Hermitian Hamiltonian equivalent to a given non-Hermitian one. Manifestation of spectral singularity

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Abstract. One of the simplest non-Hermitian Hamiltonians first proposed by Schwartz (1960 Commun. Pure Appl. Math. 13 609) which may possess a spectral singularity is analyzed from the point of view of non-Hermitian generalization of quantum mechanics. It is shown that \( \eta \) operator, being a second order differential operator, has supersymmetric structure. Asymptotic behavior of 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 the 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, one can notice a growing interest to non-Hermitian Hamiltonians possessing a real spectrum and spectral singularities [1]-[8]. Probably this is due to a 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 [3].

This is well known that for any selfadjoint (or essentially selfadjoint) scattering Hamiltonian, continuous spectrum eigenfunctions can be expressed in terms of Jost solution \( f(k, x) \) and Jost function \( F(k) \), which, in the simplest case, is the Jost solution taken at \( x = 0 \), \( F(k) = f(k, 0) \), see e. g. [9]. One of the characteristic features of any selfadjoint scattering Hamiltonian is that its Jost function never vanishes if \( k \) is a spectral point, \( F(k) \neq 0 \forall k > 0 \) [9].

An essential feature of the spectral singularity \( k_0 \) is that this point belongs to a continuous part of the spectrum of a non-Hermitian Hamiltonian \( H \) and corresponding Jost function vanishes at this point \( F(k_0) = 0 \). As a result there is no way to construct
a Hermitian\footnote{An operator $A$ in a Hilbert space is said to be selfadjoint 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 $\langle \psi | B \varphi \rangle = \langle B \psi | \varphi \rangle \forall \psi, \varphi \in D_B$, see e.g. [13]. In this paper we do not make difference between symmetric and Hermitian operators.} operator $h$ related to $H$ by an equivalence transformation (see e.g. [6]). In other words, there is no way to redefine the inner product in the spirit of paper [10] with respect to which $H$ would become Hermitian.

Probably, just for this reason some authors claimed that for a Hamiltonian possessing the spectral singularity no resolution of identity operator is possible [1, 2]. In paper [4] the completeness of biorthogonal sets of eigenfunctions of non-Hermitian Hamiltonians possessing spectral singularities were carefully analyzed. Obtained results are illustrated by a number of concrete examples. In particular, the authors [4] showed that the contribution of the spectral singularity to the resolution of identity operator depends on the class of functions employed for physical states. Further progress was made in [5] where a special regularization procedure for the resolution of identity operator has been proposed. We also note the paper [7] where a concise analysis of the general concept of the spectral singularity of non-Hermitian Hamiltonians is given.

Till now Hamiltonians possessing spectral singularities are studied mainly as a possible source of new properties of optical media [1]-[3]. Probably this is because of the fact that their association with quantum mechanical observables is involved. Nevertheless, as shown in [4], 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 [11]. Such a transformation does not exist if the Hamiltonian is not diagonalizable. (Such 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 [12].)

For scattering Hamiltonians additional obstruction appears for existing a similarity transformation between $H$ and $h$. Such a transformation does not exist if in the continuous spectrum of $H$ the spectral singularity is present. 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 Hermitian conjugate of $H(d)$, then one can construct Hermitian counterpart $h(d)$ of the operator $H(d)$. Below, using a very simple example, we 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 we present a careful analysis of Schwartz’s example of a non-Hermitian Hamiltonian $H$ with the possible presence of the spectral singularity. This is one of the simplest examples since 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 we define this Hamiltonian and give a definition of the spectral singularity. In Section 3 we introduce a Hermitian Hamiltonian $h$ together with $\eta$ operator which intertwines $H$ and $H^\dagger$. In the next section we reveal a supersymmetric nature of $\eta$ operator and introduce its superpartner $\tilde{\eta}$. In Section 5 we construct an integro-differential operator which being applied to the function $(2/\pi)^{1/2} \sin(kx)$ gives eigenfunctions $\Phi_k(x)$ of $h$. In the next section we calculate asymptotic behavior of $\Phi_k(x)$ and scattering matrix for $h$. In Section 7 we show that if $H$ has the spectral singularity, operator $h$ becomes undetermined. In the last section we review shortly our main findings and draw some conclusions.

2. Non-Hermitian Hamiltonian $H$

Following Schwartz [14] we consider a non-Hermitian operator (Hamiltonian)

$$H = -d^2/dx^2, \quad x \geq 0$$

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. This is a simple exercise to find its eigenfunctions $\phi_k(x)$

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

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

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

$$\langle \phi_k^* | \phi_{k'} \rangle = \int_0^\infty \phi_k(x)\phi_k(x') \, dx = \delta(k - k')$$

with the completeness condition of the form

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

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

We would like to emphasize that if $d > 0$ then the Hamiltonian $H$ has a discrete level (see, e.g., [7]), the possibility that we would like to avoid and therefore in what follows we assume $d < 0$.

There are several equivalent definitions of spectral singularities (see e.g. [7]). The one which is suitable for our 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 a continuous part of the spectrum of $H$ such that

$$\lim_{\lambda \to \lambda_0} R(x, \xi, \lambda) = \infty.$$
where the limit should be taken along any path belonging to the resolvent set of \( H \). The function \( R(x, \xi, \lambda) \) (see e.g. [7]) is constructed with the help of two linearly independent solutions \( \varphi(x, \lambda) \) and \( e(\xi, k) \) of the differential equation
\[
-\varphi''(x) = \lambda \varphi(x), \quad \lambda = k^2
\]
as follows
\[
R(x, \xi, \lambda) = \frac{R_1(x, \xi, \lambda)}{W(\lambda)}, \quad R_1(x, \xi, \lambda) = \begin{cases} 
\varphi(x, \lambda) e(\xi, k) & \text{for } 0 \leq x \leq \xi < \infty, \\
\varphi(\xi, \lambda) e(x, k) & \text{for } 0 \leq \xi \leq x < \infty.
\end{cases}
\]
Here \( W(\lambda) \) is the Wronskian of the functions \( \varphi(x, \lambda) \) and \( e(\xi, k) \),
\[
W(\lambda) = \varphi(x, \lambda) e'(x, k) - \varphi'(x, \lambda) e(x, k).
\]

In particular, if the function \( \varphi(x, \lambda) \) is such that
\[
\varphi(0, \lambda) = 1, \quad \varphi'(0, \lambda) + (d + ib)\varphi(0, \lambda) = 0
\]
and \( e(x, k) \) is the Jost solution of equation (5) defined by its asymptotic behavior
\[
e(x, k) = e^{ikx} [1 + o(1)], \quad x \to \infty, \quad \text{Im} \ k \geq 0
\]
then the Wronskian \( W(\lambda) \) coincides with the Jost function for the Hamiltonian \( H \)
\[
W(\lambda) = e'(0, k) + (d + ib) e(0, k) = ik + d + ib, \quad \lambda = k^2.
\]
Since 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 the spectral singularity at point \( \lambda = b^2 \), i.e., at \( d = 0 \). Just at this point, as it was mentioned in Introduction, the Jost function for \( H \) vanishes. As shown in [5] in this case the corresponding continuous spectrum eigenfunction has zero binorm and the resolution of 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 \( h \), we will use ideas formulated in [15] for quasi-Hermitian Hamiltonians and further developed in [16] 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 our case the adjoint operator \( H^\dagger \) is defined by the same differential expression (1) with the domain
\[
D_{H^\dagger} = \{ \varphi \in L^2(0, \infty) : \varphi''(x) \in L^2(0, \infty), \varphi'(0) + (d - ib)\varphi(0) = 0 \}.
\]
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 (7). Evidently, equation (7) defines $\eta$ up to a transformation $\eta \rightarrow A^\dagger \eta A$ with any invertible $A$ such that $[A, H] = 0$ (see e.g. [17]). We find convenient to use the form (9) of $\eta$ operator.

If $\eta$ were bounded its domain would be the whole Hilbert space and no problems occurred to act by both the left and the right hand sides of (7) on functions belonging to $D_H$. Unfortunately, this is not our case since operator (9) is unbounded and should have its own domain in $L^2(0, \infty)$. We find reasonable to assume that the domain of $\eta$ coincides with that of $H$,

$$D_\eta = D_H.$$  \hspace{1cm} (10)

As we show below, this assumption is justified by the property that operator $\eta$ defined in this way is selfadjoint as well as positive definite and invertible on $D_\eta$. It is not difficult to find its eigenfunctions and eigenvalues,

$$\eta \Psi_k(x) = (k^2 + d^2) \Psi_k(x), \quad k \geq 0,$$  \hspace{1cm} (11)

where

$$\Psi_k(x) = \sqrt{\frac{2}{\pi}}(k^2 + d^2)^{-1/2} e^{-ibx} [d \sin(kx) - k \cos(kx)].$$  \hspace{1cm} (12)

From here we conclude that $\eta$ (9) is positive definite. Moreover, since 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 $L^2(0, \infty)$.

We note also that functions (12) form a complete and orthonormal set in $L^2(0, \infty)$,

$$\langle \Psi_k | \Psi_{k'} \rangle = \delta(k - k'), \quad \int_0^\infty dk \, |\Psi_k\rangle \langle \Psi_k| = I.$$  \hspace{1cm} (13)

This property follows form the fact that $\eta$ is selfadjoint 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

$$\langle \psi_2 | \eta \psi_1 \rangle = \int_0^{\infty} \psi_2^\ast [-\psi_1'' + (w^* - w)\psi_1' + (ww^* - w')\psi_1] dx$$

$$= [\psi_2'\psi_1 - \psi_2^\ast \psi_1' + \psi_2^\ast \psi_1(w^* - w)]^{\infty}_{x=0}$$

$$+ \int_0^{\infty} [-\psi_2'' + (w - w^*)\psi_2' \psi_1 - (ww^* - w')\psi_2^\ast \psi_1 + (ww^* - w')\psi_1 \psi_2^\ast] dx$$

$$= \int_0^{\infty} [-\psi_2' + (w - w^*)\psi_2 + (ww^* - w')\psi_2^\ast] \psi_1 dx$$

$$= \langle \eta \psi_2 | \psi_1 \rangle.$$  \hspace{1cm} (11)

To justify the last equality we consider the integrated term at $x = 0$

$$[\psi_2'\psi_1 - \psi_2^\ast \psi_1' + \psi_2^\ast \psi_1(w^* - w)]_{x=0} = [\psi_2'\psi_1 - \psi_2^\ast (-w\psi_1) + \psi_2^\ast \psi_1(w^* - w)]_{x=0}$$

$$= \psi_1(0) [\psi_2' + \psi_2^\ast w^*]_{x=0}$$

$$= 0.$$  \hspace{1cm} (12)
The first line here follows from the property that \( \psi_1 \in D_\eta = D_H \) given in (2) and in the last line we used \( \psi_2 \in D_\eta = D_H \).

In the next step we have to check that \( \eta \) (9) is invertible on \( D_\eta \). For that we compute the kernel space of the differential expression (9). This is a two-dimensional linear space with the basis vectors

\[
f_\pm(x) = e^{-ibx^\mp dx}.
\]

Evidently, \( f_\pm(x) \) does not satisfy the boundary condition given in equation (2) while \( f_-(x) \) satisfies this condition. Therefore, for \( d < 0 \), when \( f_-(x) \notin L^2(0, \infty) \), we have \( f_-(x) \notin D_\eta \) and, hence, \( \eta \) (9) is invertible on \( D_\eta \). Thus, as it was already mentioned, in what follows we assume \( d < 0 \) except for Section 7 where we consider the case \( d = 0 \).

From Intertwining relation (7) it follows that the operator defined as

\[
h = \eta^{1/2} H \eta^{-1/2} = \eta^{-1/2} H^\dagger \eta^{1/2} \tag{14}
\]

is Hermitian, \( h = h^\dagger \), and at the same time is related to \( H \) by equivalence transformation (14). According to the first equality (14) if \( \psi_1 \in D_h \) then \( \varphi_1 = \eta^{-1/2} \psi_1 \) should belong to \( D_H \), \( \varphi_1 \in D_H \). Note that since both \( \eta^{-1} \) and \( \eta^{-1/2} \) are bounded, the function \( \varphi_1 \) is well defined. Hence we can define \( D_h^{(1)} \) as a set of functions \( \psi_1 = \eta^{1/2} \varphi_1 \) when \( \varphi_1 \) runs through \( \tilde{D}_H \subset D_H \) where \( \tilde{D}_H \) will be specified below. The function \( \psi_1 \) here is also well defined since \( \tilde{D}_H \subset D_H = D_\eta \subset D_\eta^{1/2} \). Similarly, according to the second equality in (14), we can define \( D_h^{(2)} \) as a set of functions \( \psi_2 = \eta^{-1/2} \varphi_2 \) when \( \varphi_2 \) runs through \( \tilde{D}_H^{\dagger} \subset D_H^{\dagger} \). It is not difficult to see that for any \( \varphi_1(x) \) satisfying the boundary condition (2) the function

\[
\varphi_2(x) = \eta \varphi_1(x) \in \tilde{D}_H^{\dagger} \subset D_H^{\dagger}, \quad (\varphi_1 \in \tilde{D}_H) \tag{15}
\]

satisfies the boundary condition (8). Note that since \( \eta \) is a second order differential expression and \( \varphi_2(x) \in D_H^{\dagger} \), the function \( \varphi_1(x) \) should be smoother than this is required by equation (2), namely it should be such that \( \varphi^{(iv)}(x) \in L^2(0, \infty) \) where \( \varphi^{(iv)}(x) \) is the fourth derivative of \( \varphi(x) \). Thus we have

\[
\tilde{D}_H = \{ \varphi(x) : \varphi(x) \in D_H, \varphi^{(iv)}(x) \in L^2(0, \infty) \} \subset D_H.
\]

Moreover from (15) it follows that

\[
\eta^{-1/2} \varphi_2(x) = \eta^{1/2} \varphi_1(x).
\]

This means that we can put \( D_h^{(1)} = D_h^{(2)} = D_h \) with

\[
D_h = \{ \psi(x) : \psi(x) = \eta^{1/2} \varphi(x), \varphi(x) \in \tilde{D}_H \subset D_H \}.
\]

Furthermore, since \( \eta \) has an empty kernel on \( D_H \), the set \( D_h \) is dense in \( L^2(0, \infty) \) and it can be taken as an initial domain for \( h \) where it is Hermitian, i.e.

\[
\langle \psi_2 | h \psi_1 \rangle = \langle h \psi_2 | \psi_1 \rangle \quad \forall \psi_1, \psi_2 \in D_h.
\]

This property follows from the following chain of equalities:

\[
\langle \psi_2 | h \psi_1 \rangle = \langle \psi_2 | h \eta^{1/2} \varphi_1 \rangle = \langle \psi_2 | \eta^{1/2} H \varphi_1 \rangle = \langle \eta^{1/2} \psi_2 | H \varphi_1 \rangle = \langle \eta^{-1/2} H^\dagger \eta^{1/2} \psi_2 | \psi_1 \rangle = \langle h \psi_2 | \psi_1 \rangle.
\]
4. SUSY partner of $\eta$ operator

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

$$\eta = LL^\dagger, \quad L = -d/dx + d - ib, \quad L^\dagger = d/dx + d + ib$$

(16)

thus revealing its supersymmetric (SUSY) nature. Corresponding SUSY algebra is based on the above factorization properties and intertwining relations (see e.g. [18])

$$L^\dagger \eta = \tilde{\eta} L^\dagger, \quad \eta L = L \tilde{\eta}$$

(17)

where

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

(18)

Note that intertwining relations (17) are nothing but identities

$$(L^\dagger L)L^\dagger = L^\dagger (LL^\dagger), \quad (LL^\dagger)L = L(L^\dagger L).$$

Although operator $\tilde{\eta}$, which is a SUSY partner of $\eta$, is defined by the same differential expression as operator $\eta$ (9), its domain $D_{\tilde{\eta}}$ is different than $D_{\eta}$ (10). This, in particular, follows from intertwining relations (17). Indeed, according to these relations, operator $L^\dagger$ transforms eigenfunctions of $\eta$ to eigenfunctions of $\tilde{\eta}$ and operator $L$ realizes an inverse mapping. Taking unto account factorization properties (16) and (18), we find

$$\tilde{\Psi}_k = (k^2 + d^2)^{-1/2} L^\dagger \Psi_k, \quad \Psi_k = (k^2 + d^2)^{-1/2} L \tilde{\Psi}_k.$$  

(19)

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

$${\langle \Psi_k | \Psi_{k'} \rangle = \delta(k - k'), \quad {\langle \tilde{\Psi}_k | \tilde{\Psi}_{k'} \rangle = \delta(k - k')}.$$  

Thus using (19) and (12) one finds the eigenfunctions of $\tilde{\eta}$

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

(20)

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

$$D_{\tilde{\eta}} = \{ \Psi \in L^2(0, \infty) : \Psi''(x) \in L^2(0, \infty), \quad \Psi(0) = 0 \}$$

by the differential expression (9) is selfadjoint.

Evidently, the functions (20) are $d$-independent and form an orthonormal and complete (in the sense of distributions) basis in $L^2(0, \infty)$

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

(21)

Another remarkable property of intertwining operators (16), that we need below, is the value of the composition

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

(22)
5. Eigenfunctions of $h$

First we note that the eigenfunctions $\varphi_k$ of $H$ (3) may be obtained by applying operator $L^*$ (22) to the functions

$$\psi_k(x) = \sqrt{\frac{2}{\pi}} \sin(kx),$$  \hspace{1cm} (23)

which yields

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

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 $\psi_k$

$$\Phi_k(x) = [k^2 + (d + ib)^2]^{-1/2} \eta^{1/2} \varphi_k(x)$$

$$= [k^2 + (d + ib)^2]^{-1} \eta^{1/2} L^* \psi_k(x).$$  \hspace{1cm} (24)

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

Note that function (23) is an eigenfunction of the operator (22)

$$L^1 L^* \psi_k(x) = [k^2 + (d + ib)^2] \psi_k(x).$$  \hspace{1cm} (25)

We find it useful expressing $\Phi_k(x)$ as result of the action on the functions $\tilde{\Psi}_k$ (20) by an integro-differential operator. To this end we first insert the identity operator (13) between $\eta^{1/2}$ and $L$ in (24) and use equation (11)

$$\Phi_k(x) = [k^2 + (d + ib)^2]^{-1} \int_0^\infty dk' \sqrt{(k')^2 + b^2} \Psi_k(x) \langle \Psi_k | L^* \psi_k \rangle$$  \hspace{1cm} (26)

and then in the obtained expression replace $\Psi_k(x)$ according to (19)

$$\Phi_k(x) = L \int_0^\infty \frac{dk'}{(k')^2 + d^2} \tilde{\Psi}_k(x) \langle \tilde{\Psi}_k | \psi_k \rangle.$$  \hspace{1cm} (27)

Here we moved the operator $L$ from the left side in the inner product to the right side where it becomes adjoint $L^\dagger$, replaced the action of the the superposition $L^1 L^*$ by its explicit expression (22) and used formula (25).

An advantage of using the functions $\tilde{\Psi}_k$ in (27) with respect to using $\Psi_k$ in (26) is that the integral operator in (27) is the positive and Hermitian square root of a resolvent operator and therefore it is bounded in $L^2(0, \infty)$ whereas the integral operator in (26) is unbounded.

6. Asymptotic behavior of functions $\Phi_k(x)$. Scattering matrix and cross section for $h$

Note that according to formula (27), the eigenfunctions $\Phi_k(x)$ of the Hermitian operator $h$ are expressed in terms of elementary functions (20) and (23). Nevertheless, no simple
explicit expression for these functions exists. Below we calculate their asymptotic behavior as $x \to \infty$.

Inserting formulas (22) and (25) into (27) yields

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

(28)

where

$$J(x, y) = \int_0^\infty dk' \frac{\sin(k'x) \sin(k'y)}{\sqrt{(k')^2 + d^2}}.$$ 

Expanding the product of sine functions into the difference of cosine functions reduces the above integral to the one published in [19] (see formula N 3.754.2),

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

Here $K_0(z)$ is the standard modified Bessel function (see e.g. [19]). Accordingly, integral from (28) has two contributions

$$I(x) = \frac{1}{2} I_1(x) - \frac{1}{2} I_2(x)$$

(29)

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

$$I_2(x) \to 0.$$ 

(30)

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

$$I_1(x) \to \frac{1}{d} e^{ibx} I_{11}(x)$$

where

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

With the help of standard trigonometric formulas 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 semi-axis $(0, \infty)$. As a result, both these terms reduce to the standard integral (see [19], equation No 6.671.14)

$$\int_0^\infty K_0(x) \cos(\alpha x) \, dx = \frac{\pi}{2\sqrt{1 + \alpha^2}}.$$
so that

\[ I_{11}(x) = \frac{i\pi d}{2} \left[ \frac{e^{-ikx}}{\sqrt{d^2 + (k-b)^2}} - \frac{e^{ikx}}{\sqrt{d^2 + (k+b)^2}} \right] \] (31)

Now using equations (28), (29), (30) and (31) we finally obtain

\[ \Phi_k(x) \to \sqrt{\frac{2}{\pi}} e^{-i(\varphi_1-\varphi_2)/2} \sin[kx + \frac{1}{2} (\varphi_1 + \varphi_2)], \quad x \to \infty \]

where

\[ \varphi_1 = \frac{1}{2i} \log \left[ \frac{d - ik + ib}{d + ik - ib} \right], \quad \varphi_2 = \frac{1}{2i} \log \left[ \frac{d - ik - ib}{d + ik + ib} \right]. \]

From here we find the phase shift

\[ \delta = \frac{1}{2} (\varphi_1 + \varphi_2) = \frac{1}{4i} \log \left[ \frac{b^2 + (d - ik)^2}{b^2 + (d + ik)^2} \right] \] (32)

and the \( S \)-matrix

\[ S = e^{2i\delta} = \left[ \frac{b^2 + (d - ik)^2}{b^2 + (d + ik)^2} \right]^{1/2}. \] (33)

This result perfectly agrees with the general formula for the \( S \)-matrix obtained in [6]. We note that the scattering matrix

\[ S_{BW} = S^2 = \frac{b^2 + (d - ik)^2}{b^2 + (d + ik)^2} \] (34)

leads to a Breit-Wigner resonance formula (see e.g. [20])

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

which in the energy scale reads

\[ \sigma_{BW} = \frac{4\pi}{b^2} \left( \frac{(\Gamma/2)^2}{(E - E_0)^2 + (\Gamma/2)^2} \right) \] (35)

with \( \Gamma = 4bd \) and \( E_0 = b^2 - d^2 \). We 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 Eq. (35) reduces to the celebrated Breit-Wigner formula (see e.g. [21]). From here we conclude that the \( S \)-matrix (33) is a square root of the Breit-Wigner \( S \)-matrix \( S_{BW} \) given in (34).

The phase shift \( \delta \) (32) corresponding to \( S \) (33) 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 [6]

\[ \sigma(k) = \frac{2\pi}{k^2} \left[ 1 + \frac{k^2 - b^2 - d^2}{\sqrt{(k^2 + d^2 - b^2)^2 + 4b^2d^2}} \right]. \] (36)

We choose here that sign of the square root which corresponds to positive definite operator \( \rho = \eta^{1/2} \) [6]. 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 \( 0 \leq k < \infty \) 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 \( \sigma(k) \) (36) has a maximum and therefore exhibits a resonance behavior. 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 Section 2 spectral singularity appears in $H$ only when $d = 0$. Note that the functions $\Psi_k$ (12) as well as operator $\eta$ has no singularity at $d = 0$:

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

(37)

Thus 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 $L^2(0, \infty)$,

$$\langle \Psi_k | \Psi_{k'} \rangle = \delta(k - k'), \quad \int_0^\infty dk |\Psi_k\rangle \langle \Psi_k| = 1.$$  

(38)

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

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

(39)

is also well defined for $d = 0$. This means that using this operator one is able to construct a physical Hilbert 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 we will calculate eigenfunctions $\Phi_k(x)$ of $h$ at $d = 0$.

Let us denote

$$A(x, y) = \int_0^\infty \frac{dk'}{k'} \bar{\Psi}_{k'}(x) \bar{\Psi}_{k'}(y).$$

(40)

Then the integro-differential operator (27), applied to function $\psi_k(y)$, yields

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

(41)

Integral in (40) with functions $\bar{\Psi}_k(x)$ given in (20) is standard (see [19], formula No 3.741.1) so that the kernel $A(x, y)$ reads

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

(42)

Further integration in (41) with $\psi_k$ given in (23) can also be made explicitly if one uses formulas 4.382.1 and 4.382.2 from [19]. Finally after some tedious calculations assuming, for instance, $b > 0$, one gets

$$\Phi_k(x) = \sqrt{\frac{2}{\pi^2}} e^{-ibx}$$

$$\times \left\{ \frac{1}{2} \cos[(b-k)x] \left( Ci[(b-k)x] + Ci[(b+k)x] \right) \right.$$  

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

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

were

$$\text{Ci} (z) = - \int_1^\infty \frac{\cos z}{z} \, dz, \quad \text{Si} (z) = \int_0^z \frac{\sin z}{z} \, dz.$$
We note that the last term here is undetermined for \( k = b \). We thus conclude that the point \( k = b \) cannot belong to the continuous spectrum neither it can 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 (41) is divergent.

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

8. Conclusion

In this paper we analyzed one of the simplest non-Hermitian Hamiltonian \( H \), which at a specific value of a parameter may possesses a spectral singularity in its continuous spectrum, first proposed by Schwartz [14]. It contains only kinetic energy but the functions from its domain of definition satisfy a complex boundary condition at \( x = 0 \). We have shown that \( \eta \) operator \( (\eta = \rho^2) \) is a second order differential operator with constant coefficients and revealed its supersymmetric nature. This approach permitted us to express eigenfunctions \( \Phi_k(x) \) of \( h \), where \( h \) is Hermitian and related to \( H \) by a similarity transformations, in terms of a bounded integral operator defined in the Hilbert space \( L^2(0, \infty) \). With the help of this bounded operator we succeeded to find asymptotic behavior of the functions \( \Phi_k(x) \) and calculate the scattering matrix and cross section for \( h \). Finally we have shown that at the point in the parameter space where \( H \) has the spectral singularity the Hermitian operator \( h \) becomes undetermined. Thus, using this specific example we demonstrated that a non-Hermitian Hamiltonian possessing the spectral singularity cannot be mapped to a Hermitian Hamiltonian by any similarity transformation. Nevertheless, the possible presence of the spectral singularity in \( H \) may be detected as a resonance in the scattering cross section in \( h \).

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