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ABSTRACT

In this article, we review the quantum mechanical setting associated with a non-self-adjoint Hamiltonian with a real spectrum. The spectral properties of the Hamiltonian of a Swanson-like model are investigated. The eigenfunctions associated with the real simple eigenvalues are shown to form complete systems but not a (Riesz) basis, which gives rise to difficulties in the rigorous mathematical formulation of quantum mechanics. A new inner product, appropriate for the physical interpretation of the model, has been consistently introduced. The dynamics of the system is described. Some specificities of the theory of non-self-adjoint operators with implications in quantum mechanics are discussed.

I. INTRODUCTION

In non-relativistic quantum mechanics, the state of a particle is described, at the instant t, by a function $\Psi_t(x)$, where x denotes the particle coordinate. This function is called the *wave function*. Its time evolution is described by the time dependent *Schrödinger equation*,

$$i\frac{d\Psi_t(x)}{dt} = H\Psi_t(x),$$

where H is the *Hamiltonian operator* of the system. In most relevant cases, H acts on an infinite dimensional separable Hilbert space $\mathcal{H}$, endowed with the inner product $\langle\cdot,\cdot\rangle$ and the corresponding norm $\|\cdot\|$. Throughout, $\mathcal{D}(\cdot)$ will denote the domain of the operator under consideration. The fundamental axiom of conventional formulations of quantum mechanics is that H is *Hermitian* or, synonymously, *self-adjoint*. That is, for H^* the *adjoint operator*,

$$\langle Hf, g\rangle := \langle f, H^*g\rangle, \quad f \in \mathcal{D}(H), \quad g \in \mathcal{D}(H^*),$$

we have $H = H^*$ and $\mathcal{D}(H) = \mathcal{D}(H^*)$. In addition, the *observables* of the system are Hermitian, which ensures that the involved eigenvalues are real and the corresponding eigenfunctions can be taken orthonormal in such a way that they form a basis of the Hilbert space. As a consequence, meaningful properties on the dynamics of the system follow.

A formal solution of the time dependent Schrödinger equation, which rules the system dynamics, is given by

$$\Psi_t(x) = e^{-iHt}\Psi_0(x),$$

where $\Psi_0(x)$ is the wave function in the initial state $t = 0$. In conventional quantum mechanics,

$$\int_{x_1}^{x_2} \overline{\psi(x)}\psi(x)\mathrm{d}x$$

is the probability that the result of the physical measurement of the position, performed in the state $\psi(x)$, lies in the interval $[x_1, x_2]$. A simple consequence of the hermiticity of H is the invariance of the norm of the wave function with time, that is, $\|\Psi_t\|^2 = \|\Psi_0\|^2$, as $\exp(-iHt)$ is *unitary*. This property is physically important because it is related to the conservation of the number of particles of the system or of the probability of the position measurement. If the energy of a particle is measured in the state described by the wave function $\Psi(x)$, the *expectation value* of the measurement, in a statistical sense, is given by the *Rayleigh quotient*

$$E := \frac{\langle H\Psi, \Psi\rangle}{\langle \Psi, \Psi\rangle},$$

which is real if H is Hermitian.[1–3,7,9,11,13,18]

During the second half of the last century, energy states of atoms, molecules, and atomic nuclei have been usually described as eigenfunctions of self-adjoint *Schrödinger operators*. The publication of the seminal paper in 1998 by Bender and Boettcher on non-Hermitian Hamiltonians with PT-*symmetry*,[8] where P and T are, respectively, the *parity* (or *space reflexion*) and the *time reversal* operators

$$\mathrm{P}\Psi(x) := \Psi(-x), \quad \mathrm{T}\Psi(x) := \overline{\Psi(x)},$$

is a landmark. The development of PT-*symmetric quantum mechanics* was initiated, and a growing literature on PT-models found applications in different domains of physics.

Certain relativistic extensions of quantum mechanics lead naturally to non-Hermitian Hamiltonian operators, $H \neq H^*$. In this case, the Rayleigh quotient $\langle H\Psi, \Psi\rangle/\langle \Psi, \Psi\rangle$ does not provide the energy expectation value because in general it is not real, and the norm $\langle \exp(-iHt)\Psi_0, \exp(-iHt)\Psi_0\rangle$ may become time dependent, which is undesirable in the physical context. It became fundamental to investigate formulations of quantum mechanics for non-Hermitian Hamiltonian operators, mathematically consistent and physically meaningful. This objective has been the aim of intense research activity in the last two decades. We refer to Ref. 6 and references therein. New results opened new directions both in theoretical and experimental fronts, in classical and quantum domains. Non-Hermitian Hamiltonians having real spectra exhibit a pathological behavior. In Sec. I A, we illustrate the difficulties originated by these operators in the development of mathematically rigorous quantum theories.

A. Quasi-Hermitian (QM)

The problem of how to construct a consistent non-Hermitian quantum theory has been investigated, mainly inspired by the knowledge that PT symmetric Hamiltonians possess real spectra and allow for a unitary time evolution with a redefined inner product in the Hilbert space where the operator lives. A necessary condition for developing such a theory is obviously the reality of the spectrum of the Hamiltonian, $\sigma(H)$, but it is far from being sufficient. In this context, there have been attempts to develop the so called *quasi-Hermitian quantum mechanics*, where the Hamiltonian H is a *quasi-selfadjoint* operator, that is, which satisfies the quasi-selfadjointness operator relation

$$H^*\Theta = \Theta H, \tag{1}$$

with $\Theta = \mathrm{T}^*\mathrm{T}$ a positive, bounded, and boundedly invertible operator, called a *metric*. An operator H with the above property is actually Hermitian for the new inner product

$$\langle \phi, \psi\rangle := \langle \Theta\phi, \psi\rangle = \langle \mathrm{T}\phi, \mathrm{T}\psi\rangle,$$

that is,

$$\langle H\phi, \psi\rangle := \langle \Theta H\phi, \psi\rangle = \langle H^*\Theta\phi, \psi\rangle = \langle \Theta\phi, H\psi\rangle = \langle \phi, H\psi\rangle.$$

The concept of quasi-selfadjointness, which goes back to Dieudonné,[12] is of remarkable interest in the setup of non-Hermitian quantum mechanics. A modified inner product in the underlying Hilbert space, relatively to which H becomes self-adjoint via the similarity transformation THT^{-1},

$$\widetilde{H} = THT^{-1}, \tag{2}$$

where $\widetilde{H}$ is Hermitian, has been searched. If T is bounded and boundedly invertible, then the spectra of THT^{-1} and H coincide and the eigenfunctions share basis properties. Then, some fundamental issues of self-adjoint operators remain valid, such as spectral

stability with respect to perturbations, unitary evolution, etc. It is not very common to find in the literature non-self-adjoint models for which such a metric is constructed, neither the existence of a metric operator is guaranteed. Problems arise if T or T^{-1} are unbounded, such as it may happen that the eigenvalues of H are not preserved by the similarity transformation THT^{-1}, as argued in Ref. 16.

In the finite dimensional setting, all the involved operators are bounded. In particular, if T^{-1} exists it is automatically bounded, and the concepts of quasi-Hermiticity and similarity to a self-adjoint operator work without difficulty because we are dealing essentially with finite matrices. The adjoint of H is simply the transconjugate. If the Hamiltonian is Hermitian, the time evolution deduced from the Hamiltonian is unitary, and so it preserves the total probability of the system given by $\int|\Psi_t(x)|^2dx$.[6]

The rest of this note is organized as follows. In Sec. II, we consider a simple *Swanson-like* model[20] and review the general quantum mechanical setting associated with a non-self-adjoint Hamiltonian with a real spectrum. In Subsection II C, the matrix representation of the operator is investigated. In Sec. III, the spectral properties of the Hamiltonian are investigated. The eigenfunctions associated with the real simple eigenvalues are shown to form complete systems but not a Riesz basis. In Sec. IV, the dynamics of the system is described and a new inner product, which is appropriate for the physical interpretation, is consistently introduced. In Sec. V, some specificities of non-self-adjoint operators with implications in quantum mechanics are discussed and useful mathematical background in this context is pointed out.

II. A GENERALIZED HARMONIC OSCILLATOR

We will be concerned with a model on the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$ of square integrable functions in one real variable, endowed with the standard inner product

$$\langle\Phi_\alpha,\Phi_\beta\rangle = \int_{-\infty}^{+\infty}\Phi_\alpha(x)\overline{\Phi_\beta(x)}dx, \quad \Phi_\alpha,\Phi_\beta \in L^2(\mathbb{R}).$$

The system we wish to study is a very simple model of the *Swanson type*,[20] characterized by the following Hamiltonian operator on $L^2(\mathbb{R})$,

$$H := -\frac{1}{4}\frac{d^2}{dx^2} + x^2 - \gamma\left(\frac{1}{2} + x\frac{d}{dx}\right), \quad \gamma \in \mathbb{R}\backslash\{0\}, \quad |\gamma| \le 1. \tag{3}$$

Observe that, on $L^2(\mathbb{R})$,

$$H^* = -\frac{1}{4}\frac{d^2}{dx^2} + x^2 + \gamma\left(\frac{1}{2} + x\frac{d}{dx}\right)$$

so that $H \neq H^*$ for $\gamma \neq 0$. For $\gamma = 0$, it is obvious that $H = H^*$.

Most relevant operators in quantum mechanics are unbounded. Unboundedness of operators in the infinite dimensional setting unavoidably restricts their domains of definition to nontrivial subspaces of the Hilbert space. The real parameter γ must be carefully chosen so that the spectral theory of the operator can be developed in a rigorous mathematical framework. The real parameter γ, which *measures* the degree on non-Hermiticity of the Hamiltonian, is assumed to be non-zero to avoid the well-known Hermitian case. We will consider H as a perturbation of the famous *harmonic oscillator* H_{ho},

$$H_{ho} = -\frac{1}{4}\frac{d^2}{dx^2} + x^2,$$

which coincides with $\Re(H) = (H + H^*)/2$. For our purposes, we impose the condition of smallness of γ, $|\gamma| < 1$, in order to ensure that the non-Hermitian term $V = -\gamma\left(\frac{1}{2} + x\frac{d}{dx}\right)$ does not completely change the behavior of H_{ho}.

The domain $\mathcal{D}$ of H is

$$\mathcal{D} := \{\Psi(x) \in W^{1,2}(\mathbb{R}) : x^2\Psi(x) \in L^2(\mathbb{R})\}.$$

Here, $W^{1,2}(\mathbb{R})$ denotes the usual Sobolev space of functions on $L^2(\mathbb{R})$ whose weak first and second derivatives belong to $L^2(\mathbb{R})$. Observe that the domain contains the set $\widetilde{\mathcal{S}}$ of functions $f(x)$ such that $\exp(\gamma x^2)f(x) \in L^2(\mathbb{R})$,

$$\widetilde{\mathcal{S}} := \{\Psi(x) \in \mathcal{D} : e^{\gamma x^2}\Psi(x) \in L^2(\mathbb{R})\},$$

which is dense in $L^2(\mathbb{R})$ since it contains the set of all C^∞ functions with compact support. Thus, H is densely defined in this domain, which ensures the existence and uniqueness of its adjoint H^*. As $\Re(H)$ is closed, and V is relatively bounded with respect

to $\mathfrak{R}(H)$, with the relative bound smaller than 1, then H is closed (Ref. 14, Theorem 3.3). The closedness of H is a crucial starting point for the investigation of its spectrum because the spectrum is only meaningfully defined for closed operators. We will show that H has a purely discrete real spectrum if $|\gamma|$ is sufficiently small.

A. A basis of $L^2(\mathbb{R})$

We also consider the auxiliary operator $H_0 : \mathcal{D}(H_0) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R})$,

$$H_0 := -\frac{1}{4}\frac{d^2}{dx^2} + (1+\gamma^2)x^2, \tag{4}$$

with $\mathcal{D}(H_0) = \mathcal{D}$.

Notice that the following operator identity *formally* holds,

$$H_0 = e^{\gamma x^2} H e^{-\gamma x^2}, \tag{5}$$

in the sense that the operators in the left and in the right hand sides act in the same manner on any wave function $\Phi \in \mathcal{D}(H_0)$,

$$H_0\Phi(x) = e^{\gamma x^2} H e^{-\gamma x^2}\Phi(x).$$

The word "formal" refers to the fact that $\exp(\gamma x^2)$ is unbounded. We may also write the operator equality in (5) as

$$H = e^{-\gamma x^2} H_0 e^{\gamma x^2},$$

where it is implicitly assumed that the operators in both sides of the operator equality act on wave functions $\Psi(x) \in \widetilde{\mathcal{S}} \subset \mathcal{D}$. However, while H_0 goes from $\mathcal{S}(\mathbb{R})$ to $\mathcal{S}(\mathbb{R})$, with $\mathcal{S}(\mathbb{R})$ being the set of the C^∞ functions which decrease to zero, together with their derivatives, faster than any inverse power of x, H goes from $\widetilde{\mathcal{S}}$ to $\widetilde{\mathcal{S}}$.

The spectrum and eigenvectors of H_0 are easily obtained with the help of the *annihilation* bosonic operator

$$a := (1+\gamma^2)^{1/4} x + \frac{1}{2}\,\frac{1}{(1+\gamma^2)^{1/4}}\,\frac{d}{dx},$$

and its adjoint, the *creation* bosonic operator,

$$a^* := (1+\gamma^2)^{1/4} x - \frac{1}{2}\,\frac{1}{(1+\gamma^2)^{1/4}}\,\frac{d}{dx},$$

which satisfy the commutation relation

$$[a, a^*] = aa^* - a^*a = \mathbf{1},$$

where as usual, $\mathbf{1}$ denotes the identity operator. This means that $(aa^* - a^*a)\phi(x) = \phi(x)$ for all $\phi(x) \in \mathcal{D}$, which is stable under the action of a and a^* (that is, $a^*\mathcal{D} \subset \mathcal{D}$ and $a\mathcal{D} \subset \mathcal{D}$).

The factorization of H_0 in terms of the bosonic operators is straightforwardly obtained,

$$H_0 = \sqrt{1+\gamma^2}\; a^*a + \frac{1}{2}\sqrt{1+\gamma^2}\;\mathbf{1}.$$

The wave function

$$\Phi_0(x) = e^{-x^2/\sqrt{1+\gamma^2}} \in L^2(\mathbb{R})$$

satisfies $a\Phi_0 = 0$ and describes the so-called *groundstate* of H_0, as it is an eigenfunction of H_0 associated with the lowest eigenvalue,

$$E_0 = \frac{1}{2}\sqrt{1+\gamma^2}.$$

The wave function

$$\Phi_n(x) = a^{*\,n}\Phi_0(x),\ n \geq 0,$$

is an eigenfunction of H_0 and describes the so called nth *bosonic state*. The associated eigenvalue is

$$E_n = \left(n + \frac{1}{2}\right)\sqrt{1+\gamma^2},\ n = 0, 1, 2, 3, \ldots.$$

The wave functions $\Phi_n(x)$ are orthogonal

$$\langle \Phi_n, \Phi_m \rangle = n! \delta_{nm} \langle \Phi_0, \Phi_0 \rangle, \quad m, n \geq 0$$

for δ_{mn} the *Kronecker symbol* (=1 for $m = n$ and 0 otherwise) and constitute a basis for $L^2(\mathbb{R})$,

$$\mathcal{F}_\Phi := \{\Phi_n = a^{*n}\Phi_0 : n \geq 0\}, \tag{6}$$

as for any $\Phi \in \mathcal{H}$, there exists a set of complex coefficients such that Φ can be uniquely expressed as

$$\Phi = \sum_k c_k \Phi_k.$$

B. Eigenvalues and eigenfunctions of *H*

Next, we consider the functions

$$\Psi_n(x) = e^{-\gamma x^2} \Phi_n(x),$$

which belong to $\widetilde{\mathcal{S}} \subset \mathcal{D}$ since we clearly have $\exp(\gamma x^2)\Psi_n(x) \in L^2(\mathbb{R})$. If

$$\gamma > -\sqrt{\frac{\sqrt{5}-1}{2}},$$

then $\Psi_n(x) \in L^2(\mathbb{R})$ because

$$e^{-\gamma x^2}\Phi_0(x) = e^{-\gamma x^2} e^{-x^2/\sqrt{1+\gamma^2}}$$

belongs to $L^2(\mathbb{R})$ if $(\gamma + 1/\sqrt{1+\gamma^2}) > 0$. Moreover, $e^{\gamma x^2}\Phi_n(x)$ also belongs to $L^2(\mathbb{R})$ because it is the product of a polynomial in x by $e^{\gamma x^2}\Phi_0(x)$.

Observing that

$$H\Psi_n(x) = He^{-\gamma x^2}\Phi_n(x) = e^{-\gamma x^2} e^{\gamma x^2} He^{-\gamma x^2}\Phi_n(x) = e^{-\gamma x^2} H_0 \Phi_n(x),$$

we obtain

$$H\Psi_n(x) = \left(n + \frac{1}{2}\right)\sqrt{1+\gamma^2}\Psi_n(x).$$

That is, $\Psi_n(x)$, for $n = 0, 1, 2, \ldots$, are eigenfunctions of H and $(n + 1/2)\sqrt{1+\gamma^2}$ are the associated eigenvalues. If the similarity relation (2) holds for a bounded and boundedly invertible T, the eigenvalues of H are the same of H^*. As in this case $T = \exp(\gamma x^2)$ is unbounded, this is not guaranteed. In Sec. II C, this will be confirmed.

C. Matrix representation of *H*

Let us also consider the bosonic operators

$$b := x + \frac{1}{2}\frac{d}{dx}, \quad b^* := x - \frac{1}{2}\frac{d}{dx},$$

which satisfy the commutation relation

$$[b, b^*] = \mathbf{1}.$$

Analogous considerations to those concerning a and a^*, in Subsection II A, are in order. In terms of the bosonic operators, H becomes

$$H = b^*b + \frac{\gamma}{2}(b^{*2} - b^2) + \frac{\mathbf{1}}{2}.$$

We notice that the *parity operator* P commutes with H, and the eigenspaces of P are invariant subspaces of H.

With respect to the basis constituted by the eigenfunctions of the *number operator* $N := b^*b$,

$$\mathcal{F}_\phi = \{\phi_n = \frac{b^{*n}}{\sqrt{n!}}\phi_0 : \ b\phi_0 = 0, \ n \geq 0\},$$

the operator b is represented by the upper shifted matrix

$$B = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix},$$

and the operator b^* is represented by the transpose of B, B^T. These matrices satisfy the commutation relation,

$$[B, B^T] = I,$$

where I denotes the identity matrix. In the same basis, the operator b^*b is represented by the matrix $A_0 = \mathrm{diag}(0, 1, 2, 3, \dots)$. The matrix B^T is a *raising matrix* because if Φ is an eigenvector of A_0 associated with the eigenvalue Λ,

$$A_0\Phi = \Lambda\Phi,$$

then $B^T\Phi$ is an eigenvector of A_0 associated with the upwardly shifted eigenvalue $\Lambda + 1$,

$$A_0B^T\Phi = (\Lambda + 1)B^T\Phi,$$

and similarly B is a *lowering matrix*, as

$$A_0B\Phi = (\Lambda - 1)B\Phi,$$

if $B\Phi \neq 0$.

In the same basis, the operator b^{*2} is represented by the matrix A_+,

$$A_+ = \begin{bmatrix} 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \sqrt{1\times 2} & 0 & 0 & \dots \\ 0 & \sqrt{2\times 3} & 0 & \dots \\ 0 & 0 & \sqrt{3\times 4} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

and the operator b^2 is represented by the matrix $A_- = {A_+}^T$. Notice that

$$[A_0, A_+] = 2A_+, \quad [A_0, A_-] = -2A_-.$$

Thus, H is represented by the pentadiagonal matrix

$$B^TB + \frac{\gamma}{2}((B^T)^2 - B^2) + \frac{I}{2} = A_0 + \frac{\gamma}{2}(A_+ - A_-) + \frac{I}{2}$$
$$= \begin{bmatrix} 1/2 & 0 & -\frac{\gamma}{2}\sqrt{1\times 2} & 0 & \dots \\ 0 & 3/2 & 0 & -\frac{\gamma}{2}\sqrt{2\times 3} & \dots \\ \frac{\gamma}{2}\sqrt{1\times 2} & 0 & 5/2 & 0 & \dots \\ 0 & \frac{\gamma}{2}\sqrt{2\times 3} & 0 & 7/2 & \dots \\ 0 & 0 & \frac{\gamma}{2}\sqrt{3\times 4} & 0 & \dots \\ 0 & 0 & 0 & \frac{\gamma}{2}\sqrt{4\times 5} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix},$$

which may be written as

$$\begin{bmatrix} 1/2 & -\frac{\gamma}{2}\sqrt{1\times 2} & 0 & \dots \\ \frac{\gamma}{2}\sqrt{1\times 2} & 5/2 & -\frac{\gamma}{2}\sqrt{3\times 4} & \dots \\ 0 & \frac{\gamma}{2}\sqrt{3\times 4} & 9/2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \oplus \begin{bmatrix} 3/2 & -\frac{\gamma}{2}\sqrt{2\times 3} & 0 & \dots \\ \frac{\gamma}{2}\sqrt{2\times 3} & 7/2 & -\frac{\gamma}{2}\sqrt{4\times 5} & \dots \\ 0 & \frac{\gamma}{2}\sqrt{4\times 5} & 11/2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

The eigenfunctions of N, $\phi_0(x)$, $\phi_2(x)$, $\phi_4(x)$, ... are even functions, while $\phi_1(x)$, $\phi_3(x)$, $\phi_5(x)$, ... are odd functions. The eigenspaces of P are invariant subspaces of H. Thus, H is represented by real tridiagonal matrices called *pseudo-Jacobi matrices* in the bases of these subspaces, that is, Jacobi matrices pre-multiplied by $J = \mathrm{diag}(1, -1, 1, -1, \ldots)$.

Next, in order to determine raising and lowering matrices for $(A_0 + (A_+ - A_-)/2 + I/2)$, we look for linear combinations of B^T and B satisfying

$$\left[\left(B^TB + \frac{\gamma}{2}((B^T)^2 - B^2) + \frac{I}{2}\right), (xB^T + yB)\right] = \lambda(xB^T + yB).$$

By some computations, we find that $\lambda = \pm\sqrt{1+\gamma^2}$ and we obtain, for lowering and raising matrices, respectively,

$$D = \frac{1}{2}\left((1+\gamma^2)^{1/4} + \frac{1+\gamma}{(1+\gamma^2)^{1/4}}\right)B + \frac{1}{2}\left((1+\gamma^2)^{1/4} - \frac{1-\gamma}{(1+\gamma^2)^{1/4}}\right)B^T,$$
$$D^\ddagger = \frac{1}{2}\left(1+\gamma^{2^{1/4}} - \frac{1+\gamma}{(1+\gamma^2)^{1/4}}\right)B + \frac{1}{2}\left((1+\gamma^2)^{1/4} + \frac{1-\gamma}{(1+\gamma^2)^{1/4}}\right)B^T.$$

These matrices satisfy the following commutation relations:

$$[D, D^\ddagger] = I.$$
$$\left[\left(A_0 + \frac{\gamma}{2}(A_+ - A_-) + \frac{I}{2}\right), D^\ddagger\right] = \sqrt{1+\gamma 2}D^\ddagger,$$
$$\left[\left(A_0 + \frac{\gamma}{2}(A_+ - A_-) + \frac{I}{2}\right), D\right] = -\sqrt{1+\gamma^2}D.$$

This means that, if Υ is an eigenvector of $(A_0 + \gamma/2(A_+ - A_-) + I/2)$ associated with the eigenvalue Λ, then $D^\ddagger\Upsilon$ and $D\Upsilon$ are eigenvectors associated, respectively, with the eigenvalues $\Lambda + \sqrt{1+\gamma^2}$ and $\Lambda - \sqrt{1+\gamma^2}$. Moreover,

$$A_0 + \frac{\gamma}{2}(A_+ - A_-) + \frac{I}{2} = \sqrt{1+\gamma^2}\, D^\ddagger D + \frac{1}{2}\sqrt{1+\gamma^2}\, I.$$

Thus

$$\sigma\left(A_0 + \frac{\gamma}{2}(A_+ - A_-) + \frac{I}{2}\right) = \left(n + \frac{1}{2}\right)\sqrt{1+\gamma^2}, \quad n \geq 0.$$

An eigenvector Υ_0 of $\left(A_0 + \frac{\gamma}{2}(A_+ - A_-) + I/2\right)$ associated with the lowest eigenvalue $\sqrt{1+\gamma^2}$ is such that

$$D\Upsilon_0 = 0.$$

We find

$$\Upsilon_0 = \left[1, 0, \sqrt{\frac{1}{2}}\,\eta, 0, \sqrt{\frac{1\times 3}{2\times 4}}\,\eta^2, 0, \sqrt{\frac{1\times 3\times 5}{2\times 4\times 6}}\,\eta^3, 0, \ldots\right]^T,$$

where

$$\eta = \frac{1-\gamma-\sqrt{1+\gamma^2}}{1+\gamma+\sqrt{1+\gamma^2}}.$$

An eigenvector of $(A_0 + \gamma/2(A_+ - A_-) + I/2)$ associated with the eigenvalue $(n+1/2)\sqrt{1+\gamma^2}$ is given by

$$\Upsilon_n = D^{\ddagger n}\Upsilon_0.$$

III. SPECTRUM OF H

The spectrum of an operator on a finite dimensional Hilbert space is exhausted by the eigenvalues, but, in the infinite dimensional setting, there are additional parts of the spectrum of H to be considered.

The *resolvent set* of H, denoted by $\rho(H)$, is constituted by all the complex numbers λ for which $(H - \lambda)^{-1}$ exists as a bounded operator on $\mathcal{H}$. The *spectrum* of H is the complement of the resolvent set

$$\sigma(H) = \mathbb{C}\backslash\rho(H).$$

The set of all eigenvalues of H is the *point spectrum*, denoted by $\sigma_p(H)$, and is formed by the complex numbers λ for which $H-\lambda : \mathcal{D}(H) \to \mathcal{H}$ is not injective. The *continuous spectrum* is constituted by those λ such that $H-\lambda$ is injective and its range is dense. The *residual spectrum* consists of those λ for which $H-\lambda$ is injective and its range is not dense. The spectrum $\sigma(H)$ is the union of these three disjoint spectra.

The spectrum of selfadjoint operators is non-empty, real, and the residual spectrum is empty, while the spectrum of non-self-adjoint operators can be empty or coincide with the whole complex plane (see, e.g., Refs. 21 and 22). As already mentioned, the spectrum of an operator is meaningfully defined only for closed operators, that is, those for which the set

$$\{\langle H\psi,\psi\rangle : \psi \in \mathcal{D}\}$$

is a linear closed subspace of $\mathcal{H}\times\mathcal{H}$. In Subsection III B, we show that H is closed and that $\sigma(H)$ reduces to the point spectrum. For this purpose, we next introduce the central auxiliary concept of numerical range.

A. Numerical range

The *numerical range* of H is denoted and defined as

$$W(H) := \{\langle H\psi,\psi\rangle : \psi \in \mathcal{D}(H), \|\psi\| = 1\}.$$

In general, $W(H)$ is neither open nor closed, even when H is a closed operator (Fig. 1). For H bounded, the following spectral inclusion holds:

$$\sigma(H) \subset \overline{W(H)}.$$

Theorem 3.1 .*The boundary of the numerical range of H is given by*

$$y^2 = \gamma^2\left(x-\frac{1}{2}\right)^2, \quad x \geq \frac{1}{2}. \tag{7}$$

Proof. By the Toeplitz-Hausdorff theorem, the numerical range of H is convex. So, let us consider the supporting line of $W(H)$ perpendicular to the direction θ. The distance of this line to the origin is the lowest eigenvalue of

$$\Re(e^{-i\theta}H) = b^*b\cos\theta - i\frac{\gamma}{2}(b^{*2}-b^2)\sin\theta + \frac{\cos\theta}{2},$$

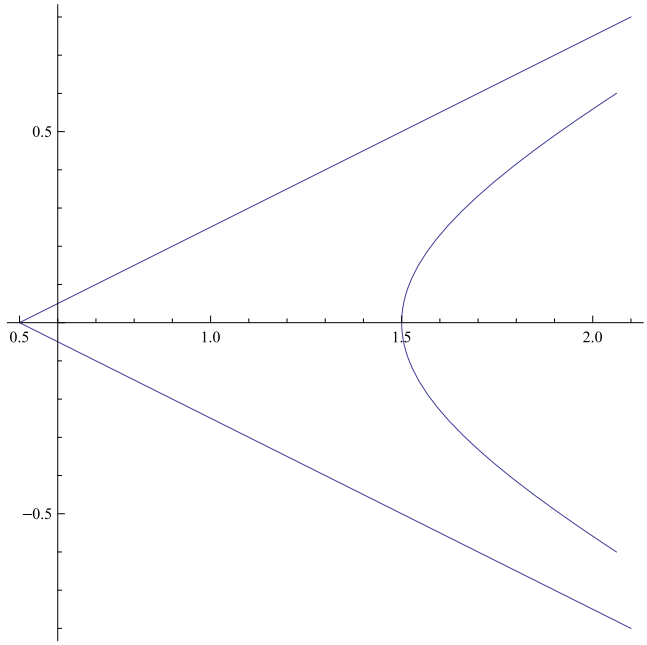

FIG. 1. Numerical range of H, $\gamma = 1/2$.

provided this operator is bounded from below, which occurs for $-\pi/2 \le \theta < \pi/2$. The eigenvalues of $\Re(e^{-i\theta}H)$ are readily determined by the EMM,[10] and they are found to be

$$E_n(\theta) = \frac{1}{2}\cos\theta + n\sqrt{\cos^2\theta - \gamma^2\sin^2\theta}, \quad n \ge 0,$$

with $E_0(\theta) < E_1(\theta) < E_2(\theta) < \cdots$, provided θ is such that $\cos^2\theta - \gamma^2\sin^2\theta \ge 0$. Let us consider, for a fixed n, the line perpendicular to the direction θ at a distance $E_n(\theta)$ from the origin. Its equation is given by

$$x\cos\theta + y\sin\theta = E_n(\theta). \tag{8}$$

The envelope of these lines is the n-th boundary generating curve and is obtained eliminating θ between (8) and

$$-x\sin\theta + y\cos\theta = \frac{dE_n(\theta)}{d\theta}.$$

Easy computations show that it is given by

$$\left(x - \frac{1}{2}\right)^2 - \frac{y^2}{\gamma^2} = n^2.$$

The boundary generating curves, $n = 0, 1, 2, 3, \ldots$, form a family of nested hyperbola branches, in which the outward one degenerates into the asymptotes.

The boundary of $W(H)$ corresponds to $n = 0$ and is given by (7). ∎

B. Accretivity of *H*

An operator is said to be *accretive* if its numerical range is a subset of the sector with vertex at the origin and *semi-angle* $0 \le \omega < \pi/2$,

$$S_{0,\omega} = \{z \in \mathbb{C} : 0 \le |\arg z| \le \omega\}.$$

An operator H is *m-accretive* if its numerical range is contained in the closed right half-plane and the so called *resolvent bound* holds

$$\forall \lambda \in \mathbb{C},\ \Re(\lambda) < 0,\ \|(H-\lambda)^{-1}\| \le 1/|\Re(\lambda)|.$$

Theorem 3.2 .*The operator H is m-accretive.*

Proof. Obviously, the operator H is *accretive* because $W(H) \subset S_{0,\pi/2}$. We show that for any $z \in \mathbb{C}$, with $\Re(z) < 0$, the resolvent bound holds. We have

$$\operatorname{dist}(z, \overline{W(H)}) \le |\langle H\psi,\psi\rangle - z| = |\langle (H-z)\psi,\psi\rangle| \le \|(H-z)\psi\|.$$

As $\operatorname{dist}(z, \overline{W(H)}) \ge |\Re(z)|$, having in mind Theorem 3.1, the result follows. ∎

The closed operator H on $\mathcal{H}$ has a *compact resolvent* if $\rho(H) \neq \emptyset$ and the inverse operator, $(H-\lambda)^{-1}$, for some $\lambda \in \rho(H)$, is compact. Notice that $\Re(H)$ is an m-accretive operator since $\Re(H)$ is Hermitian and $W(\Re(H))$ lies in the positive real axis.

Moreover, $\Re(H)$ is a closed operator and has a compact resolvent and since the perturbation operator V is relatively bounded with respect to $\Re(H)$ with relative bound smaller than 1, then $H = \Re(H) + \lambda V$ has a compact resolvent (Ref. 15, Theorem 5.4.1). Now, by (Ref. 15, Theorem IX, 2.3), if H has a compact resolvent, then $\sigma(H) = \sigma_p(H)$.

C. Pseudospectrum

The set of the eigenfunctions of a self-adjoint operator with a purely discrete real spectrum can be orthonormalized so that it forms an orthonormal basis. Eigenfunctions of a non-Hermitian operator H are typically non-orthogonal. The eigenfunctions of H, which has a purely discrete real spectrum, form a *Riesz basis* if H is quasi-Hermitian [see (1)] with bounded and boundedly invertible metric Θ. Riesz basicity is not preserved by an unbounded operator.

Our objective is to show that the eigenfunctions Ψ_n do not form a Riesz basis, and so any metric Θ in (1) is necessarily *singular*, that is, no bounded metric with bounded inverse exists.

For this purpose, we consider the ϵ-*pseudospectrum* of H, $\epsilon > 0$, denoted and defined as follows:

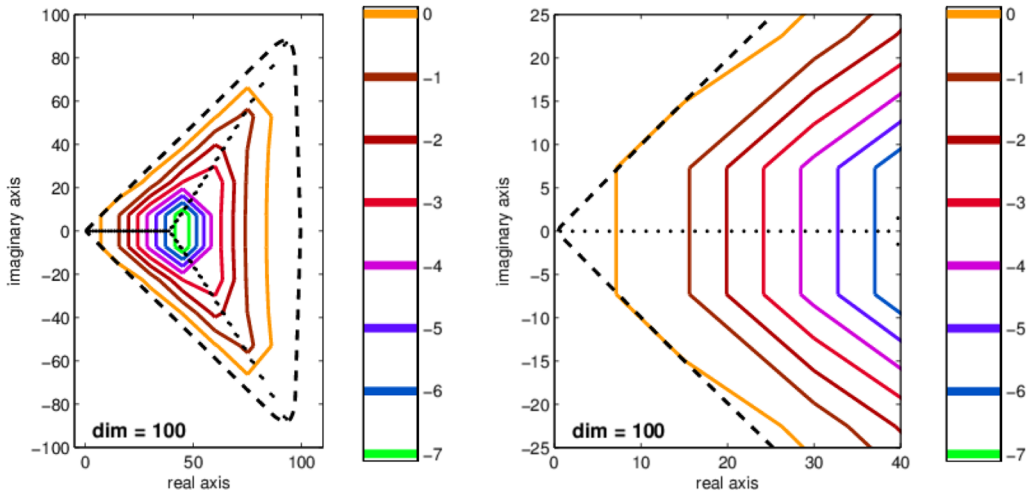

FIG. 2. (a) Pseudospectral lines. (b) Enlargement of the relevant portion: Pseudospectral lines of the 100 × 100 principal submatrix of the matrix representation of the operator *H*. The dashed lines represent the numerical range boundary, and the dots are the eigenvalues.

$$\sigma_\epsilon(H) := \{z \in \mathbb{C} : \|(H - z)^{-1}\| > \epsilon^{-1}\}$$

with the convention $\|(H - z)^{-1}\| = \infty$ for $z \in \sigma(H)$. The ϵ-pseudospectrum always contains an ϵ-neighborhood of the spectrum. If the operator is self-adjoint, equality holds and H is said to have a *trivial* pseudospectrum. A non-self-adjoint operator has a typically much larger pseudospectrum, although contained in an ϵ-neighborhood of the numerical range. This means that very small perturbations may drastically change the spectrum.

Numerical computations carried out with *Matlab* suggest that the pseudo-spectrum of H is far from being trivial. By adapting the Proof of Theorem 7 in Ref. 16, it can be shown that there are complex pseudo-eigenvalues contained in the numerical range. A non-trivial pseudospectrum implies the non-existence of a bounded metric.[21] In Fig. 2, the pseudospectrum of the 100 × 100 principal submatrix of the matrix representation of the operator H, for $\gamma = 1/2$, is shown, as computed with MATHLAB pseudospectra, Tom Wright, Oxford University Computing Laboratory. The portion of the pseudospectrum bounded by a parallel to the imaginary axis and containing all real eigenvalues remains (practically) unchanged as n increases.

D. Completeness of eigenfunctions

We will show that the eigenfunctions of H form a complete set in $L^2(R)$. Completeness of the system $\{\Psi_n\}$ means that its span is dense in $L^2(\mathbb{R})$. A basis is complete, but the converse may not be true.

The m-accretivity of H implies that $-iH$ is dissipative, i.e.,

$$\Im\langle H\Psi, \Psi\rangle \le 0, \ \forall \Psi \in \mathcal{D}(H).$$

As a consequence, the imaginary part of $(-iH - \epsilon)^{-1}$, for $\epsilon < 0$, is non-negative,

$$\frac{1}{2i}((-iH - \epsilon)^{-1} - (iH^* - \epsilon)^{-1}) \ge 0.$$

Since the resolvent is trace class [Ref. 17, p. 201], applying [Ref. 14, Theorem VII, 8.1], the completeness of $\{\Psi_n\}$ follows.

E. $\mathcal{G}$-quasi-bases

Let $\widetilde{\Psi}_n(x)$ be the eigenfunction of H^* sharing with $\Psi_n(x)$ the same eigenvalue of H. The set

$$\mathcal{F}_{\widetilde{\Psi}} = \{\widetilde{\Psi}_k(x) : k \ge 0\}$$

is complete but not necessarily a basis. The completeness follows exchanging H with H^*. It is known[21] that eigenfunctions of an operator H with a purely discrete real spectrum form a Riesz basis if and only if H is quasi-Hermitian with bounded and boundedly invertible metric.

The eigenfunctions $\Psi_n(x)$, $\widetilde{\Psi}_m(x)$, $m, n = 0, 1, 2, 3, \ldots$, constitute biorthogonal systems, as

$$\langle \Psi_m, \widetilde{\Psi}_n \rangle = \delta_{mn}.$$

Let

$$\mathcal{G} := \text{span}\{\Psi_n(x)\} \cap \text{span}\{\widetilde{\Psi}_n(x)\}.$$

The following *resolution of the identity* holds, for any $f, g \in \mathcal{G}$.

$$\langle f, g \rangle = \sum_{m,n} \frac{\langle f, \widetilde{\Psi}_n \rangle \langle \Psi_n, g \rangle}{\langle \Psi_n, \widetilde{\Psi}_n \rangle} = \sum_{m,n} \frac{\langle f, \Psi_n \rangle \langle \widetilde{\Psi}_n, g \rangle}{\langle \widetilde{\Psi}_n, \Psi_n \rangle}.$$

Since F_Ψ is complete, $\text{span}\{\Psi_n(x)\}$ is dense. Analogously, since $\mathrm{F}_{\widetilde{\Psi}}$ is complete, $\text{span}\{\widetilde{\Psi}_n(x)\}$ is dense. If $\mathcal{G}$ is dense, the wave functions Ψ_n and $\widetilde{\Psi}_n$ are $\mathcal{G}$-*quasi-basis*, in Bagarello sense, as it can be easily verified.[4,5]

For our purposes, it is enough to consider

$$\langle f, g \rangle = \sum_{m,n} \frac{\langle f, \widetilde{\Psi}_n \rangle \langle \Psi_n, g \rangle}{\langle \Psi_n, \widetilde{\Psi}_n \rangle}$$

for $f \in \text{span}\{\Psi_n(x)\}$, $g \in \text{span}\{\widetilde{\Psi}_n(x)\}$, a situation which Bagarello also envisages.

IV. THE DYNAMICS OF THE SYSTEM

For the physical interpretation of the model, we consider the following subset of $\mathcal{H}$:

$$\mathcal{D}_{phys} = \left\{ \psi(x) \in \mathcal{H} : \psi(x) = \sum_{k=0}^{\infty} c_k \, \Psi_k(x), \quad c_k \in \mathbb{C} \right\}.$$

It is assumed that this set contains all the physically relevant wave functions of the physical system. This assumption is convenient because it allows the easy solution of the time dependent Schrödinger equation

$$i \frac{\mathrm{d}\psi(x)}{\mathrm{d}t} = H\psi_t(x).$$

Indeed, if $\psi_0(x) = \sum_{n=0}^{\infty} c_n \Psi_n(x)$, then $\psi_t(x) = \sum_{n=0}^{\infty} c_n \mathrm{e}^{-\mathrm{E}_n t} \Psi_n(x)$. Even if $\mathcal{F}_\Psi$ is not a basis of $\mathcal{H}$, it is sufficient to expand physically meaningful wave functions.

The inner product $\langle \cdot, \cdot \rangle$ is not adequate for expressing the conservation of the *particle number* and for the computation of the expectation value of energy measurements, as it may yield complex values. For functions $\Psi_\alpha(x), \Psi_\beta(x) \in \widetilde{\mathcal{S}}$, we consider the *physical inner product* defined by

$$\langle \Psi_\alpha, \Psi_\beta \rangle = \langle \mathrm{e}^{\gamma x^2} \Psi_\alpha, \mathrm{e}^{\gamma x^2} \Psi_\beta \rangle = \int_{-\infty}^{+\infty} \mathrm{e}^{2\gamma x^2} \Psi_\alpha(x) \overline{\Psi_\beta(x)} \mathrm{d}x.$$

Following Mostafazadeh,[19] we say that the *physical Hilbert space* is the space of the functions $\Psi(x) \in \mathcal{D}_{phys}$ endowed with the inner product $\langle \cdot, \cdot \rangle$.

The Hamiltonian H is symmetric with respect to the inner product $\langle \cdot, \cdot \rangle$, for wave functions $\Psi(x) \in \mathcal{D}_{phys}$, because

$$\begin{aligned} \langle H\Psi, \Psi \rangle &= \int_{-\infty}^{+\infty} \mathrm{e}^{2\gamma x^2} (H\Psi(x)) \overline{\Psi(x)} \mathrm{d}x \\ &= \int_{-\infty}^{+\infty} \mathrm{e}^{\gamma x^2} (H\Psi(x)) \overline{\mathrm{e}^{\gamma x^2} \Psi(x)} \mathrm{d}x \\ &= \langle \Psi, H\Psi \rangle. \end{aligned}$$

Since $\langle H\Psi, \Psi \rangle = \langle \Psi, H\Psi \rangle$ for wave functions $\Psi(x) \in \mathcal{D}_{phys}$, it is clear that the Rayleigh quotients of H are real for the inner product $\langle \cdot, \cdot \rangle$,

$$\frac{\langle H\Psi, \Psi \rangle}{\langle \Psi, \Psi \rangle} \in \mathbb{R}$$

and that a time-invariant norm is obtained

$$\langle e^{-iHt}\Psi, e^{-iHt}\Psi\rangle = \langle \Psi, \Psi\rangle.$$

Let us consider now the operators

$$d := e^{-\gamma x^2} a e^{\gamma x^2} = (1+\gamma^2)^{1/4} x + \frac{1}{2}\,\frac{1}{(1+\gamma^2)^{1/4}}\left(\frac{d}{dx} + 2\gamma x\right),$$
$$d^\ddagger := e^{-\gamma x^2} a^* e^{\gamma x^2} = (1+\gamma^2)^{1/4} x - \frac{1}{2}\,\frac{1}{(1+\gamma^2)^{1/4}}\left(\frac{d}{dx} + 2\gamma x\right),$$

which are pseudo-bosonic in Bagarello sense. That is, the set $\mathcal{S}(\mathbb{R})$ is stable under the action of the operators d, $d^\ddagger$, $d^*, d^{\ddagger *}$, and the vacua of the operators d and $d^{\ddagger *}$,

$$\exp\left(-\frac{x^2}{4(\sqrt{1+\gamma^2}+\gamma)}\right), \quad \exp\left(-\frac{x^2}{4(\sqrt{1+\gamma^2}-\gamma)}\right),$$

respectively, are in it. These operators are called *pseudo-bosonic*, and not bosonic, because $d^\ddagger \neq d^*$, with respect to the inner product $\langle\cdot,\cdot\rangle$. The factorization of H in terms of the pseudo-bosonic operators is straightforward

$$H = \sqrt{1+\gamma^2}\, d^\ddagger d + \frac{1}{2}\sqrt{1+\gamma^2}\,\mathbf{1}.$$

With respect to the inner product $\langle\cdot,\cdot\rangle$, $d^\ddagger$ is the adjoint of d.

The physical inner product is appropriate to characterize the transition probability amplitude from the state Ψ_α to the state Ψ_β,

$$A_{\Psi_\alpha\to\Psi_\beta} = \frac{\langle\Psi_\alpha,\Psi_\beta\rangle}{\sqrt{\langle\Psi_\alpha,\Psi_\alpha\rangle\langle\Psi_\beta,\Psi_\beta\rangle}}\,. \tag{9}$$

Remark 4.1. In the definition of $\mathcal{D}_{phys}$, it is possible, and advantageous, to replace the restriction $\psi \in \mathcal{H} = L^2(\mathbb{R})$ by $\langle\psi,\psi\rangle < \infty$. Endowed with the inner product $\langle\cdot,\cdot\rangle$, $\mathcal{D}_{phys}$ becomes a Hilbert space in which H is Hermitian and the set of eigenfunctions $\{\Psi_n\}$ a basis. In this Hilbert space, H_0 is no longer Hermitian and its eigenfunctions are no longer a basis. Indeed, for the inner product $\langle\cdot,\cdot\rangle$, the adjoint of H_0 is given by

$$H_0^\ddagger = -\frac{1}{4}\frac{d^2}{dx^2} + x^2 - \gamma\left(\frac{1}{2} + x\frac{d}{dx}\right).$$

Similarly, the bosonic raising operator $d^\ddagger$ is the adjoint of the bosonic lowering operator d.

V. FINAL REMARKS

Upon viewing the operator H as the Hamiltonian of a physical model, problems arise from non-hermiticity. The original inner product, defined in the Hilbert space $\mathcal{H}$ where H lives, is not adequate for the physical interpretation of the model. A new inner product, which is appropriate for this purpose, has been introduced. Although H is non-Hermitian with respect to the initial inner product $\langle\cdot,\cdot\rangle$, it becomes symmetric with respect to the physical inner product $\ll\cdot,\cdot\gg = \langle\Theta\cdot,\cdot\rangle$.

The concept of pseudospectrum is of great relevance for the investigation of non-Hermitian operators in the context of QM, as well as the one for the numerical range. Non-Hermitian operators have typically non-trivial pseudospectra. If the quasi-Hermiticity relation holds with a positive bounded and boundedly invertible metric, then the pseudospectrum of H is trivial. A non-trivial pseudospectrum determines the non-existence of such a metric. Moreover, it implies the non-existence of a Riesz basis and of an orthonormal basis, which are very useful for a rigorous mathematical foundation of QM.

A new inner product, which is adequate for the physical interpretation, has been consistently introduced.

The case of Hamiltonians possessing complex eigenvalues is of an entirely different nature. It arises in connection with models of dissipative or absorptive processes.

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