\psi(x, 0) = g(x - x_0)\,\mathrm{e}^{\mathrm{i}k_0 x}, \qquad k_0 > 0, \tag{47}$$

where function $g(x - x_0)$ is localized around $x = x_0$ so that $\psi(x, 0)$ represents a wavepacket. For simplicity let $g(x - x_0)$ be a real, smooth function. The factor $\mathrm{e}^{\mathrm{i}k_0 x}$ of (47) puts the wavepacket in motion at speed $v_0 = 2k_0$. (Recall $2m = 1$.) It is understood that $x_0 \ll 0$ such that the wavepacket at $t = 0$ is far to the left, outside the potential region. We denote the Fourier transform of $\psi(x, 0)$ with $f(k)$,

$$\sqrt{2\pi}\, f(k) = \int_{-\infty}^{\infty} \psi(x, 0)\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x = \int_{-\infty}^{\infty} g(x - x_0)\,\mathrm{e}^{-\mathrm{i}(k-k_0)x}\,\mathrm{d}x. \tag{48}$$

We normalize $\psi(x, 0)$ as

$$\int_{-\infty}^{\infty} |\psi(x, 0)|^2\,\mathrm{d}x = \int_{-\infty}^{\infty} g^2(x - x_0)\,\mathrm{d}x = \int_{-\infty}^{\infty} |f(k)|^2\,\mathrm{d}k = 1. \tag{49}$$

Being confined in a finite region around the origin, the discrete energy states have no overlap with $\psi(x, 0)$.

Let us define the following three functions:

$$\psi_0(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k)\,\mathrm{e}^{\mathrm{i}(kx - E_k t)}\,\mathrm{d}k, \qquad x \ll 0 \quad \text{or} \quad x \gg 0, \tag{50}$$

$$\psi_T(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k)T(k)\,\mathrm{e}^{\mathrm{i}(kx - E_k t)}\,\mathrm{d}k, \qquad x \gg 0, \tag{51}$$

$$\psi_R(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k)R(k)\,\mathrm{e}^{\mathrm{i}(kx - E_k t)}\,\mathrm{d}k, \qquad x \ll 0. \tag{52}$$

Each of these three functions is a solution of the time-dependent Schrödinger equation in the asymptotic regions indicated. The $\psi_0(x, t)$ represents the wavepacket incident from the left with speed $v_0 > 0$. It can be shown that, until the front end of the wavepacket comes into the potential region, $\psi(x, t) = \psi_0(x, t)$ holds. A peculiar situation arises when v_0 is very small or the width of the incident wavepacket is very small [20]. We do not consider such cases. When the wavepacket is in the potential region, $\psi(x, t)$ generally behaves in a complicated manner. In this connection, see for example [21–23]. As t becomes sufficiently large, however, $\psi(x, t)$ becomes negligible in the potential region and it is reduced to $\psi_T(x, t) + \psi_R(x, t)$. The $\psi_T(x, t)$ and $\psi_R(x, t)$, which do not overlap, represent the transmitted and reflected wavepackets, respectively.

We define the transmission and reflection probabilities for the wavepacket by

$$P_T = \lim_{t\to\infty} \int_0^{\infty} |\psi(x, t)|^2\,\mathrm{d}x, \tag{53}$$

$$P_R = \lim_{t\to\infty} \int_{-\infty}^{0} |\psi(x, t)|^2\,\mathrm{d}x. \tag{54}$$

The $\psi(x, t)$ of (53) can be replaced by $\psi_T(x, t)$. The range of the integral can be extended to $[-\infty, \infty]$ because $\psi_T(x < 0, t \to \infty)$ is negligible. The P_R can be treated in a similar

manner. Thus we obtain

$$P_T = \int_{-\infty}^{\infty} |f(k)T(k)|^2 \, \mathrm{d}k, \tag{55}$$

$$P_R = \int_{-\infty}^{\infty} |f(k)R(k)|^2 \, \mathrm{d}k. \tag{56}$$

The probability conservation for the wave packet, $P_T + P_R = 1$, simply follows from the unitarity for stationary states, i.e., $|T(k)|^2 + |R(k)|^2 = 1$.

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