Hermitian Hamiltonian equivalent to a given non-Hermitian one: manifestation of spectral singularity

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One of the simplest non-Hermitian Hamiltonians, first proposed by Schwartz in 1960, that may possess a spectral singularity is analysed from the point of view of the non-Hermitian generalization of quantum mechanics. It is shown that the \( \eta \) operator, being a second-order differential operator, has supersymmetric structure. Asymptotic behaviour of the eigenfunctions of a Hermitian Hamiltonian equivalent to the given non-Hermitian one is found. As a result, the corresponding scattering matrix and cross section are given explicitly. It is demonstrated that the possible presence of a spectral singularity in the spectrum of the non-Hermitian Hamiltonian may be detected as a resonance in the scattering cross section of its Hermitian counterpart. Nevertheless, just at the singular point, the equivalent Hermitian Hamiltonian becomes undetermined.

1. Introduction

Recently, there has been a growing interest in non-Hermitian Hamiltonians possessing a real spectrum and spectral singularities [1–15]. Probably, this is due to the remark that they may produce a resonance-like effect in some optical experiments and may find an optical realization as a certain type of lasing effect that occurs at the threshold gain [6–9].

It is well known that, for any self-adjoint (or essentially self-adjoint) scattering Hamiltonian, continuous spectrum eigenfunctions can be expressed in terms of the Jost solution \( f(k, x) \) and Jost function \( F(k) \), which,
in the simplest case, is the Jost solution taken at \( x = 0, F(k) = f(k, 0) \) [16]. One of the characteristic features of any self-adjoint scattering Hamiltonian is that its Jost function never vanishes if \( k \) is a spectral point, \( F(k) \neq 0 \) for all \( k > 0 \) [16].

An essential feature of the spectral singularity \( k_0 \) is that this point belongs to the continuous part of the spectrum of a non-Hermitian Hamiltonian \( H \) and the corresponding Jost function vanishes at this point, \( F(k_0) = 0 \). As a result, there is no way to construct a Hermitian\(^1 \) operator \( h \) related to \( H \) by an equivalence transformation [12]. In other words, there is no way to redefine the inner product in the spirit of the study by Bender et al. [18] with respect to which \( H \) would become Hermitian.

Probably, just for this reason, some authors have claimed that for a Hamiltonian possessing the spectral singularity no resolution of the identity operator is possible [1–5]. In the study of Andrianov et al. [10], the completeness of biorthogonal sets of eigenfunctions of non-Hermitian Hamiltonians possessing spectral singularities was carefully analysed. The results obtained are illustrated by a number of concrete examples. In particular, the authors [10] showed that the contribution of the spectral singularity to the resolution of the identity operator depends on the class of functions used for physical states. Further progress was made in Samsonov [11], where a special regularization procedure for the resolution of the identity operator was proposed. Note that in Guseinov [13] a concise analysis of the general concept of the spectral singularity of non-Hermitian Hamiltonians is given.

Till now Hamiltonians possessing spectral singularities have been studied mainly as a possible source of new properties of optical media [1–9]. Probably, this is because of the fact that their association with quantum mechanical observables is involved. Nevertheless, as shown in Andrianov et al. [10], spectral singularities ‘are physical’ since ‘they contribute to transmission and reflection coefficients of a non-Hermitian Hamiltonian dramatically enhancing their values’.

On the other hand, any non-Hermitian diagonalizable Hamiltonian \( H \) with real and purely discrete spectrum possesses a Hermitian counterpart \( h = h^\dagger \) that is related to \( H \) by a similarity transformation [19]. Such a transformation does not exist if the Hamiltonian is not diagonalizable. (Such a Hamiltonian cannot be reduced to a diagonal form by changing the basis. The interested reader can find a discussion about quantum mechanics with non-diagonalizable Hamiltonians in Sokolov et al. [20] and Andrianov et al. [21].)

For scattering Hamiltonians, additional obstruction appears for the existence of a similarity transformation between \( H \) and \( h \). Such a transformation does not exist if the spectral singularity is present in the continuous spectrum of \( H \). In many cases \( H \) depends on a parameter, \( H = H(d) \), and the spectral singularity appears at \( d = d_0 \). If \( d \neq d_0 \) the continuous spectrum of \( H \) is regular. If there exists an invertible and positive definite operator \( \eta \) such that \( \eta H(d) = H^\dagger(d) \eta \), where \( H^\dagger(d) \) is the Hermitian conjugate of \( H(d) \), then one can construct the Hermitian counterpart \( h(d) \) of the operator \( H(d) \). Below, using a very simple example, I show that the possible presence of a spectral singularity in \( H(d) \), for \( d \approx d_0 \), may be detected indirectly as a resonance in the scattering cross section for \( h(d) \).

In this paper, I present a careful analysis of Schwartz’s example of a non-Hermitian Hamiltonian \( H \) with the possible presence of a spectral singularity. This is one of the simplest examples because the Hamiltonian contains only the kinetic energy, and its non-Hermitian character is hidden in a boundary condition at \( x = 0 \). In the next section, I define this Hamiltonian and give a definition of the spectral singularity. In §3, I introduce a Hermitian Hamiltonian \( h \) together with an \( \eta \) operator that intertwines \( H \) and \( H^\dagger \). In §4, I reveal the supersymmetric (SUSY) nature of the \( \eta \) operator and introduce its superpartner \( \tilde{\eta} \). In §5, I construct an integro-differential operator that being applied to the function \((2/\pi)^{1/2} \sin(kx)\) gives eigenfunctions \( \Phi_k(x) \) of \( h \). In §6, I calculate the asymptotic behaviour of \( \Phi_k(x) \) and scattering matrix for \( h \). In §7, I show that, if \( H \)

\(^1\) An operator \( A \) in a Hilbert space is said to be self-adjoint if \( A = A^\dagger \) where \( A^\dagger \) is Hermitian adjoint to \( A \). This definition assumes that \( D_A = D_{A^\dagger} \). A densely defined operator \( B \) in a Hilbert space is said to be symmetric if \( \langle \psi | B \phi \rangle = \langle B \psi | \phi \rangle \) for all \( \psi, \phi \in D_B \) [17]. In this paper, I do not differentiate between symmetric and Hermitian operators.
has the spectral singularity, operator $h$ becomes undetermined. In §8, I review briefly our main findings and draw some conclusions.

2. Non-Hermitian Hamiltonian $H$

Following Schwartz [22], consider a non-Hermitian operator (Hamiltonian)

$$H = -\frac{d^2}{dx^2}, \quad x \geq 0,$$

with the domain

$$D_H = \{ \phi \in L^2(0, \infty) : \phi''(x) \in L^2(0, \infty), \phi'(0) + (d + ib)\phi(0) = 0 \},$$

where $d$ and $b$ are real numbers. It is a simple exercise to find its eigenfunctions $\phi_k(x)$,

$$H\phi_k = k^2\phi_k, \quad \phi_k \in D_H,$$

and

$$\phi_k(x) = \sqrt{\frac{2}{\pi}} \sqrt[2]{k^2 + (d + ib)^2}^{-1/2} \left((d + ib)\sin(kx) - k\cos(kx)\right),$$

which for $d < 0$ form a bi-orthonormal set in $L^2(0, \infty)$,

$$\langle \phi_k^\ast | \phi_k \rangle = \int_0^\infty \phi_k(x)\phi_k(x') \, dx = \delta(k - k'),$$

with the completeness condition of the form

$$\int_0^\infty dk |\phi_k\rangle \langle \phi_k^\ast| = I.$$

Here and in what follows I denote the identity operator by $I$ and the asterisk means the complex conjugate.

I would like to emphasize that if $d > 0$ then the Hamiltonian $H$ has a discrete level [13], the possibility that I would like to avoid, and, therefore, in what follows I assume $d < 0$.

There are several equivalent definitions of spectral singularities [13]. The one that is suitable for my purpose uses the kernel $R(x, \xi, \lambda)$ of the resolvent $R_\lambda$ of $H$,

$$R_\lambda f(x) = \int_0^\infty R(x, \xi, \lambda) f(\xi) \, d\xi.$$

A point $\lambda_0$ belonging to the continuous part of the spectrum of $H$ satisfies

$$\lim_{\lambda \to \lambda_0} R(x, \xi, \lambda) = \infty,$$

where the limit should be taken along any path belonging to the resolvent set of $H$. The function $R(x, \xi, \lambda)$ [13] is constructed with the help of two linearly independent solutions $\phi(x, \lambda)$ and $e(\xi, k)$ of the differential equation

$$-\phi''(x) = \lambda\phi(x), \quad \lambda = k^2,$$

as follows:

$$R(x, \xi, \lambda) = \frac{R_1(x, \xi, \lambda)}{W(\lambda)}, \quad R_1(x, \xi, \lambda) = \begin{cases} \phi(x, \lambda)e(\xi, k) & \text{for } 0 \leq x \leq \xi < \infty, \\ \phi(\xi, \lambda)e(x, k) & \text{for } 0 \leq \xi \leq x < \infty. \end{cases}$$

Here $W(\lambda)$ is the Wronskian of the functions $\phi(x, \lambda)$ and $e(\xi, k)$,

$$W(\lambda) = \phi(x, \lambda)e'(x, k) - \phi'(x, \lambda)e(x, k).$$

In particular, if the function $\phi(x, \lambda)$ is such that

$$\phi(0, \lambda) = 1 \quad \text{and} \quad \phi'(0, \lambda) + (d + ib)\phi(0, \lambda) = 0$$
and \( e(x, k) \) is the Jost solution of equation (2.5) defined by its asymptotic behaviour
\[
e(x, k) = e^{ikx}[1 + o(1)], \quad x \to \infty, \quad \text{Im} \ k \geq 0,
\]
then the Wronskian \( W(\lambda) \) coincides with the Jost function for the Hamiltonian \( H \),
\[
W(\lambda) = e'(0, k) + (d + i b)e(0, k) = ik + d + ib, \quad \lambda = k^2.
\]
Because the resolvent becomes infinite at any point where \( W(\lambda) = 0 \), i.e. in the current case at \( \lambda = -(d + ib)^2 \), the Hamiltonian \( H \) has a spectral singularity at point \( \lambda = b^2 \), i.e. at \( d = 0 \). Just at this point, as mentioned in §1, the Jost function for \( H \) vanishes. As shown in Samsonov [11], in this case the corresponding continuous spectrum eigenfunction has zero binorm and the resolution of the identity operator needs a special regularization procedure.

### 3. Equivalent Hermitian operator \( h \)

To establish an equivalence between the non-Hermitian operator \( H \) and a Hermitian operator \( h \), I will use ideas formulated in Scholtz *et al.* [23] for quasi-Hermitian Hamiltonians and further developed in Mostafazadeh [24] for pseudo-Hermitian Hamiltonians. First, one has to find a Hermitian positive definite and invertible operator \( \eta \) such that
\[
\eta H = H^\dagger \eta.
\]
In the present case the adjoint operator \( H^\dagger \) is defined by the same differential expression (2.1) with the domain
\[
D_{H^\dagger} = \{ \phi \in L^2(0, \infty) : \phi''(x) \in L^2(0, \infty), \phi'(0) + (d - i b)\phi(0) = 0 \}.
\]
It is not difficult to check that a second-order differential operator,
\[
\eta = -\partial_x^2 - 2ib\partial_x + d^2 + b^2,
\]
satisfies equation (3.1). Evidently, equation (3.1) defines \( \eta \) up to a transformation \( \eta \to A^\dagger \eta A \), with any invertible \( A \) such that \([A, H] = 0 \) [25]. It is convenient to use the form (3.3) of the \( \eta \) operator.

If \( \eta \) were bounded, its domain would be the whole Hilbert space, and no problems would occur in acting by both the left- and the right-hand sides of (3.1) on functions belonging to \( D_H \). Unfortunately, this is not the case here because operator (3.3) is unbounded and should have its own domain in \( L^2(0, \infty) \). It is reasonable to assume that the domain of \( \eta \) coincides with that of \( H \),
\[
D_\eta = D_H.
\]
As I show below, this assumption is justified by the property that the operator \( \eta \) defined in this way is self-adjoint as well as positive definite and invertible on \( D_\eta \). It is not difficult to find its eigenfunctions and eigenvalues,
\[
\eta \Psi_k(x) = (k^2 + d^2)\Psi_k(x), \quad k \geq 0,
\]
where
\[
\Psi_k(x) = \sqrt{\frac{2}{\pi}}(k^2 + d^2)^{-1/2}e^{-ibx}[d \sin(kx) - k \cos(kx)].
\]
From here I conclude that \( \eta \) in (3.3) is positive definite. Moreover, because its spectrum is bounded below by \( d^2 \neq 0 \), the operator \( \eta^{-1} \) is bounded in \( L^2(0, \infty) \) and can be continued from any initial domain to the whole \( L^2(0, \infty) \).

I note also that functions (3.6) form a complete and orthonormal set in \( L^2(0, \infty) \),
\[
\langle \Psi_k | \Psi_{k'} \rangle = \delta(k - k') \quad \text{and} \quad \int_0^\infty dk |\Psi_k\rangle \langle \Psi_k | = \mathbb{I}. \quad (3.7)
\]
This property follows from the fact that \( \eta \) is self-adjoint with respect to the usual inner product in \( L^2(0, \infty) \). Indeed, as usual, assuming that \( \psi_1 \in D_\eta \) and integrating by parts twice the term with
the second derivative and once the term with the first derivative yields
\[
\langle \psi_2 | \eta \psi_1 \rangle = \int_0^\infty \psi_2^* \left[-\psi_1'' + (\omega^* - \omega) \psi_1' + (\omega \omega^* - \omega') \psi_1 \right] dx \\
= \left[ \psi_2^* \psi_1 - \psi_2 \psi_1' + \psi_2 \psi_1 (\omega^* - \omega) \right]_{x=0}^{\infty} \\
+ \int_0^\infty \left[-\psi_2'' + (\omega - \omega^*) \psi_2' \psi_1 - (\omega^* - \omega') \psi_2^* \psi_1 + (\omega \omega^* - \omega') \psi_1 \right] dx \\
= \int_0^\infty \left[-\psi_2'' + (\omega^* - \omega) \psi_2 + (\omega \omega^* - \omega') \psi_2^* \right] dx \\
= \langle \eta \psi_2 | \psi_1 \rangle.
\]

To justify the last equality, consider the integrated term at \( x = 0 \):
\[
[\psi_2^* \psi_1 - \psi_2 \psi_1' + \psi_2 \psi_1 (\omega^* - \omega)]_{x=0} = [\psi_2^* \psi_1 - \psi_2 \psi_1' + \psi_2 \psi_1 (\omega^* - \omega)]_{x=0} \\
= \psi_1 (0) [\psi_2' + \psi_2 \omega^*]_{x=0} \\
= 0.
\]

The first line here follows from the property that \( \psi_1 \in D_\eta = D_H \) given in (2.2) and in the last line I have used \( \psi_2 \in D_\eta = D_H \).

In the next step, I have to check that \( \eta \) in (3.3) is invertible on \( D_\eta \). For that, compute the kernel space of the differential expression (3.3). This is a two-dimensional linear space with the basis vectors
\[
f_\pm(x) = e^{\pm i bx} dx.
\]

Evidently, \( f_+ (x) \) does not satisfy the boundary condition given in equation (2.2) while \( f_- (x) \) does satisfy this condition. Therefore, for \( d < 0 \), when \( f_- (x) \notin L^2(0, \infty) \), we have \( f_- (x) \notin D_\eta \) and, hence, \( \eta \) in (3.3) is invertible on \( D_\eta \). Thus, as already mentioned, in what follows I assume that \( d < 0 \) except for §7 where I consider the case \( d = 0 \).

From intertwining relation (3.1), it follows that the operator defined as
\[
h = \eta^{1/2} H \eta^{-1/2} = \eta^{-1/2} H^\dagger \eta^{1/2}
\]
is Hermitian, \( h = h^\dagger \), and at the same time is related to \( H \) by equivalence transformation (3.8). According to the first equality (3.8), if \( \psi_1 \in D_h \), then \( \psi_1 = \eta^{-1/2} \psi_1' \) should belong to \( D_H, \eta \psi_1 \in D_H \). Note that because both \( \eta^{-1} \) and \( \eta^{-1/2} \) are bounded, the function \( \psi_1 \) is well defined. Hence, I can define \( D_h^{(1)} \) as a set of functions \( \psi_1 = \eta^{1/2} \psi_1' \) when \( \psi_1 \) runs through \( D_H \subset D_H \), where \( D_H \) will be specified below. The function \( \psi_1 \) here is also well defined because \( D_H \subset D_H = D_\eta \subset D_{\eta^{1/2}} \).

Similarly, according to the second equality in (3.8), I can define \( D_h^{(2)} \) as a set of functions \( \psi_2 = \eta^{-1/2} \psi_2 \) when \( \psi_2 \) runs through \( D_H \subset D_H \). It is not difficult to see that, for any \( \psi_1(x) \) satisfying the boundary condition (2.2), the function
\[
\psi_2(x) = \eta \psi_1(x) \in \hat{D}_H \subset D_H \quad (\psi_1 \in \hat{D}_H)
\]
satisfies the boundary condition (3.2). Note that, because \( \eta \) is a second-order differential expression and \( \eta \psi_2(x) \in D_H \), the function \( \psi_1(x) \) should be smoother than is required by equation (2.2), namely it should be such that \( \phi^{(iv)}(x) \in L^2(0, \infty) \) where \( \phi^{(iv)}(x) \) is the fourth derivative of \( \phi(x) \). Thus, we have
\[
\hat{D}_H = \{ \phi(x) : \phi(x) \in D_H, \phi^{(iv)}(x) \in L^2(0, \infty) \} \subset D_H.
\]

Moreover, from (3.9) it follows that
\[
\eta^{-1/2} \psi_2(x) = \eta^{1/2} \psi_1(x).
\]

This means that I can put \( D_h^{(1)} = D_h^{(2)} = D_h \) with
\[
D_h = \{ \psi(x) : \psi(x) = \eta^{1/2} \psi(x), \, \psi(x) \in \hat{D}_H \subset D_H \}.
\]
Furthermore, because $\eta$ has an empty kernel on $D_H$, the set $D_{\eta}$ is dense in $L^2(0, \infty)$ and it can be taken as an initial domain for $h$ where it is Hermitian, i.e.

$$\langle \psi_2 | h \psi_1 \rangle = \langle h \psi_2 | \psi_1 \rangle \quad \forall \psi_1, \psi_2 \in D_{\eta}.$$  

This property follows from the following chain of equalities:

$$\langle \psi_2 | h \psi_1 \rangle = \langle \psi_2 | h^{1/2} \psi_1 \rangle = \langle \psi_2 | \eta^{1/2} H \psi_1 \rangle = \langle \eta^{1/2} \psi_2 | H \psi_1 \rangle = \langle (\eta^{-1/2} H^{1/2})^{1/2} \psi_2 | \psi_1 \rangle = \langle h \psi_2 | \psi_1 \rangle.$$  

### 4. Supersymmetric partner of the $\eta$ operator

Like any positive definite second-order differential operator, $\eta$ admits a factorization by first-order operators $L$ and $L^\dagger$,

$$\eta = LL^\dagger, \quad L = -\frac{d}{dx} + d - ib \quad \text{and} \quad L^\dagger = \frac{d}{dx} + d + ib,$$  

(4.1)

thus revealing its SUSY nature. The corresponding SUSY algebra is based on the above factorization properties and intertwining relations [26]

$$L^\dagger \eta = \bar{\eta} L^\dagger \quad \text{and} \quad \eta L = L \bar{\eta},$$  

(4.2)

where

$$\bar{\eta} = L^\dagger L.$$  

(4.3)

Note that intertwining relations (4.2) are nothing but identities:

$$\langle L^\dagger L \rangle L^\dagger = L^\dagger (LL^\dagger) \quad \text{and} \quad (LL^\dagger)L = L (L^\dagger L).$$

Although the operator $\bar{\eta}$, which is a SUSY partner of $\eta$, is defined by the same differential expression as operator $\eta$ in (3.3), its domain $D_{\bar{\eta}}$ is different from $D_{\eta}$ in (3.4). This, in particular, follows from intertwining relations (4.2). Indeed, according to these relations, operator $L^\dagger$ transforms eigenfunctions of $\eta$ to eigenfunctions of $\bar{\eta}$, and operator $L$ realizes an inverse mapping. Taking into account factorization properties (4.1) and (4.3), we find

$$\tilde{\psi}_k = (k^2 + d^2)^{-1/2} L^\dagger \psi_k \quad \text{and} \quad \psi_k = (k^2 + d^2)^{-1/2} L \tilde{\psi}_k.$$  

(4.4)

Factor $(k^2 + d^2)^{-1/2}$ guarantees the normalization of these functions,

$$\langle \psi_k | \psi_{k'} \rangle = \delta(k - k') \quad \text{and} \quad \langle \tilde{\psi}_k | \tilde{\psi}_{k'} \rangle = \delta(k - k').$$

Thus, using (4.4) and (3.6) one finds the eigenfunctions of $\bar{\eta}$,

$$\tilde{\psi}_k(x) = \sqrt{\frac{2}{\pi}} e^{-ibx} \sin(kx) \quad \text{and} \quad \bar{\eta} \tilde{\psi}_k = (k^2 + d^2) \tilde{\psi}_k.$$  

(4.5)

Note that these functions satisfy the Dirichlet boundary condition at $x = 0$. One can check that the operator $\bar{\eta}$ defined on the domain

$$D_{\bar{\eta}} = \{ \psi \in L^2(0, \infty) : \psi''(x) \in L^2(0, \infty), \psi(0) = 0 \}$$

by the differential expression (3.3) is self-adjoint. Evidently, the functions (4.5) are $d$-independent and form an orthonormal and complete (in the sense of distributions) basis in $L^2(0, \infty)$,

$$\int_0^\infty dk |\tilde{\psi}_k| \langle \tilde{\psi}_k \rangle = I.$$  

(4.6)

Another remarkable property of intertwining operators (4.1), which will be needed below, is the value of the composition

$$L^\dagger L^* = -\frac{d^2}{dx^2} + (d + ib)^2, \quad L^* = -\frac{d}{dx} + d + ib.$$  

(4.7)
5. Eigenfunctions of $h$

First, note that the eigenfunctions $\varphi_k$ of $H$ (2.3) may be obtained by applying operator $L^*(4.7)$ to the functions

$$\psi_k(x) = \sqrt{\frac{2}{\pi}} \sin(kx),$$

(5.1)

which yields

$$\varphi_k(x) = \left[k^2 + (d + ib)^2\right]^{-1/2} L^* \psi_k(x).$$

Therefore, the eigenfunctions $\Phi_k$ of $h$, obtained by operating with the metric operator $\eta^{1/2}$ on the eigenfunctions of $H$, may also be expressed in terms of the functions $\psi_k$:

$$\Phi_k(x) = \left[k^2 + (d + ib)^2\right]^{-1/2} \eta^{1/2} \varphi_k(x) = \left[k^2 + (d + ib)^2\right]^{-1/2} L^* \psi_k(x).$$

(5.2)

Here, the factor $\left[k^2 + (d + ib)^2\right]^{-1/2}$ guarantees the normalization of the functions on the Dirac delta function. Also note that $L^* \psi_k(x) \notin D_{\eta^{1/2}}$, but this should not cause trouble because all continuous spectrum eigenfunctions are here generalized eigenfunctions of the corresponding operators and should be understood in the sense of distributions.

Note that function (5.1) is an eigenfunction of the operator (4.7),

$$L^*L^* \psi_k(x) = [k^2 + (d + ib)^2] \psi_k(x).$$

(5.3)

It will be useful to express $\Phi_k(x)$ as the result of the action on the functions $\Psi_k$ (4.5) by an integro-differential operator. To this end, first insert the identity operator (3.7) between $\eta^{1/2}$ and $L$ in (5.2) and use equation (3.5) to obtain

$$\Phi_k(x) = \left[k^2 + (d + ib)^2\right]^{-1} \int_0^\infty \frac{dk'}{\sqrt{(k')^2 + d^2}} \psi_k(x) \langle \Psi_k \mid L^* \psi_k \rangle,$$

(5.4)

and then in the obtained expression replace $\psi_k(x)$ according to (4.4):

$$\Phi_k(x) = L \int_0^\infty \frac{dk'}{\sqrt{(k')^2 + d^2}} \tilde{\psi}_k(x) \langle \tilde{\Psi}_k \mid \psi_k \rangle.$$  

(5.5)

Here, the operator $L$ has been moved from the left side in the inner product to the right side, where it becomes adjoint $L^\dagger$, the action of the superposition $L^\dagger L^*$ has been replaced by its explicit expression (4.7) and formula (5.3) has been used.

An advantage of using the functions $\tilde{\Psi}_k$ in (5.5) with respect to using $\psi_k$ in (5.4) is that the integral operator in (5.5) is positive and Hermitian square root of a resolvent operator and, therefore, it is bounded in $L^2(0, \infty)$, whereas the integral operator in (5.4) is unbounded.

6. Asymptotic behaviour of functions $\Phi_k(x)$: scattering matrix and cross section for $h$

Note that, according to formula (5.5), the eigenfunctions $\Phi_k(x)$ of the Hermitian operator $h$ are expressed in terms of elementary functions (4.5) and (5.1). Nevertheless, no simple explicit expression for these functions exists. Below I calculate their asymptotic behaviour as $x \to \infty$.

Inserting formulae (4.7) and (5.3) into (5.5) yields

$$\Phi_k(x) = \left(\frac{2}{\pi}\right)^{3/2} e^{-ibx} I(x) \quad \text{and} \quad I(x) = \int_0^\infty dy e^{iby} \sin(ky) J(x,y),$$

(6.1)

where

$$J(x,y) = \int_0^\infty \frac{dk'}{\sqrt{(k')^2 + d^2}} \sin(k'x) \sin(k'y).$$
Expanding the product of sine functions into the difference of cosine functions reduces the above integral to the one published in Gradshteyn & Ryzhik [27] (see formula no. 3.754.2),

\[ f(x, y) = \frac{1}{2}K_0(d|y - x|) - \frac{1}{2}K_0(d|y + x|). \]

Here \( K_0(z) \) is the standard modified Bessel function [27]. Accordingly, the integral from (6.1) has two contributions,

\[ I(x) = \frac{1}{2}I_1(x) - \frac{1}{2}I_2(x), \quad (6.2) \]

where the first term \( I_1(x) \) contains the function \( K_0(d|y - x|) \),

\[ I_1(x) = \int_0^\infty dy \sin(ky)K_0(d|y - x|), \]

and the second term \( I_2(x) \) is expressed in terms of the function \( K_0(d|y + x|) \),

\[ I_2(x) = \int_0^\infty dy \sin(ky)K_0(d|y + x|). \]

With the change of the integration variable in the last integral, \( d(y + x) = t \), and letting \( x \) tend to infinity, we see that

\[ I_2(x) \to 0. \quad (6.3) \]

Making a similar replacement in the first integral, \( d(y - x) = t \), and also letting \( x \to \infty \), we obtain a non-zero result

\[ I_1(x) \to \frac{1}{d}e^{i\phi x}I_{11}(x), \]

where

\[ I_{11}(x) = \int_{-\infty}^\infty dt \frac{K_0(|t|)\sin k(x + \frac{t}{d})}{\sqrt{d^2 + k^2}} e^{ibt/d}. \]

With the help of standard trigonometric formulae, we reduce the product of sine and exponential into a sum of four terms, two of which are even and two others are odd with respect to the replacement \( t \to -t \). Because of the symmetric integration limits, the odd terms vanish and the integration limits in the integrals with the even terms can be reduced to the semiaxis \((0, \infty) \). As a result, both these terms reduce to the standard integral (see [27], formula no. 6.671.14)

\[ \int_0^\infty \frac{K_0(x)\cos(\alpha x)}{\sqrt{x^2 + \alpha^2}} \, dx = \frac{\pi}{2\sqrt{1 + \alpha^2}}, \]

so that

\[ I_{11}(x) = \frac{i\pi d}{2} \left[ \frac{e^{-ikx}}{\sqrt{d^2 + (k - b)^2}} - \frac{e^{ikx}}{\sqrt{d^2 + (k + b)^2}} \right]. \quad (6.4) \]

Now using equations (6.1)–(6.4), we finally obtain

\[ \Phi_k(x) \to \sqrt{\frac{2}{\pi}} e^{-i(\phi_1 - \phi_2)/2} \sin \left( kx + \frac{1}{2}(\phi_1 + \phi_2) \right), \quad x \to \infty, \]

where

\[ \phi_1 = \frac{1}{2i} \log \left( \frac{d - ik + ib}{d + ik - ib} \right) \quad \text{and} \quad \phi_2 = \frac{1}{2i} \log \left( \frac{d - ik - ib}{d + ik + ib} \right). \]

From here the phase shift is found to be

\[ \delta = \frac{1}{2}(\phi_1 + \phi_2) = \frac{1}{4i} \log \left( \frac{b^2 + (d - ik)^2}{b^2 + (d + ik)^2} \right), \quad (6.5) \]

and the S-matrix is

\[ S = e^{2i\delta} = \left[ \frac{b^2 + (d - ik)^2}{b^2 + (d + ik)^2} \right]^{1/2}. \quad (6.6) \]

This result agrees perfectly with the general formula for the S-matrix obtained in Samsonov [12].
Note that the scattering matrix

$$S_{BW} = S^2 = \frac{b^2 + (d - ik)^2}{b^2 + (d + ik)^2}$$

(6.7)

leads to a Breit–Wigner resonance formula [28]

$$\sigma_{BW} = \frac{16\pi d^2}{(k^2 + d^2 - b^2)^2 + 4b^2d^2},$$

which in the energy scale reads

$$\sigma_{BW} = \frac{4\pi}{b^2} \frac{(\Gamma/2)^2}{(E - E_0)^2 + (\Gamma/2)^2},$$

(6.8)

with $\Gamma = 4bd$ and $E_0 = b^2 - d^2$. Now assume that $|d|$ is small enough so that $b^2 > d^2$. Near the resonance, $E \approx E_0$ and $k \approx b$, so that equation (6.8) reduces to the celebrated Breit–Wigner formula [29]. From here I conclude that the $S$-matrix (6.6) is the square root of the Breit–Wigner $S$-matrix $S_{BW}$ given in (6.7).

The phase shift $\delta$ (6.5) corresponding to $S$ (6.6) is one half of $\delta_{BW}$, $\delta_R = \frac{1}{2}\delta_{BW}$. It leads to a cross section with a square root branch point [12],

$$\sigma(k) = \frac{2\pi}{k^2} \left[ 1 + \frac{k^2 - b^2 - d^2}{\sqrt{(k^2 + d^2 - b^2)^2 + 4b^2d^2}} \right].$$

(6.9)

I choose here that sign of the square root which corresponds to positive definite operator $\rho = \eta^{1/2}$ [12]. It is not difficult to see that $\sigma(0) = 4\pi d^2/(b^2 + d^2)^2 > 0$, $\lim_{k \to \infty} \sigma_R(k) = 0$, $\sigma(k) > 0$ for $0 < k < \infty$ and $d\sigma_R(0)/dk > 0$ for $b^2 > \frac{1}{2}d^2$. These results mean that, for any fixed value of $b$ and small enough value of $|d|$, the function $\sigma(k)$ in (6.9) has a maximum and, therefore, exhibits a resonance behaviour. This is just a consequence of the fact that the Hamiltonian $H$ is, in a sense, close to that which has a spectral singularity.

7. Spectral singularity, $d = 0$

As was discussed in §2, a spectral singularity appears in $H$ only when $d = 0$. Note that the functions $\psi_k$ (3.6) as well as the operator $\eta$ have no singularity at $d = 0$:

$$\psi_k(x) = \sqrt{\frac{2}{\pi}} e^{-ibx} \cos(kx).$$

(7.1)

Thus, the operator $\eta$ is well defined in $L^2(0, \infty)$ at the spectral singularity of $H$, and its eigenfunctions form an orthonormal and complete set in $L^2(0, \infty)$,

$$\langle \psi_k | \psi_{k'} \rangle = \delta(k - k') \quad \text{and} \quad \int_0^\infty dk |\psi_k \rangle \langle \psi_k | = 1.$$  

(7.2)

It is apparent that operator $\rho$, being the positive and Hermitian square root of $\eta$,

$$\rho = \eta^{1/2} = \int_0^\infty dk \sqrt{k^2 + d^2} |\psi_k \rangle \langle \psi_k |,$$

(7.3)

is also well defined for $d = 0$. This means that, using this operator, one is able to construct a physical Hilbert space, but this does not mean that the non-Hermitian Hamiltonian $H$ will be mapped to a Hermitian Hamiltonian by a similarity transformation. To illustrate this impossibility, I will calculate the eigenfunctions $\psi_k(x)$ of $h$ at $d = 0$.

Let us denote

$$A(x, y) = \int_0^\infty \frac{dk'}{k'} \psi_k^*(x) \psi_k^*(y).$$

(7.4)
Then the integro-differential operator (5.5), applied to function $\psi_k(y)$, yields

$$\Phi_k(x) = L \int_0^\infty A(x, y) \psi_k(y) \, dy. \quad (7.5)$$

The integral in (7.4) with functions $\Psi_k(x)$ given in (4.5) is standard (see [27], formula no. 3.741.1) so that the kernel $A(x, y)$ reads

$$A(x, y) = \frac{1}{\pi} e^{ib(y-x)} \log \left| \frac{x+y}{x-y} \right|. \quad (7.6)$$

Further integration in (7.5) with $\psi_k$ given in (5.1) can also be carried out explicitly if one uses formulae 4.382.1 and 4.382.2 from Gradshteyn & Ryzhik [27]. Finally, after some tedious calculations, assuming, for instance, $b > 0$, one gets

$$\Phi_k(x) = \sqrt{\frac{2}{\pi^3}} e^{-ibx} \left\{ \frac{1}{2} \cos[(b-k)x] [\text{Ci}(b-k)x + \text{Ci}((b-k)x)] - \cos[(b+k)x] \text{Ci}((b+k)x) \right. $$

$$+ \sin[(b-k)x] \text{Si}((b-k)x) - \sin[(b+k)x] \text{Si}((b+k)x) \left. \right\} $$

$$+ \sqrt{\frac{2}{\pi}} e^{-ibx} \sin(bx) \sin(kx) + \frac{1}{\sqrt{2\pi}} \frac{|b-k|}{b-k} e^{-ibx} \cos[(b-k)x],$$

where

$$\text{Ci}(z) = -\int_z^\infty \frac{\cos \frac{z}{z}}{z} \, dz \quad \text{and} \quad \text{Si}(z) = \int_0^z \frac{\sin \frac{z}{z}}{z} \, dz.$$  

Note that the last term here is undetermined for $k = b$. I thus conclude that the point $k = b$ cannot belong to the continuous spectrum, nor can it belong to a discrete spectrum. Therefore, an operator that has such eigenfunctions cannot be Hermitian in $L^2(0, \infty)$. This conclusion is also supported by the fact that for $k = b$ the imaginary part of the integral in (7.5) is divergent.

This result is not surprising. Indeed, at $d = 0$ the eigenfunction of $H$ corresponding to $k = \pm b$ is proportional to $\exp(-ibx) \in \text{ker } \eta$. Although $\eta$ remains invertible on $D_H$, it is not invertible when applied to generalized eigenfunctions of $H$.

8. Conclusion

In this paper, I have analysed one of the simplest non-Hermitian Hamiltonians $H$, which at a specific value of a parameter may possesses a spectral singularity in its continuous spectrum, first proposed by Schwartz [22]. It contains only kinetic energy, but the functions from its domain of definition satisfy a complex boundary condition at $x = 0$. I have shown that the $\eta$ operator ($\eta = \rho^2$) is a second-order differential operator with constant coefficients and revealed its SUSY nature. This approach permitted me to express the eigenfunctions $\Phi_k(x)$ of $h$, where $h$ is Hermitian and related to $H$ by a similarity transformation, in terms of a bounded integral operator defined in the Hilbert space $L^2(0, \infty)$. With the help of this bounded operator, I succeeded in finding asymptotic behaviour of the functions $\Phi_k(x)$ and calculating the scattering matrix and cross section for $h$. Finally, I have shown that, at the point in the parameter space where $H$ has a spectral singularity, the Hermitian operator $h$ becomes undetermined. Thus, using this specific example I demonstrated that a non-Hermitian Hamiltonian possessing a spectral singularity cannot be mapped to a Hermitian Hamiltonian by any similarity transformation. Nevertheless, the possible presence of a spectral singularity in $H$ may be detected as a resonance in the scattering cross section.

References


