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Non-Hermitian quantum mechanics of non-diagonalizable Hamiltonians: puzzles with self-orthogonal states

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Abstract
We consider quantum mechanics with non-Hermitian quasi-diagonalizable Hamiltonians, i.e. the Hamiltonians having a number of Jordan cells, in particular, biorthogonal bases. The 'self-orthogonality' phenomenon is clarified in terms of a correct spectral decomposition and it is shown that 'self-orthogonal' states never jeopardize a resolution of identity and thereby quantum averages of observables. The example of a complex potential leading to one Jordan cell in the Hamiltonian is constructed and its origin from level coalescence is elucidated. Some puzzles with zero-binorm bound states in a continuous spectrum are unravelled with the help of a correct resolution of identity.

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1. Introduction

The variety of complex potentials in quantum physics is associated typically with open systems when a control of information is partially lost and thereby the unitarity of observable evolution is broken. For this class of quantum systems, the energy eigenvalues may have an imaginary part which signals the opening of new channels not directly measured in a given experiment. In this context, non-Hermitian interactions have been used in field theory and statistical mechanics for many years with applications to condensed matter, quantum optics and hadronic and nuclear physics [1–4]. The subject of non-self-adjoint operators has been also under intensive mathematical investigations [5–7], in particular, interesting examples of non-Hermitian effective Hamiltonian operators have been found for the Faddeev equations [8].

An important class of complex Hamiltonians deals with a real spectrum [9, 10], in particular, in the PT-symmetric quantum mechanics [11–14] and its pseudo-Hermitian generalization [15, 16]. Scattering problems for such Hamiltonians have been investigated in [4, 17] .

For complex, non-Hermitian potentials the natural spectral decomposition exploits the sets of biorthogonal states [18], and within this framework one can discover new features that never happen for closed systems with Hermitian Hamiltonians possessing a real spectrum[3], namely, certain Hamiltonians may not be diagonalizable [26] with the help of biorthogonal bases and can be reduced only to a quasi-diagonal form with a number of Jordan cells [15]. Such a feature can be realized by a level crossing which, in fact, occurs (after some kind of complexification) in atomic and molecular spectra [26] and optics [27] (see more examples in [28]) as well as in PT-symmetric quantum systems [29–31]. In this case, some eigenstates seem to be 'self-orthogonal' with respect to a binorm [28, 32]. The latter quite intriguing phenomenon has been interpreted as a sort of phase transition [28] .

The main purpose of the present work is to clarify the 'self-orthogonality' in terms of a correct spectral decomposition both for discrete and continuous spectra and to show that, at least, in one-dimensional quantum mechanics such states never jeopardize a resolution of identity for the discrete or bound state spectrum and thereby do not affect quantum averages of observables.

We start introducing the notion of biorthogonal basis and, correspondingly, the resolution of identity for a non-Hermitian diagonalizable Hamiltonian. In section 2 the appearance of associated functions is discussed and in section 3 the non-diagonalizable (but quasi-diagonalizable) Hamiltonians with finite-size Jordan cells are analysed. Special attention is paid to the definition of a biorthogonal *diagonal* basis and the meaning of zero-binorm states is clarified. Namely, it is shown that the apparent self-orthogonality of eigenfunctions and associated functions is misleading as they never replicate themselves as relative pairs in a diagonal resolution of identity. Instead, the 'self-orthogonality' involves the different elements in the related basis thereby being addressed to a conventional orthogonality. The construction of such biorthogonal bases with pairs of mutually complex-conjugated base functions is described. In section 4 another representation of non-diagonalizable Hamiltonians, manifestly symmetric under transposition is given, compatible with the diagonal resolution of identity. In section 5 the example of a (transparent) complex potential leading to the non-diagonalizable Hamiltonian with one Jordan 2×2 cell is constructed and its origin from level coalescence is illustrated.

On the other hand, some puzzles with zero-binorm bound states arise in a continuous spectrum and they are unravelled in section 6 with the help of a correct resolution of identity. Its proof is relegated to the appendix. In section 7 we complete our analysis with discussion of singularities in the spectral parameter for resolvents and of scattering characteristics for previous examples. We conclude with some proposals for probabilistic interpretation of wavefunctions defined with respect to a biorthogonal basis which does not allow any negative or zero-norm states.

There are certain links of our approach to the works [33] on Jordan cells associated with the occurrence of non-Hermitian degeneracies for essentially Hermitian Hamiltonians where the description has been developed for complex eigenvalue Gamow states (resonances) unbounded

[3] An exception concerns the action of the Hamiltonian operator on zero-mode subspaces of supercharges in nonlinear SUSY [19–23]. For confluent NSUSY, a Hermitian Hamiltonian may produce a non-Hermitian matrix, with Jordan cells [24, 25] after quasi-diagonalization. In this case, zero-mode subspaces of supercharges also include non-normalizable solutions of the Schrödinger equation which do not belong to the energy spectrum of the original self-adjoint Hamiltonian.

in their asymptotics and, in general, not belonging to the Hilbert space. In contrast, we instead examine non-Hermitian Hamiltonians with normalizable bound and associated states.

In our paper we deal with complex one-dimensional potentials $V(x) \neq V^*(x)$ and respectively with non-Hermitian Hamiltonians h of the Schrödinger type, defined on the real axis:

$$h \equiv -\partial_x^2 + V(x), \tag{1}$$

which are assumed to be t-symmetric or self-transposed under the t transposition operation, $h = h^t$. Only scalar local potentials will be analysed which are obviously symmetric under transposition (for some matrix non-diagonalizable problems, see [32, 34]). Throughout this work the units will be used with $m = 1/2, \hbar = 1, c = 1$ which leads to dimensionless energies.

Let us first define a class of one-dimensional non-Hermitian *diagonalizable* Hamiltonian h with a discrete spectrum such that

(a) a biorthogonal system $\{|\psi_n\rangle, |\tilde{\psi}_n\rangle\}$ exists,

$$h|\psi_n\rangle = \lambda_n|\psi_n\rangle, \qquad h^\dagger|\tilde{\psi}_n\rangle = \lambda_n^*|\tilde{\psi}_n\rangle, \qquad \langle\tilde{\psi}_n|\psi_m\rangle = \langle\psi_m|\tilde{\psi}_n\rangle = \delta_{nm}, \tag{2}$$

(b) the complete resolution of identity in terms of these bases and the spectral decomposition of the Hamiltonian hold,

$$I = \sum_n |\psi_n\rangle\langle\tilde{\psi}_n|, \qquad h = \sum_n \lambda_n|\psi_n\rangle\langle\tilde{\psi}_n|. \tag{3}$$

In the coordinate representation,

$$\psi_n(x) = \langle x|\psi_n\rangle, \qquad \tilde{\psi}_n(x) = \langle x|\tilde{\psi}_n\rangle, \tag{4}$$

the resolution of identity has the form

$$\delta(x - x') = \langle x'|x\rangle = \sum_n \psi_n(x')\tilde{\psi}_n^*(x). \tag{5}$$

The differential equations,

$$h\psi_n = \lambda_n\psi_n, \qquad h^\dagger\tilde{\psi}_n = \lambda_n^*\tilde{\psi}_n, \tag{6}$$

and the fact that there is only one normalizable eigenfunction of h for the eigenvalue λ_n (up to a constant factor), allow one to conclude that

$$\tilde{\psi}_n^*(x) \equiv \alpha_n\psi_n(x), \qquad \alpha_n = \text{const} \neq 0. \tag{7}$$

Hence, the system $\{|\psi_n\rangle, |\tilde{\psi}_n\rangle\}$ can be redefined,

$$|\psi_n\rangle \to \frac{1}{\sqrt{\alpha_n}}|\psi_n\rangle, \qquad |\tilde{\psi}_n\rangle \to \sqrt{\alpha_n^*}|\tilde{\psi}_n\rangle, \tag{8}$$

so that

$$\tilde{\psi}_n^*(x) \equiv \psi_n(x), \qquad \int_{-\infty}^{+\infty} \psi_n(x)\psi_m(x)\,\mathrm{d}x = \delta_{nm}. \tag{9}$$

We stress that the non-vanishing binorms in equation (9) support the completeness of this basis, i.e. the resolution of identity:

$$\delta(x - x') = \sum_n \psi_n(x)\psi_n(x'). \tag{10}$$

Indeed if some of the states in equation (10) were 'self-orthogonal' (as has been accepted in [32]), i.e. had zero binorms in (9), the would-be unity in (10) would annihilate such states thereby signalling the incompleteness.

2. Non-diagonalizable Hamiltonians and zero-binorm states

For complex Hamiltonians one can formulate the extended eigenvalue problem, searching not only for normalizable eigenfunctions but also for normalizable associated functions for the discrete part of the energy spectrum. Some related problems have been known for a long time in mathematics of linear differential equations (see, for instance, [35]).

Let us give the formal definition.

Definition. *The function $\psi_{n,i}(x)$ is called a formal associated function of the ith order of the Hamiltonian h for a spectral value λ_n, if*

$$(h-\lambda_n)^{i+1}\psi_{n,i} \equiv 0, \qquad (h-\lambda_n)^{i}\psi_{n,i} \not\equiv 0, \tag{11}$$

where 'formal' emphasizes that a related function is not necessarily normalizable.

In particular, the associated function of zero order $\psi_{n,0}$ is a formal eigenfunction of h (a solution of the homogeneous Schrödinger equation, not necessarily normalizable).

Let us single out normalizable associated functions and the case when h maps them into normalizable functions. Evidently, this may occur only for non-Hermitian Hamiltonians. Then for any normalizable associated functions $\psi_{n,i}(x)$ and $\psi_{n',i'}(x)$, the transposition symmetry holds

$$\int_{-\infty}^{+\infty} h\psi_{n,i}(x)\psi_{n',i'}(x)\,\mathrm{d}x = \int_{-\infty}^{+\infty} \psi_{n,i}(x)h\psi_{n',i'}(x)\,\mathrm{d}x. \tag{12}$$

Furthermore, one can prove the following relations:

$$\int_{-\infty}^{+\infty} \psi_{n,i}(x)\psi_{n',i'}(x)\,\mathrm{d}x \equiv (\psi^*_{n,i}, \psi_{n',i'}) = 0, \qquad \lambda_n \neq \lambda_{n'}, \tag{13}$$

where $(\ldots,\ldots)$ is a scalar product.

As well, let us take two normalizable associated functions $\psi_{n,k}(x)$ and $\psi_{n,k'}(x)$ so that, in general, $k \neq k'$ and there are two different sequences of associated functions for $i \leqslant k$ and $i' \leqslant k'$

$$\psi_{n,i}(x) = (h-\lambda_n)^{k-i}\psi_{n,k}(x), \qquad \psi_{n,i'}(x) = (h-\lambda_n)^{k'-i'}\psi_{n,k'}(x). \tag{14}$$

Then

$$\int_{-\infty}^{+\infty} \psi_{n,i}(x)\psi_{n,i'}(x)\,\mathrm{d}x = (\psi^*_{n,i}, \psi_{n,i'}) = 0, \qquad i+i' \leqslant \max\{k,k'\}-1. \tag{15}$$

In particular, for some normalizable associated function $\psi_{n,l}(x)$, the 'self-orthogonality' [32] is realized,

$$\int_{-\infty}^{+\infty} \psi^2_{n,l}(x)\,\mathrm{d}x = 0, \qquad \psi_{n,l}(x) = (h-\lambda)^{i-l}\psi_{n,i}(x), \qquad l = 0,\ldots,\left[\frac{i-1}{2}\right]. \tag{16}$$

Thus, when assigning [28] the probabilistic meaning for the binorm (Ψ^*, Ψ), one comes to a conclusion that a sort of intriguing phase transition occurs in such a system, signalled by the puzzling divergence of some averages of observables,

$$\langle O\rangle = \frac{(\psi^*_{n,l}, O\psi_{n,l})}{(\psi^*_{n,l}, \psi_{n,l})} = \frac{\int_{-\infty}^{+\infty}\psi_{n,l}(x)O\psi_{n,l}(x)\,\mathrm{d}x}{\int_{-\infty}^{+\infty}\psi^2_{n,l}(x)\,\mathrm{d}x} \to \infty. \tag{17}$$

All the above relations are derived from the symmetry of a Hamiltonian under transposition and the very definition of associated functions and therefore the existence of self-orthogonal states seems to be inherent for any non-diagonalizable Hamiltonians with normalizable associated functions.

3. Towards resolution of puzzle with self-orthogonal states for Hamiltonians with finite-size Jordan cells

Let us show that the puzzle with self-orthogonal states may appear, in fact, due to misinterpretation of what are the pairs of orthogonal states in a true biorthogonal basis. We proceed to the special class of Hamiltonians for which the spectrum is discrete and there is a complete biorthogonal system $\{|\psi_n, a, i\rangle, |\tilde{\psi}_n, a, i\rangle\}$ such that

$$\begin{aligned}
&h|\psi_n, a, 0\rangle = \lambda_n|\psi_n, a, 0\rangle, \qquad (h - \lambda_n)|\psi_n, a, i\rangle = |\psi_n, a, i - 1\rangle,\\
&h^\dagger|\tilde{\psi}_n, a, p_{n,a} - 1\rangle = \lambda_n^*|\tilde{\psi}_n, a, p_{n,a} - 1\rangle,\\
&(h^\dagger - \lambda_n^*)|\tilde{\psi}_n, a, p_{n,a} - i - 1\rangle = |\tilde{\psi}_n, a, p_{n,a} - i\rangle,
\end{aligned} \tag{18}$$

where $n = 0, 1, 2, \ldots$ is an index of an h eigenvalue λ_n, $a = 1, \ldots, d_n$ is an index of a Jordan cell (block) for the given eigenvalue λ_n, d_n is a number of Jordan cells for λ_n, $i = 0, \ldots, p_{n,a} - 1$ is an index of an associated function in the Jordan cell with indices n, a and $p_{n,a}$ is a dimension of this Jordan cell. We have taken a general framework which is also applicable for matrix and/or multidimensional Hamiltonians. But the main results of this and the next sections are guaranteed only for scalar one-dimensional Hamiltonians with local potentials.

We remark that the number d_n is called a geometric multiplicity of the eigenvalue λ_n. For a scalar one-dimensional Schrödinger equation, it cannot normally exceed 1 (but may reach 2 in specific cases of periodic potentials and of potentials unbounded from below). In turn, the sum $\sum_a p_{n,a}$ is called an algebraic multiplicity of the eigenvalue λ_n.

The completeness implies the biorthogonality relations (in line with the enumeration of states $|\tilde{\psi}_n, a, i\rangle$ given in (18))

$$\langle\tilde{\psi}_n, a, i|\psi_m, b, j\rangle = \delta_{nm}\delta_{ab}\delta_{ij} \tag{19}$$

and the resolution of identity

$$I = \sum_{n=0}^{+\infty}\sum_{a=1}^{d_n}\sum_{i=0}^{p_{n,a}-1} |\psi_n, a, i\rangle\langle\tilde{\psi}_n, a, i|. \tag{20}$$

The spectral decomposition for the Hamiltonian can be constructed as well,

$$h = \sum_{n=0}^{+\infty}\sum_{a=1}^{d_n}\left[\lambda_n \sum_{i=0}^{p_{n,a}-1} |\psi_n, a, i\rangle\langle\tilde{\psi}_n, a, i| + \sum_{i=0}^{p_{n,a}-2} |\psi_n, a, i\rangle\langle\tilde{\psi}_n, a, i + 1|\right]. \tag{21}$$

It represents the analogue of the block-diagonal Jordan form for arbitrary non-Hermitian matrices [36].

If existing such biorthogonal systems are not unique. Indeed, relations (18) remain invariant under the group of triangle transformations:

$$|\psi_n', a, i\rangle = \sum_{0\leqslant j\leqslant i} \alpha_{ij}|\psi_n, a, j\rangle, \qquad |\tilde{\psi}_n', a, k\rangle = \sum_{k\leqslant l\leqslant p_{n,a}-1} \beta_{kl}|\tilde{\psi}_n, a, l\rangle, \tag{22}$$

where the matrix elements must obey the following equations:

$$\begin{aligned}
&\alpha_{ij} = \alpha_{i+1,j+1} = \alpha_{i-j,0}, && \alpha_{00} \neq 0,\\
&\beta_{kl} = \beta_{k+1,l+1} = \beta_{k-l+p_{n,a}-1,p_{n,a}-1}, && \beta_{p_{n,a}-1,p_{n,a}-1} \neq 0.
\end{aligned} \tag{23}$$

Biorthogonality (19) restricts the choice of pairs of matrices $\hat{\alpha}$ and $\hat{\beta}$ in (22) to be

$$\hat{\alpha}\hat{\beta}^\dagger = \hat{\beta}^\dagger\hat{\alpha} = \mathbb{I}. \tag{24}$$

This freedom in the redefinition of the biorthogonal basis is similar to equation (8) and it can be exploited to define the pairs of biorthogonal functions $\psi_{n,a,i}(x) \equiv \langle x|\psi_n, a, i\rangle$ and $\tilde{\psi}_{n,a,i}(x) \equiv \langle x|\tilde{\psi}_n, a, i\rangle$, in accordance with (9). However, one has to take into account our enumeration of associated functions $\psi_{n,a,i}(x)$ versus their conjugated ones $\tilde{\psi}_{n,a,i}(x)$ as is introduced in equations (18):

$$\psi_{n,a,i}(x) = \tilde{\psi}^*_{n,a,p_{n,a}-i-1}(x) \equiv \langle\tilde{\psi}_n, a, p_{n,a} - i - 1|x\rangle. \tag{25}$$

Then the analogue of equation (9) reads

$$\int_{-\infty}^{+\infty} \psi_{n,a,i}(x)\psi_{m,b,p_{m,b}-j-1}(x)\,\mathrm{d}x = \delta_{nm}\delta_{ab}\delta_{ij}. \tag{26}$$

We stress that this kind of biorthogonal systems is determined uniquely up to an overall sign.

In these terms, it becomes clear that relations (15) have the meaning of orthogonality of some off-diagonal pairs in the biorthogonal system $\{|\psi_n, a, i\rangle, |\tilde{\psi}_n, a, j\rangle\}$ as

$$\begin{aligned} \psi_{n,a,i}(x) &= (h - \lambda_n)^{p_{n,a}-1-i}\psi_{n,a,p_{n,a}-1}(x), \\ \tilde{\psi}^*_{n,a,j}(x) &= \psi_{n,a,p_{n,a}-1-j}(x) = (h - \lambda_n)^j\psi_{n,a,p_{n,a}-1}(x). \end{aligned} \tag{27}$$

When comparing with specification of indices in equation (15), one identifies $p_{n,a} - 1 - j \leftrightarrow i, i \leftrightarrow i'$. In both cases $k = k' = p_{n,a} - 1$. Then inequality (15) singles out off-diagonal binorms, $i \leqslant j - 1$. From equation (27) it follows that in order to have all diagonal binorms non-vanishing, it is sufficient to prove that at least one of them is not zero because

$$\begin{aligned} \int_{-\infty}^{+\infty} \psi_{n,a,0}(x)\psi_{n,a,p_{n,a}-1}(x)\,\mathrm{d}x &= \int_{-\infty}^{+\infty} [(h - \lambda_n)^{p_{n,a}-1}\psi_{n,a,p_{n,a}-1}(x)]\psi_{n,a,p_{n,a}-1}(x)\,\mathrm{d}x \\ &= \int_{-\infty}^{+\infty} \psi_{n,a,i}(x)\psi_{n,a,p_{n,a}-1-i}(x)\,\mathrm{d}x \neq 0. \end{aligned} \tag{28}$$

The latter is necessary for the completeness of the basis (because of the absence of self-orthogonal pairs of basis elements made of bound and associated functions when the resolution of identity is diagonal).

Going back to the definition of quantum-state averages of certain observables, we realize that the matrix element used in (17) is *not diagonal* and therefore this relation cannot be interpreted as an average (compare with [28, 32]) of a putative order-parameter-like operator.

4. *t*-symmetric representation of non-diagonalizable Hamiltonians

We still note that the biorthogonal basis (25) does not provide a manifestly *t*-symmetric representation of the Hamiltonian (which is symmetric under transposition $h = h^t$ in the coordinate representation as a finite-order differential operator). One can obtain another biorthogonal basis using the canonical set of (normalizable) associated functions given by equation (18) and their complex conjugates in an analogy to (8). It can be achieved by means of renumbering of conjugated elements of the biorthogonal system (18):

$$|\hat{\psi}_n, a, j\rangle = |\tilde{\psi}_n, a, p_{n,a} - j - 1\rangle, \qquad j = 0, \ldots, p_{n,a} - 1. \tag{29}$$

Eventually, one arrives at the *t-symmetric* spectral decomposition for h:

$$\begin{aligned} h = \sum_{n=0}^{+\infty}\sum_{a=1}^{d_n}\Bigg[\lambda_n \sum_{j=0}^{p_{n,a}-1} |\psi_n, a, j\rangle\langle\hat{\psi}_n, a, p_{n,a} - j - 1| \\ + \sum_{i=0}^{p_{n,a}-2} |\psi_n, a, j\rangle\langle\hat{\psi}_n, a, p_{n,a} - j - 2|\Bigg], \end{aligned} \tag{30}$$

which looks like a Jordan decomposition along the secondary diagonal. Evidently in the coordinate representation the Hamiltonian operator is manifestly t-symmetric when the special biorthogonal basis (25),

$$\psi_{n,a,j}(x) = \hat{\psi}^*_{n,a,j}(x) \equiv \langle \hat{\psi}_n, a, j|x\rangle, \tag{31}$$

is chosen.

But the resolution of identity in this case is not diagonal,

$$I = \sum_{n=0}^{+\infty} \sum_{a=1}^{d_n} \sum_{j=0}^{p_{n,a}-1} |\psi_n, a, j\rangle\langle\hat{\psi}_n, a, p_{n,a} - j - 1|, \tag{32}$$

although t-symmetric. One can diagonalize this resolution of identity by a non-degenerate orthogonal transformation Ω of sub-bases in each non-diagonal sub-block,

$$|\psi_n, a, j\rangle = \sum_{k=0}^{p_{n,a}-1} \Omega_{jk}|\psi'_n, a, k\rangle, \qquad \langle\hat{\psi}_n, a, j| = \sum_{k=0}^{p_{n,a}-1} \Omega_{jk}\langle\hat{\psi}'_n, a, k|, \tag{33}$$

retaining the type of basis (31). Then one finds a number of eigenvalues ± 1. In order to come to the canonical form of basis (19), one has to rotate by the complex unit i the pairs in the basis (31) normalized on -1. Evidently, the combination of the transformation Ω and such a rotation contains complex elements and is not orthogonal.

The remaining freedom of basis redefinition with the help of orthogonal rotations cannot provide the consequent diagonalization of the symmetric Hamiltonian matrix in each non-diagonal block. The reason is that some of the eigenvectors of the Hamiltonian sub-matrices have zero binorms, in particular, those which are related to the true Hamiltonian eigenfunctions. Thus, while being a t-symmetric operator with symmetric matrix representation, the Hamiltonian remains essentially non-diagonalizable[4].

We remark that in the general case the existence and the completeness of a biorthogonal system is not obvious (especially if the continuous spectrum is present) and needs a careful examination. In particular, at the border between discrete and continuous spectra and in the continuous spectrum itself, one can anticipate to have puzzling states with non-trivial role in the spectral decomposition. These peculiarities will be discussed in the following sections.

5. A model with non-diagonalizable Hamiltonian and its origin from level coalescence

In this section we build a model[5] with non-Hermitian Hamiltonian which has a real continuous spectrum and, in addition, possesses a Jordan cell spanned on the bound state and a normalizable associated state. This model does not belong to the class of Hamiltonians with a purely discrete spectrum considered in the preceding sections, but being block-diagonal it inherits some of their properties in the bound state sector. Further on, we demonstrate how this kind of degeneracy arises from coalescence of a pair of non-degenerate levels.

[4] We note that a similar symmetric representation for the Hamiltonian has been exemplified in a specific model with one eigenstate and one associated function [31].

[5] All Hamiltonians considered in this and the following sections can be constructed with the help of SUSY methods [24, 25, 37] and are intertwined with the Hamiltonian of a free particle by differential operators of the first or second order.

5.1. Jordan cell for a bound state

The model Hamiltonian contains the potential with coordinates selectively shifted into a complex plane:

$$h = -\partial^2 - 16\alpha^2 \frac{\alpha(x-z)\mathrm{sh}(2\alpha x) - 2\mathrm{ch}^2(\alpha x)}{[\mathrm{sh}(2\alpha x) + 2\alpha(x-z)]^2}, \qquad \alpha > 0, \quad z \in \mathbb{C}, \quad \mathrm{Im}\, z \neq 0. \tag{34}$$

This Hamiltonian is not PT-symmetric unless $\mathrm{Re}\, z = 0$. It has the Jordan cell, spanned by the normalizable eigenfunction $\psi_0(x)$ and associated function $\psi_1(x)$ on the level $\lambda_1 = -\alpha^2$,

$$\psi_0(x) = \frac{(2\alpha)^{3/2}\mathrm{ch}(\alpha x)}{\mathrm{sh}(2\alpha x) + 2\alpha(x-z)}, \qquad \psi_1(x) = \frac{2\alpha(x-z)\mathrm{sh}(\alpha x) - \mathrm{ch}(\alpha x)}{\sqrt{2\alpha}[\mathrm{sh}(2\alpha x) + 2\alpha(x-z)]}, \tag{35}$$

$$h\psi_0 = \lambda_1\psi_0, \qquad (h-\lambda_1)\psi_1 = \psi_0. \tag{36}$$

In turn, the eigenfunctions of h for a continuous spectrum read

$$\psi(x;k) = \frac{1}{\sqrt{2\pi}}\left[1 + \frac{\mathrm{i}k}{\alpha^2+k^2}\frac{W'(x)}{W(x)} - \frac{1}{2(\alpha^2+k^2)}\frac{W''(x)}{W(x)}\right]\mathrm{e}^{\mathrm{i}kx},$$
$$k \in \mathbb{R}, \qquad h\psi(x;k) = k^2\psi(x;k), \qquad W(x) = \mathrm{sh}(2\alpha x) + 2\alpha(x-z). \tag{37}$$

The eigenfunctions and the associated function of h obey the biorthogonality relations,

$$\int_{-\infty}^{+\infty} \psi_{0,1}^2(x)\,\mathrm{d}x = 0, \qquad \int_{-\infty}^{+\infty} \psi_0(x)\psi_1(x)\,\mathrm{d}x = 1,$$
$$\int_{-\infty}^{+\infty} \psi_{0,1}(x)\psi(x;k)\,\mathrm{d}x = 0, \qquad \int_{-\infty}^{+\infty} \psi(x;k)\psi(x;-k')\,\mathrm{d}x = \delta(k-k'). \tag{38}$$

The functions $\psi_0(x)$, $\psi_1(x)$ can be obtained by analytical continuation of $\psi(x;k)$ in k,

$$\lim_{k\to\pm\mathrm{i}\alpha} [(k^2+\alpha^2)\psi(x;k)] = \mp\sqrt{\frac{\alpha}{\pi}}\psi_0(x), \tag{39}$$

$$\lim_{k\to\pm\mathrm{i}\alpha} \left\{\frac{1}{2k}\frac{\partial}{\partial k}[(k^2+\alpha^2)\psi(x;k)]\right\} = \mp\sqrt{\frac{\alpha}{\pi}}\left[\psi_1(x) - \frac{1\mp 2\alpha z}{4\alpha^2}\psi_0(x)\right]. \tag{40}$$

For this model, the resolution of identity built of eigenfunctions and associated functions of h can be obtained by conventional Green function methods:

$$\delta(x-x') = \int_{-\infty}^{+\infty} \psi(x;k)\psi(x';-k)\,\mathrm{d}k + \psi_0(x)\psi_1(x') + \psi_1(x)\psi_0(x'). \tag{41}$$

With the help of Dirac notations,

$$\langle x|\psi,k\rangle = \psi(x;k), \qquad \langle x|\tilde{\psi},k\rangle = \psi^*(x;-k), \tag{42}$$

$$\langle x|\psi_{0,1}\rangle = \psi_{0,1}(x), \qquad \langle x|\hat{\psi}_{0,1}\rangle = \psi_{0,1}^*(x), \tag{43}$$

this resolution of identity can be represented in the operator form,

$$I = \int_{-\infty}^{+\infty} |\psi,k\rangle\langle\tilde{\psi},k|\,\mathrm{d}k + |\psi_0\rangle\langle\hat{\psi}_1| + |\psi_1\rangle\langle\hat{\psi}_0|. \tag{44}$$

Evidently, the basis $|\hat{\psi}_{1,2}\rangle$ corresponds to the basis $|\hat{\psi}_n, a, i\rangle$ of section 4 and therefore gives the t-symmetric spectral decomposition for the Hamiltonian,

$$h = \int_{-\infty}^{+\infty} k^2|\psi,k\rangle\langle\tilde{\psi},k|\mathrm{d}k - \alpha^2|\psi_0\rangle\langle\hat{\psi}_1| - \alpha^2|\psi_1\rangle\langle\hat{\psi}_0| + |\psi_0\rangle\langle\hat{\psi}_0|. \tag{45}$$

The diagonalization of the resolution of identity (44) may be arranged in two different ways. First, one can exploit the scheme of section 3 performing renumeration of certain elements of conjugated basis,

$$h^\dagger|\tilde\psi_1\rangle = \lambda_1|\tilde\psi_1\rangle, \qquad (h^\dagger - \lambda_1)|\tilde\psi_0\rangle = |\tilde\psi_1\rangle, \qquad h^\dagger|\tilde\psi, k\rangle = k^2|\tilde\psi, k\rangle,$$

namely,

$$\langle x|\psi, k\rangle = \psi(x;k), \qquad \langle x|\tilde\psi, k\rangle = \psi^*(x;-k), \tag{46}$$

$$\langle x|\psi_{0,1}\rangle = \psi_{0,1}(x), \qquad \langle x|\tilde\psi_{0,1}\rangle = \psi^*_{1,0}(x). \tag{47}$$

With this notation, the resolution of identity reads

$$I = \int_{-\infty}^{+\infty} |\psi, k\rangle\langle\tilde\psi, k|\,\mathrm{d}k + |\psi_0\rangle\langle\tilde\psi_0| + |\psi_1\rangle\langle\tilde\psi_1|. \tag{48}$$

We stress that $|\tilde\psi_{1,2}\rangle$ are related to the basis $|\tilde\psi_n, a, i\rangle$ in section 3. The relevant spectral decomposition of the Hamiltonian takes the quasi-diagonal form with one Jordan cell,

$$h = \int_{-\infty}^{+\infty} k^2|\psi, k\rangle\langle\tilde\psi, k|\,\mathrm{d}k - \alpha^2|\psi_0\rangle\langle\tilde\psi_0| - \alpha^2|\psi_1\rangle\langle\tilde\psi_1| + |\psi_0\rangle\langle\tilde\psi_1|. \tag{49}$$

On the other hand, the resolution of identity (44) can be diagonalized by complex non-degenerate rotations, i.e. by using the construction of section 4. The relevant basis is given by

$$\Psi_1(x) = \frac{1}{\sqrt2}\left[\varkappa\psi_0(x) + \frac{\psi_1(x)}{\varkappa}\right], \qquad \Psi_2(x) = \frac{\mathrm{i}}{\sqrt2}\left[\varkappa\psi_0(x) - \frac{\psi_1(x)}{\varkappa}\right],$$

$$\psi_{0,1} = \varkappa^{\mp1}\frac{\Psi_1 \mp i\Psi_2}{\sqrt2}, \qquad \int_{-\infty}^{+\infty} \Psi_{1,2}^2(x)\,\mathrm{d}x = 1, \tag{50}$$

$$\int_{-\infty}^{+\infty} \Psi_1(x)\Psi_2(x)\,\mathrm{d}x = 0, \qquad \int_{-\infty}^{+\infty} \Psi_{1,2}(x)\psi(x;k)\,\mathrm{d}x = 0,$$

where $\varkappa$ is an arbitrary constant. The resolution of identity becomes diagonal,

$$\delta(x-x') = \int_{-\infty}^{+\infty} \psi(x;k)\psi(x';-k)\,\mathrm{d}k + \Psi_1(x)\Psi_1(x') + \Psi_2(x)\Psi_2(x'),$$

or in the operator form,

$$I = \int_{-\infty}^{+\infty} |\psi, k\rangle\langle\tilde\psi, k|\,\mathrm{d}k + |\Psi_1\rangle\langle\tilde\Psi_1| + |\Psi_2\rangle\langle\tilde\Psi_2|, \tag{51}$$

where again the Dirac notations have been used,

$$\langle x|\Psi_{1,2}\rangle = \Psi_{1,2}(x), \qquad \langle x|\tilde\Psi_{1,2}\rangle = \Psi^*_{1,2}(x). \tag{52}$$

Accordingly, the manifestly t-symmetric spectral decomposition of h can be easily obtained:

$$h = \int_{-\infty}^{+\infty} k^2|\psi, k\rangle\langle\tilde\psi, k|\,\mathrm{d}k - \left(\alpha^2 - \frac{1}{2\varkappa^2}\right)|\Psi_1\rangle\langle\tilde\Psi_1| - \left(\alpha^2 + \frac{1}{2\varkappa^2}\right)|\Psi_2\rangle\langle\tilde\Psi_2|$$
$$- \frac{\mathrm{i}}{2\varkappa^2}|\Psi_2\rangle\langle\tilde\Psi_1| - \frac{\mathrm{i}}{2\varkappa^2}|\Psi_1\rangle\langle\tilde\Psi_2|. \tag{53}$$

Note that it cannot be diagonalized further, since the symmetric 2×2 matrix in (53),

$$\begin{pmatrix} -\alpha^2 + \frac{1}{2\varkappa^2} & -\frac{\mathrm{i}}{2\varkappa^2} \\ -\frac{\mathrm{i}}{2\varkappa^2} & -\alpha^2 - \frac{1}{2\varkappa^2} \end{pmatrix}, \tag{54}$$

has one degenerate eigenvalue $-\alpha^2$ and possesses only one eigenvector $\mathbf{e}^t = (1, -i)$, with zero norm $\mathbf{e}^t \cdot \mathbf{e} = 0$. Its existence means that the orthogonal non-degenerate matrix required for diagonalization cannot be built conventionally from a set of eigenvectors. Evidently, this vector $\mathbf{e}$ maps the pair of basis functions Ψ_1, Ψ_2 into the self-biorthogonal eigenstate of the Hamiltonian ψ_0. However, its partner in the biorthogonal basis is ψ_1 with $\langle\hat{\psi}_1|\psi_0\rangle = 1$. Thus, the existence of the zero-norm vector $\mathbf{e}$ does not entail the breakdown of the resolution of identity.

5.2. Level coalescence for complex coordinates

The Hamiltonian h with a Jordan cell for bound state (34) can be obtained as a limiting case, of the Hamiltonian h_β with two non-degenerate bound states (of algebraic multiplicity 1), corresponding $\beta = 0$:

$$h_\beta = -\partial^2 - 16\alpha^2 \frac{\frac{\alpha^2+\beta^2}{2\alpha\beta}\mathrm{sh}(2\alpha x)\mathrm{sh}(2\beta(x-z)) - 2\mathrm{ch}^2(\alpha x)\mathrm{ch}(2\beta(x-z)) + 2\mathrm{sh}^2(\beta(x-z))}{\left[\mathrm{sh}(2\alpha x) + \frac{\alpha}{\beta}\mathrm{sh}(2\beta(x-z))\right]^2},$$
$$z \in \mathbb{C}, \qquad \mathrm{Im}\, z \neq 0, \qquad \alpha > 0 \quad (\text{or} - \mathrm{i}\alpha > 0), \qquad 0 \leqslant \beta < \frac{\pi}{2\,\mathrm{Im}\, z}, \qquad \beta \neq \alpha. \tag{55}$$

For this Hamiltonian h_β, there are two normalized eigenfunctions for bound states:

$$\psi_+(x) = \sqrt{2}\mathrm{i}\alpha\sqrt{\frac{1}{\beta} + \frac{1}{\alpha}}\frac{\mathrm{ch}((\alpha-\beta)x + \beta z)}{\mathrm{sh}(2\alpha x) + \frac{\alpha}{\beta}\mathrm{sh}(2\beta(x-z))},$$
$$\psi_-(x) = \sqrt{2}\alpha\sqrt{\frac{1}{\beta} - \frac{1}{\alpha}}\frac{\mathrm{ch}((\alpha+\beta)x - \beta z)}{\mathrm{sh}(2\alpha x) + \frac{\alpha}{\beta}\mathrm{sh}(2\beta(x-z))}, \tag{56}$$

with eigenvalues,

$$h_\beta\psi_\pm = \lambda_\pm\psi_\pm, \qquad \lambda_\pm = -(\alpha \pm \beta)^2. \tag{57}$$

The eigenfunctions of h_β for a continuous spectrum take the form

$$\psi(x;k) = \frac{\left[\alpha^2 + \beta^2 + k^2 + \mathrm{i}k\frac{W'(x)}{W(x)} - \frac{1}{2}\frac{W''(x)}{W(x)}\right]\mathrm{e}^{\mathrm{i}kx}}{\sqrt{2\pi}\sqrt{(k^2+\alpha^2+\beta^2)^2 - 4\alpha^2\beta^2}},$$
$$k \in \mathbb{R}, \qquad h_\beta\psi(x;k) = k^2\psi(x;k), \qquad W(x) = \mathrm{sh}(2\alpha x) + \frac{\alpha}{\beta}\mathrm{sh}(2\beta(x-z)), \tag{58}$$

where the branch of $\sqrt{(k^2+\alpha^2+\beta^2)^2 - 4\alpha^2\beta^2}$ is defined by the condition

$$\sqrt{(k^2+\alpha^2+\beta^2)^2 - 4\alpha^2\beta^2} = k^2 + o(k^2), \qquad k \to \infty$$

in the complex k-plane with cuts, linking branch points situated in the upper (lower) half-plane. One can show that the biorthogonal relations hold,

$$\int_{-\infty}^{+\infty} \psi_\pm^2(x)\,\mathrm{d}x = 1, \qquad \int_{-\infty}^{+\infty} \psi_+(x)\psi_-(x)\,\mathrm{d}x = 0, \qquad \int_{-\infty}^{+\infty} \psi_\pm(x)\psi(x;k)\,\mathrm{d}x = 0.$$

The analytical continuation of eigenfunctions for a continuous spectrum provides the bound state functions,

$$\lim_{k\to\pm\mathrm{i}(\alpha+\beta)}\left[\sqrt{(k^2+\alpha^2+\beta^2)^2 - 4\alpha^2\beta^2}\,\psi(x;k)\right] = \pm\frac{2\mathrm{i}\alpha\beta}{\sqrt{\pi}}\sqrt{\frac{1}{\beta}+\frac{1}{\alpha}}\,\mathrm{e}^{\mp\beta z}\psi_+(x),$$
$$\lim_{k\to\pm\mathrm{i}(\alpha-\beta)}\left[\sqrt{(k^2+\alpha^2+\beta^2)^2 - 4\alpha^2\beta^2}\,\psi(x;k)\right] = \mp\frac{2\alpha\beta}{\sqrt{\pi}}\sqrt{\frac{1}{\beta}-\frac{1}{\alpha}}\,\mathrm{e}^{\pm\beta z}\psi_-(x). \tag{59}$$

Now let us coalesce two levels $\lambda_\pm$ in the limit of $\beta \to 0$. One can see that the eigenfunction $\psi_0(x)$ and the associated function $\psi_1(x)$ of h (see subsection 5.1) can be derived from $\psi_\pm(x)$ as follows:

$$\psi_0(x) = -2\mathrm{i}\sqrt{\alpha}\lim_{\beta\to 0}[\sqrt{\beta}\psi_+(x)] = 2\sqrt{\alpha}\lim_{\beta\to 0}[\sqrt{\beta}\psi_-(x)],$$
$$\psi_1(x) = 2\sqrt{\alpha}\lim_{\beta\to 0}\frac{\frac{\partial}{\partial\beta}[\sqrt{\beta}(\psi_-(x) + \mathrm{i}\psi_+(x))]}{\frac{\partial}{\partial\beta}(\lambda_- - \lambda_+)}. \tag{60}$$

The resolution of identity for $\beta \neq 0$ takes the conventional form

$$\delta(x - x') = \psi_+(x)\psi_+(x') + \psi_-(x)\psi_-(x') + \int_{-\infty}^{+\infty}\psi(x;k)\psi(x;-k)\,\mathrm{d}k$$

and in the limit of $\beta \to 0$ one can reveal that in the case of $\alpha > 0$

$$\lim_{\beta\to 0}[\psi_+(x)\psi_+(x') + \psi_-(x)\psi_-(x')] = \psi_0(x)\psi_1(x') + \psi_1(x)\psi_0(x'), \tag{61}$$

i.e. the resolution of identity (41) is reproduced.

6. Puzzles with zero-binorm bound states in the continuum

In what follows we develop another type of models in which the continuous spectrum is essentially involved in a non-diagonal part of a Hamiltonian and elaborate the resolution of identity. First, we built the model with a self-orthogonal bound state which however is essentially entangled with the lower end of the continuous spectrum. As a consequence, the self-orthogonality does not lead to infinite average values of observables like kinetic or potential energies if these averages are treated with the help of wave packet regularization.

Conventionally, the continuous spectrum physics deals with reflection and transmission coefficients whose definition implies the existence of two linearly independent scattering solutions for a given spectral parameter. The second model provides an example when this is not realized for a non-Hermitian Hamiltonian defined on the whole axis.

6.1. Non-Hermitian Hamiltonian with normalizable bound state at the continuum threshold

Let us now consider the Hamiltonian

$$h = -\partial^2 + \frac{2}{(x-z)^2}, \qquad \operatorname{Im} z \neq 0. \tag{62}$$

The eigenfunctions of h for the continuous spectrum can be explicitly found,

$$\psi(x;k) = \frac{1}{\sqrt{2\pi}}\left[1 - \frac{1}{\mathrm{i}k(x-z)}\right]\mathrm{e}^{\mathrm{i}kx}, \qquad k \in \mathbb{R}\backslash\{0\}, \qquad h\psi(x;k) = k^2\psi(x;k). \tag{63}$$

In addition, there is a normalizable eigenfunction of h at the threshold of the continuous spectrum,

$$\psi_0(x) = \frac{1}{(x-z)} = -\sqrt{2\pi}\lim_{k\to 0}[\mathrm{i}k\psi(x;k)], \qquad h\psi_0 = 0. \tag{64}$$

Evidently, the eigenfunctions of h satisfy the biorthogonality relations,

$$\int_{-\infty}^{+\infty}[\mathrm{i}k\psi(x;k)][-\mathrm{i}k'\psi(x;-k')]\,\mathrm{d}x = k^2\delta(k-k'), \tag{65}$$

where the bound state wavefunction is included at the bottom of the continuous spectrum due to (64). Thus, this very eigenfunction has a zero binorm:

$$\int_{-\infty}^{+\infty} \psi_0^2(x)\,\mathrm{d}x = 0, \tag{66}$$

raising up the puzzle of 'self-orthogonality' [28].

In order to unravel this puzzle, we examine the resolution of identity made of eigenfunctions of h:

$$\delta(x - x') = \int_{\mathcal{L}} \psi(x; k)\psi(x'; -k)\,\mathrm{d}k, \tag{67}$$

where the contour $\mathcal{L}$ must be a proper integration path in the complex k-plane which allows us to regularize the singularity in (63) for $k = 0$, for instance, an integration path, obtained from the real axis by its displacement near the point $k = 0$ up or down.

To reach an adequate definition of the resolution of identity, one can instead use the Newton–Leibnitz formula and rewrite (67) in the form

$$\begin{aligned}\delta(x - x') = {} & \left(\int_{-\infty}^{-\varepsilon} + \int_{\varepsilon}^{+\infty}\right) \psi(x; k)\psi(x'; -k)\,\mathrm{d}k \\ & - \frac{\psi_0(x)\psi_0(x')}{\pi\varepsilon} + \frac{\sin\varepsilon(x - x')}{\pi(x - x')} + \frac{2\sin^2\left[\frac{\varepsilon}{2}(x - x')\right]}{\pi\varepsilon(x - x_0)(x' - x_0)}, \qquad \varepsilon > 0.\end{aligned} \tag{68}$$

One can show that the limit of the third term on the right-hand side of (68) (as a distribution function) at $\varepsilon \downarrow 0$ is zero for any test function from $C_{\mathbb{R}}^{\infty} \cap L^2(\mathbb{R})$, but the limit of the last term on the right-hand side of (68) for $\varepsilon \downarrow 0$ is zero only for test functions from $C_{\mathbb{R}}^{\infty} \cap L^2(\mathbb{R}; |x|^{\gamma}), \gamma > 1$. Thus, for test functions from $C_{\mathbb{R}}^{\infty} \cap L^2(\mathbb{R}; |x|^{\gamma}), \gamma > 1$, the resolution of identity can be reduced to

$$\delta(x - x') = \lim_{\varepsilon\downarrow 0}\left[\left(\int_{-\infty}^{-\varepsilon} + \int_{\varepsilon}^{+\infty}\right) \psi(x; k)\psi(x'; -k)\,\mathrm{d}k - \frac{\psi_0(x)\psi_0(x')}{\pi\varepsilon}\right], \tag{69}$$

and for test functions from $C_{\mathbb{R}}^{\infty} \cap L^2(\mathbb{R})$ to

$$\begin{aligned}\delta(x - x') = \lim_{\varepsilon\downarrow 0}\Bigg\{ & \left(\int_{-\infty}^{-\varepsilon} + \int_{\varepsilon}^{+\infty}\right) \psi(x; k)\psi(x'; -k)\,\mathrm{d}k \\ & - \frac{1}{\pi\varepsilon}\left[1 - 2\sin^2\left(\frac{\varepsilon}{2}(x - x')\right)\right]\psi_0(x)\psi_0(x')\Bigg\}.\end{aligned} \tag{70}$$

Decomposition (69) seems to have a more natural form than (70), but its right-hand side obviously cannot reproduce the *normalizable* eigenfunction

$$\psi_0(x) \notin C_{\mathbb{R}}^{\infty} \cap L^2(\mathbb{R}; |x|^{\gamma}), \qquad \gamma > 1$$

because of the orthogonality relations (65). Indeed, the identity holds

$$\lim_{\varepsilon\downarrow 0}\int_{-\infty}^{+\infty} \frac{2}{\pi\varepsilon}\sin^2\left(\frac{\varepsilon}{2}(x - x')\right)\psi_0^2(x)\psi_0(x')\,\mathrm{d}x = \lim_{\varepsilon\downarrow 0}[\mathrm{e}^{-\mathrm{i}\varepsilon x'}\psi_0(x')] = \psi_0(x'). \tag{71}$$

Hence, it is the third term on the right-hand side of (70) that provides the opportunity to reproduce $\psi_0(x)$ and thereby to complete the resolution of identity. Thus, one concludes that the state $\psi_0(x)$ is inseparable from the bottom of the continuous spectrum and the resolution of identity in this sense is not diagonal.

We note that the Hamiltonian (62) is PT-symmetric and can be derived from the Hamiltonian (34) in the limit $\alpha \to 0$, but the parameter z must be taken as a half of z from (34).

We also remark that the Hamiltonian (62) makes sense also for arbitrary coupling constants of 'centrifugal' potential, and for the following set,

$$h = -\partial^2 + \frac{n(n+1)}{(x-z)^2}, \tag{72}$$

with positive n, the Jordan cell, spanned by $\left[\frac{n+1}{2}\right]$ normalizable eigenfunction and associated functions, appears at the threshold of the continuous spectrum,

$$h\psi_0 = 0, \qquad h\psi_j = \psi_{j-1}, \qquad j = 0, \ldots, \left[\frac{n-1}{2}\right],$$
$$\psi_j(x) = \frac{(2(n-j)-1)!!}{(2j)!!(2n-1)!!(x-z)^{n-2j}}. \tag{73}$$

All these zero-energy bound and associated states have zero binorms and are biorthogonal to each other (the multiple puzzle of 'self-orthogonality'). The resolution of identity in such cases can be derived in a similar way although its form will be more cumbersome.

6.2. Expectation values (e.v.) of kinetic and potential energies in the vicinity of zero–energy bound state

As the binorm of the bound state (64) vanishes, it seems that the quantum averages of basic observables like the kinetic K or potential V energy in this system described by the Hamiltonian (62) $h = K + V$ tend to diverge. But it is, in fact, not the case. Indeed, the e.v.'s of these observables vanish as well:

$$h\psi_0(x) = 0, \qquad \langle\tilde{\psi}_0|V|\psi_0\rangle = -\langle\tilde{\psi}_0|K|\psi_0\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \frac{2}{(x-z)^4} = 0. \tag{74}$$

Thus, one comes to the classical uncertainty of 0/0 type. In order to unravel it, one has to build a wave packet which reproduces the function ψ_0 in the limit of its form parameters. We choose the Gaussian wave packet,

$$\psi_\epsilon(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{\sqrt{\pi\epsilon}} \left(-\mathrm{i}k + \frac{1}{x-z}\right) \exp\left(\mathrm{i}kx - \frac{k^2}{\epsilon}\right)$$
$$= \left(-\partial + \frac{1}{x-z}\right) \exp\left(-\epsilon\frac{x^2}{4}\right) = \left(\epsilon\frac{x}{2} + \frac{1}{x-z}\right) \exp\left(-\epsilon\frac{x^2}{4}\right), \tag{75}$$

which evidently approaches uniformly ψ_0 when $\epsilon \downarrow 0$. The binorm of this wave packet,

$$\langle\tilde{\psi}_\epsilon|\psi_\epsilon\rangle = \sqrt{\frac{\pi}{8}}\epsilon^{1/2}, \tag{76}$$

rapidly vanishes when $\epsilon \downarrow 0$.

In turn the e.v. of the total energy,

$$\langle\tilde{\psi}_\epsilon|H|\psi_\epsilon\rangle = \sqrt{\frac{9\pi}{128}}\epsilon^{3/2}, \tag{77}$$

decreases with $\epsilon \downarrow 0$ faster than the normalization (76). The e.v. of the potential energy,

$$\langle\tilde{\psi}_\epsilon|V|\psi_\epsilon\rangle = -\sqrt{\frac{25\pi}{36}}\epsilon^{3/2}, \tag{78}$$

behaves as the total energy and therefore the e.v. for the kinetic energy decreases also as $\epsilon^{3/2}$, much faster than the binorm (76). Thus, one concludes that their ratios, i.e. the quantum averages of the kinetic and potential energies, vanish for the self-orthogonal bound state in contrast to the superficial divergence. Therefore, the puzzle with self-orthogonality is resolved.

6.3. Hamiltonian with bound state in continuum

Let us force the bound state energy $-\alpha^2$ in the Hamiltonian (34) to move towards the continuous spectrum, $\alpha \to i\alpha$. Then for the Hamiltonian,

$$h = -\partial^2 + 16\alpha^2 \frac{\alpha(x-z)\sin(2\alpha x) + 2\cos^2(\alpha x)}{[\sin(2\alpha x) + 2\alpha(x-z)]^2}, \qquad \alpha > 0, \qquad z \in \mathbb{C}, \qquad \operatorname{Im} z \neq 0, \tag{79}$$

on the level $\lambda_1 = \alpha^2$ in the continuous spectrum, one finds the Jordan cell, spanned by the normalizable eigenfunction $\psi_0(x)$ and the associated function $\psi_1(x)$, whose asymptotics for $x \to \pm\infty$ correspond to superposition of incoming and outgoing waves (standing wave),

$$\psi_0(x) = \frac{\cos(\alpha x)}{\sin(2\alpha x) + 2\alpha(x-z)}, \qquad \psi_1(x) = \frac{2\alpha(x-z)\sin(\alpha x) + \cos(\alpha x)}{4\alpha^2[\sin(2\alpha x) + 2\alpha(x-z)]}, \tag{80}$$

$$h\psi_0 = \lambda_1\psi_0, \qquad (h - \lambda_1)\psi_1 = \psi_0. \tag{81}$$

The asymptotics of the associated state is given by the standing wave,

$$\psi_1(x) = \frac{i}{8\alpha^2}[e^{-i\alpha x} - e^{i\alpha x}] + O\left(\frac{1}{x}\right), \qquad x \to \pm\infty,$$

but it does not appear in the resolution of identity (see below). Thereby, this associated state does not belong to the physical state space.

In turn, the eigenfunctions of h for the scattering spectrum read

$$\psi(x;k) = \frac{1}{\sqrt{2\pi}}\left[1 + \frac{ik}{k^2-\alpha^2}\frac{W'(x)}{W(x)} - \frac{1}{2(k^2-\alpha^2)}\frac{W''(x)}{W(x)}\right]e^{ikx},$$
$$k \in \mathbb{R}\backslash\{\alpha, -\alpha\}, \qquad h\psi(x;k) = k^2\psi(x;k), \qquad W(x) = \sin(2\alpha x) + 2\alpha(x-z). \tag{82}$$

Then one can check that the eigenfunctions and associated functions of h obey the relations

$$\int_{-\infty}^{+\infty} [(k^2-\alpha^2)\psi(x;k)][((k')^2-\alpha^2)\psi(x;-k')]\,dx = (k^2-\alpha^2)^2\delta(k-k'),$$
$$\int_{-\infty}^{+\infty} \psi_0(x)\psi_1(x)\,dx = 0, \qquad \int_{-\infty}^{+\infty} \psi_1(x)\psi(x;k)\,dx = 0. \tag{83}$$

The last equation is understood in the sense of distributions. The limit of $\psi(x;k)$ at $k \to \mp\alpha$ gives the elements of the Jordan cell $\psi_0(x)$ and $\psi_1(x)$,

$$\lim_{k\to\mp\alpha}[(k^2-\alpha^2)\psi(x;k)] = \mp\frac{4i\alpha^2}{\sqrt{2\pi}}\psi_0(x), \tag{84}$$

$$\lim_{k\to\mp\alpha}\left[\frac{1}{2k}\frac{\partial}{\partial k}((k^2-\alpha^2)\psi(x;k))\right] = \mp\frac{4\,i\alpha^2}{\sqrt{2\pi}}\left[\psi_1(x) + \frac{1 \mp 2i\alpha z}{4\alpha^2}\psi_0(x)\right]. \tag{85}$$

For this model, the resolution of identity made of eigenfunctions and associated functions of h can be obtained by conventional Green function methods,

$$\delta(x-x') = \int_{\mathcal{L}} \psi(x;k)\psi(x';-k)\,dk, \tag{86}$$

where $\mathcal{L}$ is an integration path in the complex momentum plane, obtained from real axis by its simultaneous displacement near the points $k = \pm\alpha$ up or down.

For test functions from $C_{\mathbb{R}}^{\infty} \cap L^2(\mathbb{R}; |x|^{\gamma}), \gamma > 1$, this resolution of identity can be presented in the form

$$\delta(x-x') = \lim_{\varepsilon \downarrow 0} \left[\left(\int_{-\infty}^{-\alpha-\varepsilon} + \int_{-\alpha+\varepsilon}^{\alpha-\varepsilon} + \int_{\alpha+\varepsilon}^{+\infty} \right) \psi(x;k)\psi(x';-k)\,\mathrm{d}k - \frac{1}{\pi\varepsilon\alpha}\psi_0(x)\psi_0(x') \right], \tag{87}$$

and for test functions from $C_{\mathbb{R}}^{\infty} \cap L^2(\mathbb{R})$ it must be extended,

$$\delta(x-x') = \lim_{\varepsilon \downarrow 0} \left\{ \left(\int_{-\infty}^{-\alpha-\varepsilon} + \int_{-\alpha+\varepsilon}^{\alpha-\varepsilon} + \int_{\alpha+\varepsilon}^{+\infty} \right) \psi(x;k)\psi(x';-k)\,\mathrm{d}k - \frac{1}{\pi\varepsilon\alpha}\left[1 - 2\sin^2\left(\frac{\varepsilon}{2}(x-x')\right)\right]\psi_0(x)\psi_0(x') \right\} \tag{88}$$

(cf with (70)). One can see that operator (87) projects away the *normalizable* eigenfunction

$$\psi_0(x) \notin C_{\mathbb{R}}^{\infty} \cap L^2(\mathbb{R}; |x|^{\gamma}), \qquad \gamma > 1,$$

because of the orthogonality relations (83). Meanwhile, operator (88) is complete and acts on this eigenfunction as an identity. Thus, one concludes again that the state $\psi_0(x)$ is inseparable from the continuous spectrum and the resolution of identity in this sense is not diagonal.

7. Resolvents and scattering characteristics

The peculiar spectral properties and the specific pattern of level degeneracy for non-diagonalizable Hamiltonians have interesting consequences for the structure of their resolvents and scattering matrices.

In all the above examples the Green functions can be calculated conventionally, as follows:

$$G(x,x';\lambda) = \frac{\pi \mathrm{i}}{\sqrt{\lambda}}\psi(x_>;\sqrt{\lambda})\psi(x_<;-\sqrt{\lambda}), \qquad x_> = \max\{x,x'\}, \qquad x_< = \min\{x,x'\}, \tag{89}$$

where the solutions ψ are made by analytical continuation of $\psi(x;k)$ in k into the complex plane, and the branch of $\sqrt{\lambda}$ is uniquely defined by the condition $\mathrm{Im}\sqrt{\lambda} \geqslant 0$ in the plane with the cut on the positive part of the real axis. In virtue of (58) the Green function for the diagonalizable Hamiltonian of subsection 5.2 has two poles of the first order (if $\beta \neq 0$) at the points $\lambda = -(\alpha \pm \beta)^2$, where α can be either real or imaginary. If $\beta \to 0$ and level confluence emerges, two poles coalesce into one pole of the second order in both cases (37) and (82) when $\lambda = \mp|\alpha|^2$. However, the examples of subsections 5.1 and 6.2 have different meaning: in the first case, the double pole does not appear on the physical cut $\lambda > 0$ and its order enumerates the rank of the Jordan cell. In contrast, in the second case the double pole is placed exactly on the cut $\lambda > 0$ and strictly speaking signifies the spectral pathology as it generates only one eigenstate with the eigenvalue $\lambda = |\alpha|^2$ in resolution of identity. The second state—the associated function—represents a standing wave and does not influence the spectral decomposition. In the example of subsection 6.1, the Green function has only a branch point at $\lambda = 0$ of the following type $\lambda^{-3/2}$. This branch point can be thought of as a confluence of the double pole in the variable $\sqrt{\lambda}$ and the branch point of order $\lambda^{-1/2}$.

From the explicit form of wavefunctions, one can see that all potentials in sections 5 and 6 are transparent as the reflection coefficient is zero. The transmission coefficient in the non-degenerate case of subsection 5.2 takes the form

$$T(k) = \begin{cases} \frac{\beta^2+(k+\mathrm{i}\alpha)^2}{\beta^2+(k-\mathrm{i}\alpha)^2}, & 0 < \beta < \alpha, \\ \frac{\alpha^2+(k+\mathrm{i}\beta)^2}{\alpha^2+(k-\mathrm{i}\beta)^2}, & -\mathrm{i}\alpha > 0. \end{cases} \tag{90}$$

In different limits, one can derive the transmission coefficients for three other Hamiltonians. Namely, when $\beta \to 0$ and $\alpha > 0$ (subsections 5.1), the scattering is described by

$$T(k) = \left(\frac{k + \mathrm{i}\alpha}{k - \mathrm{i}\alpha}\right)^2, \tag{91}$$

and for $\beta \to 0$ and $\alpha \to 0$ or imaginary (subsections 6.1 and 6.2) the scattering is absent,

$$T(k) = 1. \tag{92}$$

Thus, the colliding particle in such cases is not 'influenced' by the bound states in the continuum.

8. Conclusions

In this paper we have presented a thorough analysis of the phenomenon of apparent self-orthogonality of some eigenstates for non-Hermitian Hamiltonians. For the discrete part of an energy spectrum, it has been shown that such a phenomenon should take place only for non-diagonalizable Hamiltonians, the spectrum of which consists not only of eigenfunctions but also of associated functions. However, the genuine *diagonal* biorthogonal basis related to the spectral decomposition of such Hamiltonians normally does not contain pairs made of the same eigenfunctions or the associated functions of the same order. Rather they are complementary; for instance, the eigenfunctions in the direct basis are paired to those associated functions in the conjugated basis, which have the maximal order in the same Jordan cell. One possible exception exists for the Jordan cells of odd order where one basis pair consists of the same function which is *not* self-orthogonal.

The situation in the continuous spectrum is more subtle, namely, the spectral decomposition does not include any obvious Jordan cells and associated functions. However, we have established that when a zero-binorm normalizable state arises it remains inseparable from the nearest scattering states of the continuum and eventually the existence of this state does not destroy the completeness of the resolution of identity.

Finally, let us outline the measurability of quantum observables and, for this purpose, prepare a wave packet,

$$|\psi\rangle = \sum\!\!\!\!\!\!\int_r C_r |\psi_r\rangle, \qquad C_r = \text{const}, \tag{93}$$

where the possibility of having a continuous spectrum is made explicit in the notation and, for brevity, all indices enumerating eigenvalues, Jordan cells and their elements are encoded in the index $r \equiv \{n, a, j\}$.

In order to perform the quantum averaging of an operator of observable O, one can use the conventional Hilbert space scalar product and the complex-conjugated wavefunction, $\langle\psi|x\rangle = \langle x|\psi\rangle^*$. In this way one defines the wave packet of the conjugated state and, respectively, the average values of the operator O:

$$\langle\psi| = \sum\!\!\!\!\!\!\int_r C_r^* \langle\psi_r|, \qquad \overline{O} = \frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle}, \tag{94}$$

so that the average values $\overline{O}$ remain finite as $\langle\psi|\psi\rangle > 0$.

On the other hand, the use of *complete* biorthogonal bases $\{|\psi_r\rangle, \langle\tilde{\psi}_r|\}$ from section 3 (or $\{|\psi_r\rangle, \langle\hat{\psi}_r|\}$ from section 4) seems to be more suitable to describe a non-Hermitian evolution. Accordingly, to supply the wave packet binorm with a probabilistic meaning one may introduce [18] the wave packet partner in respect to a binorm with complex-conjugated coefficients, in order that its binorm was always positive,

$$\langle\tilde{\psi}| \equiv \sum\!\!\!\!\!\!\int_r C_r^* \langle\tilde{\psi}_r|, \qquad \langle\tilde{\psi}|\psi\rangle = \sum\!\!\!\!\!\!\int_r C_r^* C_r > 0. \tag{95}$$

For such a definition, the averages of an operator of the observable $\widetilde{\widetilde{O}} = \langle\tilde{\psi}|O|\psi\rangle/\langle\tilde{\psi}|\psi\rangle$ cannot be infinite and the phenomena of (pseudo) phase transitions at the level crossing [28] cannot appear. In this relation, the basis from section 4 with $\langle\hat{\psi}_r|$ may be used equally well.

However, one has to keep in mind that such a definition of probabilities, to some extent, depends on a particular set of biorthogonal bases. We hope to examine this approach and its applications elsewhere.

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Appendix

Let $CL_\gamma = C_{\mathbb{R}}^\infty \cap L_2(\mathbb{R}; |x|^\gamma), \gamma \geqslant 0$, be the space of test functions. The sequence $\varphi_n(x) \in CL_\gamma$ is called convergent in CL_γ to $\varphi(x) \in CL_\gamma$,

$$\lim_{n\to+\infty}{}_\gamma \; \varphi_n(x) = \varphi(x) \tag{A.1}$$

if

$$\lim_{n\to+\infty} \int_{-\infty}^{+\infty} |\varphi_n(x) - \varphi(x)|^2 |x|^\gamma \, \mathrm{d}x = 0, \tag{A.2}$$

and for any $x_1, x_2 \in \mathbb{R}, x_1 < x_2$,

$$\lim_{n\to+\infty} \max_{[x_1,x_2]} |\varphi_n(x) - \varphi(x)| = 0. \tag{A.3}$$

We shall denote the value of a functional f on $\varphi \in CL_\gamma$ conventionally as (f, φ). A functional f is called continuous if for any sequence $\varphi_n \in CL_\gamma$ convergent in CL_γ to zero the equality ,

$$\lim_{n\to+\infty} (f, \varphi_n) = 0, \tag{A.4}$$

is valid. The space of distributions over CL_γ, i.e. of linear continuous functionals over CL_γ is denoted as CL'_γ. The sequence $f_n \in CL'_\gamma$ is called convergent in CL'_γ to $f \in CL_\gamma$,

$$\lim_{n\to+\infty}{}'_\gamma \; f_n = f, \tag{A.5}$$

if for any $\varphi \in CL_\gamma$ the relation takes place,

$$\lim_{n\to+\infty} (f_n, \varphi) = (f, \varphi). \tag{A.6}$$

A functional $f \in CL'_\gamma$ is called regular if there is $f(x) \in L_2(\mathbb{R}; (1+|x|^\gamma)^{-1})$ such that for any $\varphi \in CL_\gamma$ the equality

$$(f, \varphi) = \int_{-\infty}^{+\infty} f(x)\varphi(x)\,\mathrm{d}x \tag{A.7}$$

holds. In this case we shall identify the distribution $f \in CL'_\gamma$ with the function $f(x) \in L_2(\mathbb{R}; (1+|x|^\gamma)^{-1})$. In virtue of the Bunyakovskii inequality,

$$\left|\int_{-\infty}^{+\infty} f(x)\varphi(x)\,\mathrm{d}x\right|^2 \leqslant \int_{-\infty}^{+\infty} \frac{|f^2(x)|\,\mathrm{d}x}{1+|x|^\gamma} \int_{-\infty}^{+\infty} |\varphi^2(x)|(1+|x|^\gamma)\,\mathrm{d}x, \tag{A.8}$$

it is evident that $L_2(\mathbb{R}; (1+|x|^\gamma)^{-1}) \subset CL'_\gamma$.

Let us also note that the Dirac delta function $\delta(x-x')$ belongs to CL'_γ, $\gamma \geqslant 0$.

Lemma 1. *Suppose that (1)*

$$\psi(x;k) = \frac{1}{\sqrt{2\pi}}\left[1 - \frac{1}{\mathrm{i}k(x-z)}\right]\mathrm{e}^{\mathrm{i}kx};$$

(2) $\mathcal{L}(A)$ is a path in the complex plane of k, made of the segment $[-A, A]$ of the real axis by deformation of its central part up or down of zero and the positive direction of $\mathcal{L}(A)$ is specified from $-A$ to A and (3) $x' \in \mathbb{R}$, $\gamma \geqslant 0$, $\varepsilon > 0$. Then the following relations hold:

$$\mathop{\lim\nolimits'_\gamma}_{A\to+\infty} \int_{\mathcal{L}(A)} \psi(x;k)\psi(x';-k)\,\mathrm{d}k = \delta(x-x'), \tag{A.9}$$

$$\mathop{\lim\nolimits'_\gamma}_{A\to+\infty} \left(\int_{-A}^{-\varepsilon} + \int_{\varepsilon}^{A}\right) \psi(x;k)\psi(x';-k)\,\mathrm{d}k = \delta(x-x') - \int_{\mathcal{L}(\varepsilon)} \psi(x;k)\psi(x';-k)\,\mathrm{d}k. \tag{A.10}$$

Proof. In accordance with the Newton–Leibnitz formula, one obtains

$$\int_{\mathcal{L}(A)} \psi(x;k)\psi(x';-k)\,\mathrm{d}k = \frac{1}{\pi}\left[\frac{\sin A(x-x')}{x-x'} - \frac{\cos A(x-x')}{A(x-z)(x'-z)}\right]. \tag{A.11}$$

Integral (A.11) as a function of x belongs to $L_2(\mathbb{R}; (1+|x|^\gamma)^{-1})$ and therefore to CL'_γ. Thus, to prove (A.9) it is sufficient to establish that for any $\varphi(x) \in CL_\gamma$ the equality takes place,

$$\lim_{A\to+\infty} \frac{1}{\pi}\int_{-\infty}^{+\infty}\left[\frac{\sin A(x-x')}{x-x'} - \frac{\cos A(x-x')}{A(x-z)(x'-z)}\right]\varphi(x)\,\mathrm{d}x = \varphi(x'). \tag{A.12}$$

By virtue of the Bunyakovskii inequality

$$\left|\int_{-\infty}^{+\infty} \frac{\cos A(x-x')}{A(x-z)(x'-z)}\varphi(x)\,\mathrm{d}x\right|^2 \leqslant \frac{1}{A^2}\int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{|x-z|^2|x'-z|^2} \int_{-\infty}^{+\infty} |\varphi^2(x)|\,\mathrm{d}x, \tag{A.13}$$

wherefrom it follows that

$$\begin{aligned}\lim_{A\to+\infty} \frac{1}{\pi}\int_{-\infty}^{+\infty}&\left[\frac{\sin A(x-x')}{x-x'} - \frac{\cos A(x-x')}{A(x-z)(x'-z)}\right]\varphi(x)\,\mathrm{d}x \\ &= \lim_{A\to+\infty} \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\sin A(x-x')}{x-x'}\varphi(x)\,\mathrm{d}x.\end{aligned} \tag{A.14}$$

In virtue of the Riemann theorem and due to the evident inclusions

$$\frac{\varphi(x)}{x-x'} \in L_1(\mathbb{R}\backslash]x'-\delta, x'+\delta[), \qquad \frac{\varphi(x)-\varphi(x')}{x-x'} \in L_1([x'-\delta, x'+\delta])$$

for any $\delta > 0$, the following relations are valid:

$$\lim_{A\to+\infty}\left(\int_{-\infty}^{x'-\delta}+\int_{x'+\delta}^{+\infty}\right)\sin A(x-x')\frac{\varphi(x)}{x-x'}\,\mathrm{d}x = 0,$$
$$\lim_{A\to+\infty}\int_{x'-\delta}^{x'+\delta}\sin A(x-x')\frac{\varphi(x)-\varphi(x')}{x-x'}\,\mathrm{d}x = 0. \tag{A.15}$$

Hence,

$$\lim_{A\to+\infty}\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\sin A(x-x')}{x-x'}\varphi(x)\,\mathrm{d}x = \frac{\varphi(x')}{\pi}\lim_{A\to+\infty}\int_{x'-\delta}^{x'+\delta}\frac{\sin A(x-x')}{x-x'}\,\mathrm{d}x = \varphi(x')$$

and in view of (A.14) equations (A.12) and (A.9) hold. equation (A.10) follows from equation (A.9) and from additivity of classical path integrals. Lemma 1 is proved. □

Lemma 2. *For any $x' \in \mathbb{R}$ and $\gamma \geqslant 0$, the relation*

$$\mathop{\mathrm{lim}'_{\gamma}}_{\varepsilon\downarrow 0}\frac{\sin\varepsilon(x-x')}{x-x'} = 0, \qquad \gamma \geqslant 0, \tag{A.16}$$

takes place.

Proof. It is true that

$$\frac{\sin\varepsilon(x-x')}{x-x'} \in L_2(\mathbb{R}; (1+|x|^{\gamma})^{-1}) \subset CL'_{\gamma}, \qquad \gamma \geqslant 0.$$

Thus, to prove the lemma it is sufficient to establish that for any $\varphi(x) \in CL_{\gamma}, \gamma \geqslant 0$, the relation

$$\lim_{\varepsilon\downarrow 0}\int_{-\infty}^{+\infty}\frac{\sin\varepsilon(x-x')}{x-x'}\varphi(x)\,\mathrm{d}x = 0 \tag{A.17}$$

is valid. But its validity follows from the Bunyakovskii inequality:

$$\left|\int_{-\infty}^{+\infty}\frac{\sin\varepsilon(x-x')}{x-x'}\varphi(x)\,\mathrm{d}x\right|^2 \leqslant \int_{-\infty}^{+\infty}\frac{\sin^2\varepsilon(x-x')}{(x-x')^2}\,\mathrm{d}x\int_{-\infty}^{+\infty}|\varphi^2(x)|\,\mathrm{d}x$$
$$= \varepsilon\int_{-\infty}^{+\infty}\frac{\sin^2\tau}{\tau^2}\,\mathrm{d}\tau\int_{-\infty}^{+\infty}|\varphi^2(x)|\,\mathrm{d}x \to 0, \qquad \varepsilon\downarrow 0. \tag{A.18}$$

Lemma 2 is proved. □

Lemma 3. *For any $z \in \mathbb{C}$, $\mathrm{Im}\, z \neq 0$, $x' \in \mathbb{R}$ and $\gamma > 1$, the following relation holds,*

$$\mathop{\mathrm{lim}'_{\gamma}}_{\varepsilon\downarrow 0}\frac{\sin^2\left[\frac{\varepsilon}{2}(x-x')\right]}{\varepsilon(x-z)(x'-z)} = 0, \qquad \gamma > 1. \tag{A.19}$$

Proof. It is evident that

$$\frac{\sin^2\left[\frac{\varepsilon}{2}(x-x')\right]}{\varepsilon(x-z)(x'-z)} \in L_2(\mathbb{R}; (1+|x|^{\gamma})^{-1}) \subset CL'_{\gamma}, \qquad \gamma > 1.$$

Thus, to prove the lemma it is sufficient to establish that for any $\varphi(x) \in CL_{\gamma}, \gamma > 1$, the equality

$$\lim_{\varepsilon\downarrow 0}\int_{-\infty}^{+\infty}\frac{\sin^2\left[\frac{\varepsilon}{2}(x-x')\right]}{\varepsilon(x-z)(x'-z)}\varphi(x)\,\mathrm{d}x = 0 \tag{A.20}$$

holds. This equality can be obtained from the chain of inequalities

$$\left|\int_{-\infty}^{+\infty}\frac{\sin^2\left[\frac{\varepsilon}{2}(x-x')\right]}{\varepsilon(x-z)(x'-z)}\varphi(x)\,\mathrm{d}x\right|^2 \leqslant \int_{-\infty}^{+\infty}\frac{\sin^4\left[\frac{\varepsilon}{2}(x-x')\right]\mathrm{d}x}{\varepsilon^2|x-z|^2|x'-z|^2(1+|x|^\gamma)}$$
$$\times\int_{-\infty}^{+\infty}|\varphi^2(x)|(1+|x|^\gamma)\,\mathrm{d}x \leqslant \int_{-\infty}^{+\infty}\frac{(\varepsilon/2)^{2+\min\{2,(\gamma-1)/2\}}|x-x'|^{2+\min\{2,(\gamma-1)/2\}}\,\mathrm{d}x}{\varepsilon^2|x-z|^2|x'-z|^2(1+|x|^\gamma)}$$
$$\times\int_{-\infty}^{+\infty}|\varphi^2(x)|(1+|x|^\gamma)\,\mathrm{d}x \to 0, \qquad \varepsilon\downarrow 0, \tag{A.21}$$

derived with the help of the Bunyakovskii inequality and trivial inequalities $|\sin\tau| \leqslant 1$, $|\sin\tau| \leqslant |\tau|$, $\tau\in\mathbb{R}$. Lemma 3 is proved. □

Corollary 1. *Let us define*

$$\int_{\mathcal{L}}\psi(x;k)\psi(x';-k)\,\mathrm{d}k = \lim_{A\to+\infty}{}'_{\gamma}\int_{\mathcal{L}(A)}\psi(x;k)\psi(x';-k)\,\mathrm{d}k, \tag{A.22}$$

where $\mathcal{L}$ is a path, made by deformation of the real axis near zero up or down. Then in view of (A.9) the resolution of identity (67) holds.

Corollary 2. *Using the Newton–Leibnitz formula, one can rewrite the integral $\int_{\mathcal{L}(\varepsilon)}\psi(x;k)\psi(x';-k)\,\mathrm{d}k$ in the form*

$$\int_{\mathcal{L}(\varepsilon)}\psi(x;k)\psi(x';-k)\,\mathrm{d}k = -\frac{1}{\pi\varepsilon(x-z)(x'-z)} + \frac{\sin\varepsilon(x-x')}{\pi(x-x')} + \frac{2\sin^2\left[\frac{\varepsilon}{2}(x-x')\right]}{\pi\varepsilon(x-z)(x'-z)}. \tag{A.23}$$

Thus, if by definition

$$\left(\int_{-\infty}^{-\varepsilon}+\int_{\varepsilon}^{+\infty}\right)\psi(x;k)\psi(x';-k)\,\mathrm{d}k = \lim_{A\to+\infty}{}'_{\gamma}\left(\int_{-A}^{-\varepsilon}+\int_{\varepsilon}^{A}\right)\psi(x;k)\psi(x';-k)\,\mathrm{d}k, \tag{A.24}$$

then due to equations (A.10), (A.16), (A.19) and (A.23), the resolutions of identity (69) and (70) are valid.

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