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One-dimensional point interaction with three complex parameters

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Abstract
For a pair of non-Hermitian Hamiltonian H and its Hermitian adjoint $H^\dagger$, there are situations in which their eigenfunctions form a biorthogonal system. We illustrate such a situation by means of a one-particle system with a one-dimensional point interaction in the form of the Fermi pseudo-potential. The interaction consists of three terms with three strength parameters g_i ($i = 1, 2$ and 3), which are all complex. This complex point interaction is neither Hermitian nor $\mathcal{PT}$-invariant in general. The S-matrix for the transmission–reflection problem constructed with H (or with $H^\dagger$) in the usual manner is not unitary, but it conforms to the pseudo-unitarity that we define. The pseudo-unitarity is closely related to the biorthogonality of the eigenfunctions. The eigenvalue spectrum of H with the complex interaction is generally complex but there are cases where the spectrum is real. In such a case H and $H^\dagger$ form a pseudo-Hermitian pair.

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1. Introduction

A very large number of papers on quantum mechanical systems with non-Hermitian Hamiltonians have appeared since the seminal paper of Bender and Boettcher of 1998 [1]. Including some earlier works of the 1970s and 1980s, references on the subject can be traced, for example, through [2, 3]. In the present paper, we quote only the ones that are directly relevant to what we are going to deal with.

For a pair of non-Hermitian Hamiltonian H and its Hermitian adjoint $H^\dagger$, there are situations in which their eigenfunctions form a biorthogonal system [4–6]. We illustrate such a situation by means of a one-particle system with a one-dimensional point interaction in the form of the Fermi pseudo-potential, which consists of three terms with three strength parameters g_i ($i = 1, 2$ and 3) [7, 8]. If g_i's are all real, the interaction is Hermitian. If g_2 is purely imaginary while g_1 and g_3 are real, the interaction is non-Hermitian but is invariant under the $\mathcal{PT}$ transformation [9]. Here $\mathcal{P}$ performs space reflection $x \to -x$ for the position of the particle and $p \to -p$ for the momentum while $\mathcal{T}$ is complex conjugation $i \to -i$. These two cases have been examined earlier. This time we assume that g_i's are all complex. Hamiltonian H of the system with such a complex interaction is neither Hermitian nor $\mathcal{PT}$-invariant in general.

In a series of papers Mostafazadeh developed a systematic method of handling non-Hermitian Hamiltonians [10], (see also [11]). We confirm that the point interaction with three complex parameters can be accommodated into Mostafazadeh's formalism. In the transmission–reflection problem with the complex point interaction, the S-matrix constructed on the basis of H (or of $H^\dagger$) in the usual manner is not unitary but it satisfies the pseudo-unitarity that we define in due course. We show that the pseudo-unitarity is closely related to the biorthogonality of the eigenfunctions of H and those of $H^\dagger$. The eigenvalue spectrum of Hamiltonian H is generally complex but there are situations such that the spectrum is real. In such a case H and $H^\dagger$ form a pseudo-Hermitian pair. In order to see this aspect we need the metric operator that Mostafazadeh denoted with η [10]. We discuss how operator η can be constructed for our model system. Mostafazadeh recently examined the Dirac δ-function potential with a complex coefficient, which is a special case of our interaction with $g_2 = g_3 = 0$ [12]. He noted that, when g_1 is pure imaginary, spectral singularity appears giving rise to a complication. We show how that complication can be avoided.

In section 2 we summarize relevant aspects of the Fermi pseudo-potential. In section 3, we examine the transmission–reflection problem and introduce the notion of pseudo-unitarity of the S-matrix. In section 4, we examine the biorthogonality of eigenfunctions and also how to construct metric operator η. In section 5 we examine a special case, a δ-function potential with a complex coefficient. Discussions are presented in section 6.

2. Point interaction in the form of the Fermi pseudo-potential

Consider the time-independent Schrödinger equation $H\psi = E\psi$ which we write as

$$-\psi''(x) + \int_{-\infty}^{\infty} V(x, x')\psi(x')\,\mathrm{d}x' = E\psi(x) \quad (\hbar = 1, 2m = 1), \tag{1}$$

where $\psi''(x) = \mathrm{d}^2\psi(x)/\mathrm{d}x^2$. For potential $V(x, x')$, we assume the pseudo-potential of the form of [7, 8]

$$V(x, x') = g_1 v_1(x, x') + g_2 v_2(x, x') + g_3 v_3(x, x'), \tag{2}$$

where g_i's are constants and

$$\begin{aligned} &v_1(x, x') = \delta(x)\delta(x'), \qquad v_2(x, x') = \delta'_p(x)\delta(x') + \delta(x)\delta'_p(x'), \\ &v_3(x, x') = \delta'_p(x)\delta'_p(x'). \end{aligned} \tag{3}$$

The $\delta'_p(x)$ is defined by

$$\delta'_p(x)\psi(x) = \delta'(x)\tilde{\psi}(x), \tag{4}$$

where $\delta'(x) = \mathrm{d}\delta(x)/\mathrm{d}x$ and

$$\tilde{\psi}(x) = \begin{cases} \psi(x) - \frac{1}{2}(\psi_+ - \psi_-) & \text{for } x > 0, \\ \psi(x) + \frac{1}{2}(\psi_+ - \psi_-) & \text{for } x < 0. \end{cases} \tag{5}$$

Suffix $\pm$ refers to the boundary value for $x \to +0$ ($x \to -0$), e.g., $\psi_+ = \psi(+0)$. It is understood that $\psi(x)$ is generally discontinuous at $x = 0$, i.e., $\psi_+ \neq \psi_-$. Unlike

$\psi(x)$, $\tilde{\psi}(x)$ is continuous at $x = 0$ by the definition and $\tilde{\psi}(0) = (1/2)(\psi_+ + \psi_-)$. When $\psi_+ \neq \psi_-$, $\delta'(x)\psi(x)$ is ill-defined but $\delta'(x)\tilde{\psi}(x)$ is well-defined. The $\delta'_p(x)$ is anti-symmetric, i.e., $\delta'_p(-x) = -\delta'_p(x)$. Note that $V(x, x') = V(x', x)$ and

$$v_1(x, x') = v_1(-x, -x'), \qquad v_2(x, x') = -v_2(-x, -x'),$$
$$v_3(x, x') = v_3(-x, -x'). \tag{6}$$

The $V(x, x')$ is of the form of a nonlocal separable potential but it actually represents a point interaction that acts only at the origin. It is a convenient device with which we can construct general point interactions. Its first term is equivalent to the δ-function potential $g_1\delta(x)$. The effect of $V(x, x')$ on wavefunction $\psi(x)$ can be expressed by a boundary condition at $x = 0$. We assume that $\psi(x)$ is twice differentiable except at $x = 0$ but $\psi'(x) = \mathrm{d}\psi(x)/\mathrm{d}x$ is discontinuous at $x = 0$ in general. The boundary condition that ensues is

$$\begin{pmatrix} \psi'_+ \\ \psi_+ \end{pmatrix} = U \begin{pmatrix} \psi'_- \\ \psi_- \end{pmatrix} = \frac{1}{4\Delta} \begin{pmatrix} (2-g_2)^2 - g_1 g_3 & 4g_1 \\ -4g_3 & (2+g_2)^2 - g_1 g_3 \end{pmatrix} \begin{pmatrix} \psi'_- \\ \psi_- \end{pmatrix}, \tag{7}$$

$$\Delta = \frac{1}{4}[(2+g_2)(2-g_2) + g_1 g_3], \tag{8}$$

where it is understood that $\Delta \neq 0$. If the strength parameters g_i $(i = 1, 2, 3)$ are all real, $V(x, x')$ is real and Hermitian [7, 8]. If g_2 is pure imaginary, i.e., $g_2^* = -g_2$, while g_1 and g_3 remain as real parameters, then $V(x, x')$ is $\mathcal{PT}$-invariant [9]. For this $\mathcal{PT}$-invariant case, see also [13]. In the following we assume that g_i $(i = 1, 2, 3)$ are all complex in general.

3. The transmission–reflection problem: pseudo-unitarity of the *S*-matrix

Let us consider the transmission–reflection problem in which a plane wave of the form of $\mathrm{e}^{\pm \mathrm{i}kx}$ is incident either from the left or from the right. The wavefunction can be written as

$$\psi_{\mathrm{L}}(k, x) = \frac{1}{\sqrt{2\pi}}[(\mathrm{e}^{\mathrm{i}kx} + R_{\mathrm{L}}\,\mathrm{e}^{-\mathrm{i}kx})\theta(-x) + T_{\mathrm{L}}\,\mathrm{e}^{\mathrm{i}kx}\theta(x)],$$
$$\psi_{\mathrm{R}}(k, x) = \frac{1}{\sqrt{2\pi}}[T_{\mathrm{R}}\,\mathrm{e}^{-\mathrm{i}kx}\theta(-x) + (\mathrm{e}^{-\mathrm{i}kx} + R_{\mathrm{R}}\,\mathrm{e}^{\mathrm{i}kx})\theta(x)] \tag{9}$$

where $k \geqslant 0$ is related to the energy of the particle by $E = k^2$, $\theta(x) = 1(0)$ if $x > 0$ $(x < 0)$ and the T's and R's are functions of k. Wavefunction $\psi_{\mathrm{L}}(k, x)$ is for the case in which the wave is incident from the left. The *S*-matrix is a 2×2 matrix, which is related to the T's and R's by [14]

$$S = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix} = \begin{pmatrix} T_{\mathrm{L}} & R_{\mathrm{R}} \\ R_{\mathrm{L}} & T_{\mathrm{R}} \end{pmatrix}. \tag{10}$$

The $\pm$ of S_{++}, etc, refers to the direction of the wave propagation. By solving the Schrödinger equation (1) with the pseudo-potential, we find

$$\begin{aligned} S &= \begin{pmatrix} T_{\mathrm{L}} & R_{\mathrm{R}} \\ R_{\mathrm{L}} & T_{\mathrm{R}} \end{pmatrix} \\ &= \frac{1}{D}\begin{pmatrix} \frac{1}{2}(4 + g_1 g_3 - g_2{}^2) & \mathrm{i}g_3 k + 2g_2 - \mathrm{i}g_1 k^{-1} \\ \mathrm{i}g_3 k - 2g_2 - \mathrm{i}g_1 k^{-1} & \frac{1}{2}(4 + g_1 g_3 - g_2{}^2), \end{pmatrix}, \\ D &= \mathrm{i}g_3 k + \frac{1}{2}(4 - g_1 g_3 + g_2{}^2) + \frac{\mathrm{i}g_1}{k}. \end{aligned} \tag{11}$$

Note that $T_L = T_R$ but $R_L \neq R_R$. In the following we suppress suffices L and R of T. The S of (11) is not unitary, i.e., $S^\dagger S \neq 1$ unless g_i's are all real. The usual self-adjoint extensions of the kinetic energy operator can be obtained by requiring that the conventional probability current $-\mathrm{i}(\psi^*\psi' - \psi'^*\psi)$ be continuous across the origin [16]. Boundary condition (7) with complex g_i's is generally incompatible with this continuity.

When k is extended to the complex plane, $S(k)$ can have a pole if $D(k) = 0$. If this occurs for $\mathrm{Im}(k) > 0$, H obtains discrete eigenvalue $E = k^2$, which is generally complex. The eigenfunction associated with it decays like $\exp[-\mathrm{Im}(k)|x|]$ as $|x|$ increases. It is square-integrable and represents a 'bound state'. If the pole falls on the real axis, it gives rise to a spectral singularity and a complication arises [12]. We exclude such a situation in this section but discuss it in section 5. Let us examine $D(k) = 0$ with $k = \mathrm{i}\kappa$, which is a quadratic equation for unknown κ. The roots of this equation are given by

$$\kappa = \frac{1}{4g_3}\left[4 - g_1 g_3 + g_2{}^2 \pm \sqrt{(4 - g_1 g_3 + g_2{}^2)^2 + 16 g_1 g_3}\right]. \tag{12}$$

If there is a root with real and positive κ, there is a bound state with real energy $-\kappa^2$. With $k = \mathrm{i}\kappa$, $\psi_{L,R}(k, x)$ becomes of the form of

$$\psi_\kappa(x) \propto C_\pm\, \mathrm{e}^{-\kappa|x|}, \tag{13}$$

where suffix $\pm$ refers to the sign of x; C_+ (C_-) is for $x > 0$ $(x < 0)$. The ratio C_+/C_- is determined by boundary condition (7). Here we must add that actually the physical meaning of $\psi(x)$ is not clear yet. We will return to this point toward the end of section 4.

If we require that κ of (12) be real and positive, restrictions on g_i's follow. The three complex g_i's contain six real parameters. In the absence of bound states, the six parameters can be chosen arbitrarily. If there is a bound state, the condition $\mathrm{Im}(\kappa) = 0$ reduces the number of independent real parameters from six to five. The condition $\mathrm{Re}(\kappa) > 0$ restricts the range of the values of the parameters but it does not reduce the number of independent parameters. There are two simple situations of (12). If $g_2 = 0$ equation (12) has roots,

$$\kappa = -\frac{g_1}{2}, \qquad \kappa = \frac{2}{g_3}. \tag{14}$$

If we take the first root and assume that g_1 is real and negative, a discrete state emerges with a real negative eigenvalue of H. In this case g_3 can take on any complex value. (This does not mean that g_3 is unimportant. The S-matrix depends on g_3.) A similar situation occurs with the second root of (14) with $g_3 > 0$ and complex g_1.

We now turn to the Schrödinger equation $H^\dagger\phi = E^*\phi$, i.e.,

$$-\phi''(x) + \int_{-\infty}^{\infty} V^*(x, x')\phi(x')\,\mathrm{d}x' = E^*\phi(x), \tag{15}$$

where

$$V^*(x, x') = g_1^* v_1(x, x') + g_2^* v_2(x, x') + g_3^* v_3(x, x'). \tag{16}$$

For the transmission–reflection problem with $H^\dagger$, we seek solutions of the same form as (9), i.e.,

$$\begin{aligned}\phi_L(k, x) &= \frac{1}{\sqrt{2\pi}}[(\mathrm{e}^{\mathrm{i}kx} + R'_L\,\mathrm{e}^{-\mathrm{i}kx})\theta(-x) + T'\,\mathrm{e}^{\mathrm{i}kx}\theta(x)],\\ \phi_R(k, x) &= \frac{1}{\sqrt{2\pi}}[T'\,\mathrm{e}^{-\mathrm{i}kx}\theta(-x) + (\mathrm{e}^{-\mathrm{i}kx} + R'_R\,\mathrm{e}^{\mathrm{i}kx})\theta(x)],\end{aligned} \tag{17}$$

where $k \geqslant 0$. In this case it is clear that $E^* = E = k^2$. It is important to realize that equations (9) and (17) are as such not complex conjugate of each other. The asymptotic forms of the wavefunctions are not invariant under complex conjugation.

We proceed in the same way as we did with H and obtain the S-matrix for $H^\dagger$, which we denote with S'. The S' can be obtained from S by replacing g_i's with g_i^*'s, i.e.,

$$\begin{aligned} S' &= \begin{pmatrix} T' & R'_{\mathrm{R}} \\ R'_{\mathrm{L}} & T' \end{pmatrix} \\ &= \frac{1}{D'} \begin{pmatrix} \frac{1}{2}(4 + g_1^* g_3^* - g_2^{*2}) & \mathrm{i}g_3^* k + 2g_2^* - \mathrm{i}g_1^* k^{-1} \\ \mathrm{i}g_3^* k - 2g_2^* - \mathrm{i}g_1^* k^{-1} & \frac{1}{2}(4 + g_1^* g_3^* - g_2^{*2}) \end{pmatrix}, \\ D' &= \mathrm{i}g_3^* k + \frac{1}{2}(4 - g_1^* g_3^* + g_2^{*2}) + \frac{\mathrm{i}g_1^*}{k}. \end{aligned} \tag{18}$$

Then $(S')^\dagger$ is given by

$$\begin{aligned} (S')^\dagger &= \begin{pmatrix} T'^* & R'^*_{\mathrm{L}} \\ R'^*_{\mathrm{R}} & T'^* \end{pmatrix} \\ &= \frac{1}{D'^*} \begin{pmatrix} \frac{1}{2}(4 + g_1 g_3 - g_2{}^2) & -\mathrm{i}g_3 k - 2g_2 + \mathrm{i}g_1 k^{-1} \\ -\mathrm{i}g_3 k + 2g_2 + \mathrm{i}g_1 k^{-1} & \frac{1}{2}(4 + g_1 g_3 - g_2{}^2) \end{pmatrix}, \\ D'^* &= -\mathrm{i}g_3 k + \frac{1}{2}(4 - g_1 g_3 + g_2{}^2) - \frac{\mathrm{i}g_1}{k}. \end{aligned} \tag{19}$$

Recall that, when the $g_i's$ are all real, S is unitary, i.e., $S^\dagger S = 1$. *It is crucial to note that the* $(S')^\dagger$ *obtained above with complex* g_i*'s is precisely the same in form as* $S^\dagger$ *of the case in which the* g_i*'s are, although complex, treated as if they are real.* In this sense, $(T'^*, R'^*_{\mathrm{L}}, R'^*_{\mathrm{R}})$ can be replaced by $(T^*, R^*_{\mathrm{L}}, R^*_{\mathrm{R}})$. If one works out $(S')^\dagger S - 1$ by using (11) and (19), one finds that it vanishes identically. It vanishes irrespective of the values of the g_i's, real or complex. Hence follows

$$(S')^\dagger S = 1, \tag{20}$$

which we refer to as 'pseudo-unitarity'. Equation (20) implies

$$T'^* T + R'^*_{\mathrm{L}} R_{\mathrm{L}} = T'^* T + R'^*_{\mathrm{R}} R_{\mathrm{R}} = 1, \qquad T'^* R_{\mathrm{R}} + R'^*_{\mathrm{L}} T = R'^*_{\mathrm{R}} T + T'^* R_{\mathrm{L}} = 0. \tag{21}$$

When the interaction is $\mathcal{PT}$-invariant, i.e., g_1 and g_3 are real while g_2 is pure imaginary, we find that $S' = S^{\mathrm{T}}$ where superscript T means transposed and that $R'_{\mathrm{L}} = R_{\mathrm{R}}$ and $R'_{\mathrm{R}} = R_{\mathrm{L}}$.

4. Biorthogonality of eigenfunctions and construction of the metric operator

It is known that for a Hermitian conjugate pair of Hamiltonians H and $H^\dagger$, their eigenfunctions can form a biorthogonal system [4–6]. Let us illustrate this with our complex point interaction. In this section we assume for simplicity that there are no discrete eigenvalues. In section 5 we discuss a situation in which a discrete state exists.

An observation similar to that made toward the end of the last section can be made regarding the relation between $\psi(k, x)$ for H and $\phi(k, x)$ for $H^\dagger$. The expression for $\phi(k, x)$ can be obtained from $\psi(k, x)$ by replacing g_i's with g_i^*'s. Then $\phi^*(k, x)$ obtained with *complex* g_i's is the same in form as $\psi^*(k, x)$ of the case in which the g_i's are treated as if they are all real. Let us see this explicitly. The complex conjugate of (17) is

$$\begin{aligned} \phi_{\mathrm{L}}^*(k, x) &= \frac{1}{\sqrt{2\pi}}[(\mathrm{e}^{-\mathrm{i}kx} + R'^*_{\mathrm{L}}\,\mathrm{e}^{\mathrm{i}kx})\theta(-x) + T'^*\mathrm{e}^{-\mathrm{i}kx}\theta(x)], \\ \phi_{\mathrm{R}}^*(k, x) &= \frac{1}{\sqrt{2\pi}}[T'^*\mathrm{e}^{\mathrm{i}kx}\theta(-x) + (\mathrm{e}^{\mathrm{i}kx} + R'^*_{\mathrm{R}}\,\mathrm{e}^{-\mathrm{i}kx})\theta(x)]. \end{aligned} \tag{22}$$

Recall the relation between $(S')^\dagger$ and $S^\dagger$ that we pointed out below (19). In (22) if we replace $(T'^*, R'^*_{\mathrm{L}}, R'^*_{\mathrm{R}})$ with $(T^*, R^*_{\mathrm{L}}, R^*_{\mathrm{R}})$, then $\phi^*_{\mathrm{L,R}}(k, x)$ is transcribed into $\psi^*_{\mathrm{L,R}}(k, x)$ in which the g_i's are treated as if they are real.

The biorthogonality of the eigenfunctions of H and $H^\dagger$ means that

$$\int_{-\infty}^{\infty} \phi_\lambda^*(k,x)\psi_{\lambda'}(k',x)\,\mathrm{d}x = \delta_{\lambda,\lambda'}\delta(k-k'), \tag{23}$$

$$\sum_\lambda \int_0^\infty \phi_\lambda^*(k,x)\psi_\lambda(k,y)\,\mathrm{d}k = \delta(x-y), \tag{24}$$

where suffix λ stands for L or R and similarly for λ'. The summation with respect to λ is over L and R. Equations (23) and (24) are obviously valid when g_i's are all real. It remains valid when g_i's are made complex. This is because of the correspondence between $\phi_\lambda^*(k,x)$ and $\psi_\lambda^*(k,x)$ that we pointed out above.

If the above reasoning is not convincing, one can calculate, for example, the left-hand side of (24) explicitly. By using (9) and (22), apart from the overall factor of $1/(2\pi)$, the left hand side of (24) can be worked out as follows,

$$\begin{aligned}
&[\mathrm{e}^{\mathrm{i}k(x-y)} + \mathrm{e}^{-\mathrm{i}k(x-y)}(T'^*T + R'^*_{\mathrm{R}}R_{\mathrm{R}})]\theta(x)\theta(y)\\
&\quad + [\mathrm{e}^{-\mathrm{i}k(x-y)} + \mathrm{e}^{\mathrm{i}k(x-y)}(T'^*T + R'^*_{\mathrm{L}}R_{\mathrm{L}})]\theta(-x)\theta(-y)\\
&\quad + \mathrm{e}^{-\mathrm{i}k(x+y)}(TR'^*_{\mathrm{R}} + T'^*R_{\mathrm{L}})\theta(x)\theta(-y) + \mathrm{e}^{\mathrm{i}k(x+y)}(TR'^*_{\mathrm{L}} + T'^*R_{\mathrm{R}})\theta(-x)\theta(y).
\end{aligned} \tag{25}$$

We have not included terms of the form of $\mathrm{e}^{\pm\mathrm{i}k(x+y)}\theta(x)\theta(y)$, $\mathrm{e}^{\pm\mathrm{i}k(x+y)}\theta(-x)\theta(-y)$ and $\mathrm{e}^{\pm\mathrm{i}k(x-y)}\theta(x)\theta(-y)$ because they will disappear after the k-integration. The four terms of (25) are related to the four matrix elements of $S'^\dagger S = 1$. By using (21), (25) can be reduced to

$$[\mathrm{e}^{\mathrm{i}k(x-y)} + \mathrm{e}^{-\mathrm{i}k(x-y)}][\theta(x)\theta(y) + \theta(-x)\theta(-y)]. \tag{26}$$

After the k-integration

$$\frac{1}{2\pi}\int_0^\infty [\mathrm{e}^{\mathrm{i}k(x-y)} + \mathrm{e}^{-\mathrm{i}k(x-y)}]\,\mathrm{d}k = \frac{1}{2\pi}\int_{-\infty}^\infty \mathrm{e}^{\mathrm{i}k(x-y)}\,\mathrm{d}k = \delta(x-y), \tag{27}$$

(26) leads to (24).

Having confirmed biorthogonality, we can install metric operator η. Following Mostafazadeh [10] we define $\eta(x,y)$ by

$$\eta(x,y) = \sum_\lambda \int_0^\infty \phi_\lambda(k,x)\phi_\lambda^*(k,y)\,\mathrm{d}k, \tag{28}$$

which is Hermitian in the sense that $\eta^*(x,y) = \eta(y,x)$. The inverse operator $\eta^{-1}(x,y)$ is defined by

$$\eta^{-1}(x,y) = \sum_\lambda \int_0^\infty \psi_\lambda(k,x)\psi_\lambda^*(k,y)\,\mathrm{d}k. \tag{29}$$

The biorthogonality relations (23) and (24) immediately lead to $\eta\eta^{-1} = 1$, i.e.,

$$\int_{-\infty}^\infty \eta(x,y)\eta^{-1}(y,z)\,\mathrm{d}y = \delta(x-z). \tag{30}$$

It also follows from the biorthogonality that H and $H^\dagger$ form a pseudo- Hermitian pair[4],

$$H^\dagger = \eta H\eta^{-1}, \qquad H^\dagger\eta = \eta H. \tag{31}$$

[4] As we said at the beginning of this section we are assuming that there is no discrete state. Hence $E = k^2$ is real. The pseudo-Hermiticity condition (31) is not satisfied if $E^* \neq E$, which can happen for a 'bound state' as we mentioned above (12). The biorthogonality, however, holds even when $E \neq E^*$.

The integrand $[\cdots]$ of (28) can be obtained from (25) by replacing T and R's with T' and R''s, respectively. We obtain

$$\eta(x, y) = \delta(x - y) + \frac{1}{2\pi}\int_0^\infty F(k, x, y)\,\mathrm{d}k \tag{32}$$

where

$$\begin{aligned} F(k, x, y) = {} & \mathrm{e}^{\mathrm{i}k(x-y)}(U'_{\mathrm{R}} - 1)\theta(x)\theta(y) + \mathrm{e}^{-\mathrm{i}k(x-y)}(U'_{\mathrm{L}} - 1)\theta(-x)\theta(-y) \\ & + \mathrm{e}^{\mathrm{i}k(x+y)}V'^{*}\theta(x)\theta(-y) + \mathrm{e}^{-\mathrm{i}k(x+y)}V'\theta(-x)\theta(y), \end{aligned} \tag{33}$$

$$U'_{\lambda} = T'T'^{*} + R'_{\lambda}R'^{*}_{\lambda}, \qquad V' = T'R'^{*}_{\mathrm{R}} + R'_{\mathrm{L}}T'^{*}. \tag{34}$$

We have not included terms of the form of $\mathrm{e}^{\pm k(x+y)}\theta(x)\theta(y), \mathrm{e}^{\pm k(x+y)}\theta(-x)\theta(-y)$ and $\mathrm{e}^{\pm \mathrm{i}k(x-y)}\theta(x)\theta(-y)$. The U'_{L} and U'_{R} are real. The $U'_{\mathrm{L}}, U'_{\mathrm{R}}$ and V' are related to $S'^{\dagger}S'$ through

$$S'^{\dagger}S' = \begin{pmatrix} U'_{\mathrm{R}} & V'^{*} \\ V' & U'_{\mathrm{L}} \end{pmatrix}, \tag{35}$$

which is Hermitian. It is not difficult to see that $F^{*}(k, x, y) = F(k, y, x)$ and hence $\eta^{*}(x, y) = \eta(y, x)$.

For $\eta^{-1}(x, y)$ we obtain

$$\eta^{-1}(x, y) = \delta(x - y) + \frac{1}{2\pi}\int_0^\infty G(k, x, y)\,\mathrm{d}k \tag{36}$$

where

$$\begin{aligned} G(k, x, y) = {} & \mathrm{e}^{\mathrm{i}k(x-y)}(U_{\mathrm{R}} - 1)\theta(x)\theta(y) + \mathrm{e}^{-\mathrm{i}k(x-y)}(U_{\mathrm{L}} - 1)\theta(-x)\theta(-y) \\ & + \mathrm{e}^{\mathrm{i}k(x+y)}V^{*}\theta(x)\theta(-y) + \mathrm{e}^{-\mathrm{i}k(x+y)}V\theta(-x)\theta(y). \end{aligned} \tag{37}$$

The $U_{\mathrm{L}}, U_{\mathrm{R}}$ and V are obtained from (34) but without the primes. They are related to $S^{\dagger}S$ through

$$S^{\dagger}S = \begin{pmatrix} U_{\mathrm{R}} & V^{*} \\ V & U_{\mathrm{L}} \end{pmatrix}. \tag{38}$$

Note that $G(k, x, y)$ can be obtained from $F(k, x, y)$ by replacing T', R', etc with T, R, etc, respectively. By using (32) and (36), (30) can be explicitly confirmed. In doing so, $(S'^{\dagger}S')(S^{\dagger}S) = 1$ is useful but we do not delve into such details. The above is as much as what we have done for η and η^{-1}. The k-integrations involved are highly nontrivial and are yet to be worked out.

In order to be able to do physics we need $\eta^{1/2}(x, y)$ such that

$$\int_{-\infty}^{\infty} \eta^{1/2}(x, y)\eta^{1/2}(y, z)\,\mathrm{d}y = \eta(x, z), \tag{39}$$

but we have not been able to work this out in a closed form. When the interaction is weak, $\eta^{1/2}(x, y)$ can be obtained perturbatively [10]

$$\begin{aligned} \eta^{1/2}(x, y) = {} & \delta(x - y) + \frac{1}{4\pi}\int_0^\infty F(k, x, y)\,\mathrm{d}k \\ & - \frac{1}{2(4\pi)^2}\int_{-\infty}^{\infty}\mathrm{d}z\left\{\int_0^\infty F(k, x, z)\,\mathrm{d}k\int_0^\infty F(k', z, y)\,\mathrm{d}k'\right\} \\ & + \frac{1}{2(4\pi)^3}\int_{-\infty}^{\infty}\mathrm{d}z\int_{-\infty}^{\infty}\mathrm{d}z'\left\{\int_0^\infty F(k, x, z)\,\mathrm{d}k\int_0^\infty F(k', z, z')\,\mathrm{d}k'\right. \\ & \left.\times\int_0^\infty F(l, x, z')\,\mathrm{d}l\int_0^\infty F(l', z', y)\,\mathrm{d}l'\right\} + \cdots. \end{aligned} \tag{40}$$

Note that $[\eta^{1/2}(x,y)]^* = \eta^{1/2}(y,x)$. The $\eta^{-1/2}(x,y)$ can be obtained from (40) by replacing F with G.

Pretending that we know $\eta^{\pm 1/2}$ let us proceed a little further along Mostafazadeh's scheme [10]. For notational simplicity let us write (1) as $H\psi = E\psi$. Hamiltonian H is non-Hermitian and the wavefunction $\psi(x)$ cannot be interpreted as the probability amplitude. We introduce Hamiltonian h defined by

$$h = \eta^{1/2} H \eta^{-1/2}, \tag{41}$$

which is Hermitian. The transformation of (41) from H to h is not unitary. Hamiltonian h is a nonlocal operator. This is because η is a nonlocal operator. The Schrödinger equation $H\psi = E\psi$ can be transcribed into the form of

$$h\chi = E\chi. \tag{42}$$

Wavefunctions $\psi(x)$ and $\chi(x)$ are related by $\chi = \eta^{1/2}\psi$ and $\psi = \eta^{-1/2}\chi$, i.e.,

$$\chi(x) = \int_{-\infty}^{\infty} \eta^{1/2}(x,y)\psi(y)\,\mathrm{d}y, \qquad \psi(x) = \int_{-\infty}^{\infty} \eta^{-1/2}(x,y)\chi(y)\,\mathrm{d}y. \tag{43}$$

The $\chi(x)$ has a positive-definite norm and it can be interpreted exactly like the usual wavefunction; $|\chi(x)|^2$ is the probability density at x. Hermitian Hamiltonian h and wavefunction $\chi(x)$ enable us to explore the physics of the system under consideration. Note that

$$\begin{aligned}\int \chi^*(x)\chi(x)\,\mathrm{d}x &= \int \left\{ \left[\int \eta^{1/2}(x,y)\psi(y)\,\mathrm{d}y \right]^* \int \eta^{1/2}(x,z)\psi(z)\,\mathrm{d}z \right\} \mathrm{d}x \\ &= \iint \psi^*(y)\eta(y,z)\psi(z)\,\mathrm{d}y\,\mathrm{d}z, \end{aligned} \tag{44}$$

which is the 'η-norm' of ψ.

We have used words such as transmission and reflection regarding wavefunction $\psi(x)$. The physical meaning of $\psi(x)$ is however not clear. For example, $|T|^2$ and $|R_\lambda|^2$ cannot be interpreted as the transmission and reflection probabilities because the total probability so defined is not conserved. Most of the papers so far published regarding non-Hermitian Hamiltonians are concerned with energy spectra of bound systems. In contrast, little has been done for the scattering or the transmission–reflection problem. The energy of a bound system can be found by solving the Schrödinger equation with H. In order to do more physics such as finding anything related to probability, we need the physical Hamiltonian h and wavefunction $\chi(x)$. The h is not known in the beginning. It can be determined only after $H\psi = E\psi$ has been solved for all eigenfunctions and operator $\eta^{1/2}$ has been obtained. To do so is a highly nontrivial task. Even for the $\mathcal{PT}$-invariant point interaction, which is probably the simplest non-Hermitian interaction, the physics of the transmission–reflection problem is yet to be worked out. The S-matrix obtained in the usual manner, i.e., the S of (11) is of course insufficient. We have to be able to determine the physical transmission and reflection probabilities.

5. Complex δ-function potential

Let us consider a special case with complex $g_1 \neq 0$ and $g_2 = g_3 = 0$. We simply denote g_1 as g in this section. Then the $V(x,x')$ of (2) is reduced to

$$V(x) = g\delta(x). \tag{45}$$

Mostafazadeh [12] examined this model in considerable detail but we intend to present something complementary to his work. In particular, we point out that the 'spectral singularity' about which he was concerned causes no difficulty regarding the biorthogonality of the wavefunctions. The following calculations go in the same way as those of Brownstein [17] who examined a similar problem but with real g.

The T, R's and the S-matrix are given by

$$T = \frac{2k}{2k + \mathrm{i}g}, \qquad R_{\mathrm{L}} = R_{\mathrm{R}} = R = \frac{-\mathrm{i}g}{2k + \mathrm{i}g}, \tag{46}$$

$$S = \begin{pmatrix} T & R \\ R & T \end{pmatrix} = \frac{1}{2k + \mathrm{i}g} \begin{pmatrix} 2k & -\mathrm{i}g \\ -\mathrm{i}g & 2k \end{pmatrix}. \tag{47}$$

The $S(k)$ has a pole at $k = -\mathrm{i}g/2$ in the complex k plane. If $\mathrm{Re}(g) < 0$ the pole leads to a normalizable 'bound state'. If g is pure imaginary, i.e., $\mathrm{Re}(g) = 0$ the pole falls on the real k axis. Then the wavefunction associated with the pole turns out to be ill-defined for $k = -\mathrm{i}g/2$; see (49) given below. The T', R' and S' for the conjugate Hamiltonian $H^\dagger$ with $V^*(x) = g^*\delta(x)$ can be obtained from T, R and S by replacing g with g^*, respectively, i.e.,

$$(S')^\dagger = \frac{1}{2k - \mathrm{i}g} \begin{pmatrix} 2k & \mathrm{i}g \\ \mathrm{i}g & 2k \end{pmatrix}, \tag{48}$$

which is equal to $S^\dagger$ that is obtained from the S but by retaining g as such. It is easy to confirm pseudo-unitarity $(S')^\dagger S = 1$.

Let us now examine the biorthogonality of the eigenfunctions. Instead of $\psi_{\mathrm{L,R}}$ it is more convenient to use $\psi_\pm(x) = (\psi_{\mathrm{L}} \pm \psi_{\mathrm{R}})/\sqrt{2}$, which we find to be

$$\begin{aligned} \psi_+(k, x) &= (1/\sqrt{\pi})(T \cos kx + \mathrm{i}R \sin k|x|) \\ &= \frac{1}{\sqrt{\pi}} \frac{2k \cos kx + g \sin k|x|}{2k + \mathrm{i}g}, \end{aligned} \tag{49}$$

$$\psi_-(k, x) = \frac{\mathrm{i}}{\sqrt{\pi}} \sin kx. \tag{50}$$

The potential has no effect on the odd-parity wavefunction $\psi_-(k, x)$. Wavefunction $\phi_+(k, x)$ for $H^\dagger$ can be obtained from $\psi_+(k, x)$ but respectively replacing T and R with T' and R' (or replacing g with g^*). We also have $\phi_-(k, x) = \psi_-(k, x)$. Note that

$$\begin{aligned} \phi_+^*(k, x) &= (1/\sqrt{\pi})(T'^* \cos kx - \mathrm{i}R'^* \sin k|x|) \\ &= \frac{1}{\sqrt{\pi}} \frac{2k \cos kx + g \sin k|x|}{2k - \mathrm{i}g}, \end{aligned} \tag{51}$$

which is equal to $\psi_+^*(k, x)$ but obtained by treating g as if it is real. These solutions are normalized as

$$\begin{aligned} &\int_{-\infty}^{\infty} \phi_+^*(k, x)\psi_+(k', x)\,\mathrm{d}x = \frac{(4kk' + g^2)\delta(k - k')}{(2k - \mathrm{i}g)(2k' + \mathrm{i}g)} = \delta(k - k'), \\ &\int_{-\infty}^{\infty} \phi_-^*(k, x)\psi_-(k', x)\,\mathrm{d}x = \delta(k - k'), \\ &\int_{-\infty}^{\infty} \phi_\pm^*(k, x)\psi_\mp(k', x)\,\mathrm{d}x = 0. \end{aligned} \tag{52}$$

We have used

$$\begin{aligned} &\int_0^\infty \sin kx \sin k'x\,\mathrm{d}x = \int_0^\infty \cos kx \cos k'x\,\mathrm{d}x = \frac{\pi}{2}\delta(k - k'), \\ &\int_0^\infty (k' \sin kx \cos k'x + k \cos kx \sin k'x)\,\mathrm{d}x = 0, \end{aligned} \tag{53}$$

for which see the appendix of [17]. The orthogonality relation (52) is valid irrespective of the value of g, real or complex. When g is pure imaginary, wavefunctions $\psi_+(k, x)$ and $\phi_+^*(k, x)$ become ill-defined for k such that the denominator $(2k + \mathrm{i}g)$ or $(2k - \mathrm{i}g)$ vanishes. Mostafazadeh indicated that if g is pure imaginary the so-called spectral singularity problem arises [12]. It is noteworthy, however, that the orthogonality (52) as such holds even when g is pure imaginary. This is because when the problematic denominator vanishes, the numerator that appears in (52) also vanishes[5].

Next we examine the completeness of the solutions. For the odd-parity states we find

$$\int_0^\infty \phi_-^*(k, x)\psi_-(k, y)\,\mathrm{d}k = \frac{1}{2}[\delta(x - y) - \delta(x + y)]. \tag{54}$$

For the even-parity states we obtain

$$\begin{aligned}\int_0^\infty \phi_+^*(k, x)\psi_+(k, y)\,\mathrm{d}k &= \frac{1}{2}[\delta(x - y) + \delta(x + y)] \\ &\quad - \frac{g}{\pi}\int_0^\infty \frac{g\cos(|x| + |y|) - 2k\sin(|x| + |y|)}{(2k)^2 + g^2}\,\mathrm{d}k \\ &= \frac{1}{2}[\delta(x - y) + \delta(x + y)] + P(x, y)\end{aligned} \tag{55}$$

with

$$P(x, y) = -(g/2)\theta(-\mathrm{Re}g)\,\mathrm{e}^{(g/2)(|x|+|y|)}, \tag{56}$$

where $\theta(-\mathrm{Re}g) = 1(0)$ if $\mathrm{Re}(g) < 0(>0)$. For the integral containing $\cos(|x| + |y|)$ and $\sin(|x|+|y|)$, we replaced $\int_0^\infty(\cdots)\,\mathrm{d}k$ by $(1/2)\int_{-\infty}^\infty(\cdots)\,\mathrm{d}k$, wrote the sine and cosine functions in the exponential form, and completed the contour for each such term with a semi-circular path in the appropriate upper or lower half-plane of complex k. If $\mathrm{Re}(g) < 0$, there is a discrete state that gives rise to a pole of the S-matrix in the upper half-plane. The term $P(x, y)$ of (55) comes from that pole. By adding (54) and (55) we arrive at

$$\int_0^\infty [\phi_+^*(k, x)\psi_+(k, y) + \phi_-^*(k, x)\psi_-(k, y)]\,\mathrm{d}k = \delta(x - y) + P(x, y). \tag{57}$$

When $S(k)$ has a pole in the upper half-plane of complex k, H obtains a discrete eigenfunction $\psi(x)$ with complex eigenvalue $(g/2)^2$. At the same time $H^\dagger$ obtains eigenfunction $\phi(x)$ with eigenvalue $(g^*/2)^2$. When appropriately normalized, these two eigenfunctions satisfy

$$\phi^*(x)\psi(y) = -P(x, y). \tag{58}$$

Note that $\int_{-\infty}^\infty \phi^*(x)\psi(x)\,\mathrm{d}x = \theta(-\mathrm{Re}g)$. When (57) and (58) are combined the completeness relation follows exactly as explained by Brownstein [17]. The completeness clearly holds irrespective of the value of complex g.

On the basis of their analysis of analytic properties of the resolvent operator that is associated with Hamiltonian H, Fonda *et al* derived three conditions such that the biorthogonality holds for the eigenfunctions of H and $H^\dagger$ (see section 2 of [5]). Their condition (2) requires that the resolvent operator has no accumulation point of the poles E_b (associated with discrete eigenfunctions) and no pole falls on the branch cut (real axis). If g is pure imaginary a pole appears on the real axis and the quoted condition as such is not satisfied. This difficulty, however, can be avoided by adding an infinitesimal real part to g. After the

[5] For the even-parity wavefunctions Mostafazadeh [12] used $\psi_2^k(x)$ and $\phi_2^k(x)$ defined by his (16) and (17), respectively. They are related to our wavefunctions by $\psi_2^k(x) = [(2k + \mathrm{i}g)/(2k - \mathrm{i}g)]^{1/2}\psi_+(k, x)$ and $\phi_2^{k*}(x) = [(2k - \mathrm{i}g)/(2k + \mathrm{i}g)]^{1/2}\phi_+^*(k, x)$. Note that $\phi_2^{k*}(x)\psi_2^k(x) = \phi_+^*(x)\psi_+(k, x)$.

k integration is done, we let $\mathrm{Re}(g) \to 0$. The sign of $\mathrm{Re}(g)$ can be chosen arbitrarily because g disappears when (56) and (57) are combined. We have examined other conditions given in [5] and also in [6] and found that they are satisfied in the example under consideration.

If $\mathrm{Re}(g) > 0$ there is no discrete state and the model conforms to pseudo-Hermiticity. In this situation Mostafazadeh worked out metric operator η and physical Hamiltonian h perturbatively and illustrated some interesting physics aspects of the model [12]. He emphasized the nonlocal nature of the interaction that appears in h. His analysis, however, fell short of determining the transmission and reflection probabilities.

6. Discussions

If we require that the point interaction in one dimension be Hermitian, there is a three-(real) parameter family of such interactions. The interactions of the family can be interpreted as self-adjoint extensions of the kinetic energy operator[6]. For a precise definition and comprehensive treatment of the self-adjoint extensions of the kinetic energy operator, we refer the reader to [15] and other references quoted therein. For a pedestrian approach to the subject, see [16]. With such an interaction the usual probability current $-\mathrm{i}(\psi^*\psi' - \psi'^*\psi)$ is continuous across the origin where the interaction acts. If the point interaction is complex but $\mathcal{PT}$-invariant, again there is a three-parameter (but different) family of such interactions [9, 13]. In this case the usual probability current is not conserved but $-\mathrm{i}[(\mathcal{PT}\psi)^*\psi' - (\mathcal{PT}\psi)'^*\psi)]$, which might be called 'pseudo-probability current', is continuous across the origin [9, 13]. In these two situations, the reason why there cannot be more than three independent real parameters is because of the conserved currents.

If we do not require Hermiticity nor $\mathcal{PT}$ invariance, the point interaction can have three complex parameters (or six real parameters). In sections 3 and 4, we explicitly confirmed that the point interaction with three complex parameters can be accommodated into Mostafazadeh's formalism of pseudo-Hermitian Hamiltonians [10]. Non-Hermitian Hamiltonian H and its Hermitian adjoint $H^\dagger$ can form a pseudo-Hermitian pair, related by (31). If there is no discrete eigenstate, there is no restriction on the choice of the parameters. In the presence of a discrete eigenstate, the pseudo-Hermiticity requires that the associated eigenvalue be real and the number of the parameters of the interaction is reduced. The physics of the system with the complex point interaction can be described in terms of Hermitian Hamiltonian h, which is related to the non-Hermitian Hamiltonian H by (41). As Mostafazadeh emphasized and as we discussed in section 4, Hamiltonian h is a nonlocal operator. Although the interaction in H is a (complex) point interaction, the interaction that emerges in h is not a point interaction. This is also related to the following aspect. The complex point interaction of H can have more than three real parameters. The interaction in h and that in H share the same set of parameters. If the interaction in h that is Hermitian is a point interaction, we are led to a contradiction. Recall that a Hermitian point interaction cannot have more than three real parameters that are physically meaningful.

In section 5, we examined the case of a δ-function potential with a complex coefficient in some detail. This model was examined earlier by Mostafazadeh [12]. We re-examined a

[6] The most general point interaction that acts at the origin and that conforms to self-adjointness can be represented by boundary condition (7) with U replaced by $\mathrm{e}^{\mathrm{i}\theta}U$ where θ is a real constant. In this case it is understood that the g_i's are all real. There are four real parameters involved in the interaction. However, all that the fourth parameter θ does is to introduce a constant phase difference between the wavefunction for $x > 0$ and that for $x < 0$. As far as one- and two-body problems are concerned, θ is void of physical consequences [18]. The three parameters g_1, g_2 and g_3 are the only meaningful ones. When the interaction is used for a many-body system, θ may have subtle implications regarding the symmetry of the many-body wavefunction [19]. We do not consider such an aspect in this paper.

problematic aspect that emerges when g is pure imaginary and showed how such a difficulty can be avoided.

We introduced the notion of pseudo-unitarity of the S-matrix. We showed that the pseudo-unitarity is closely related to the biorthogonality of eigenfunctions of H and $H^\dagger$. The validity of pseudo-unitarity and biorthogonality is not confined to point interactions. Consider a potential $V(\alpha, x)$ that depends on parameter α (which may represent a set of parameters). The x-dependence of the potential is arbitrary. Assume that $V(\alpha, x)$ is real if α is real. If α is complex, then we have $V^*(\alpha, x) = V(\alpha^*, x)$. Let S be the S-matrix based on $V(\alpha, x)$ and S' based on $V^*(\alpha, x)$ of this system. They satisfy the pseudo-unitarity relation $(S')^\dagger S = 1$. This holds irrespective of the value of α. The pseudo-unitarity does not introduce any new restriction on the number of independent parameters involved in the interaction. Let us add that pseudo-Hermiticity does not hold unless the eigenvalue spectrum associated with the complex potential is real.

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