Physical aspects of pseudo-Hermitian and *PT*-symmetric quantum mechanics

2004 J. Phys. A: Math. Gen. 37 11645

(http://iopscience.iop.org/0305-4470/37/48/009)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 11645–11679 PII: S0305-4470(04)84912-6

Physical aspects of pseudo-Hermitian and PT-symmetric quantum mechanics

Ali Mostafazadeh and Ahmet Batal

Department of Mathematics, Koç University, Rumelifeneri Yolu, 34450 Sariyer, Istanbul, Turkey

E-mail: amostafazadeh@ku.edu.tr and abatal@ku.edu.tr

Received 11 August 2004
Published 17 November 2004
Online at stacks.iop.org/JPhysA/37/11645
doi:10.1088/0305-4470/37/48/009

Abstract

For a non-Hermitian Hamiltonian H possessing a real spectrum, we introduce a canonical orthonormal basis in which a previously introduced unitary mapping of H to a Hermitian Hamiltonian h takes a simple form. We use this basis to construct the observables O_α of the quantum mechanics based on H. In particular, we introduce pseudo-Hermitian position and momentum operators and a pseudo-Hermitian quantization scheme that relates the latter to the ordinary classical position and momentum observables. These allow us to address the problem of determining the conserved probability density and the underlying classical system for pseudo-Hermitian and in particular PT-symmetric quantum systems. As a concrete example we construct the Hermitian Hamiltonian h, the physical observables O_α, the localized states and the conserved probability density for the non-Hermitian PT-symmetric square well. We achieve this by employing an appropriate perturbation scheme. For this system, we conduct a comprehensive study of both the kinematical and dynamical effects of the non-Hermiticity of the Hamiltonian on various physical quantities. In particular, we show that these effects are quantum mechanical in nature and diminish in the classical limit. Our results provide an objective assessment of the physical aspects of PT-symmetric quantum mechanics and clarify its relationship with both conventional quantum mechanics and classical mechanics.

PACS number: 03.65.−w

1. Introduction

Most of the recent publications on PT-symmetric quantum mechanics focus on the study of the spectral properties of various (non-Hermitian) PT-symmetric Hamiltonians. The results reported in these publications are mainly mathematical. The purpose of the present paper is to

address some of the most basic problems related to the physical aspects of PT-symmetric and more generally pseudo-Hermitian quantum mechanics. In particular, we will offer a complete description of the nature and the construction of the physical observables and provide a method to compute various physical quantities in these theories. We will also elucidate the relationship between these theories and conventional classical and quantum mechanics.

As our approach is motivated by the mathematical results obtained within the framework of the theory of pseudo-Hermitian operators [1–3], we begin our discussion by a brief review of the relevant developments.

A central question that arises in connection with the current interest in PT-symmetric quantum mechanics [4, 5] is: 'What are the necessary and sufficient conditions for the reality of the spectrum of a linear operator?' Reference [2] provides the following answer to this question. If the operator acts in a Hilbert space $\mathcal{H}$ and has a complete set of eigenvectors (i.e., it is diagonalizable) then its spectrum is real if and only if (one and consequently all of) the following equivalent conditions holds:

(C1) There exists a positive-definite operator[1] $\eta_+ : \mathcal{H} \to \mathcal{H}$ that fulfils

$$H^\dagger = \eta_+ H \eta_+^{-1}, \tag{1}$$

i.e., H is pseudo-Hermitian [1] and the set[2] of all the metric operators η satisfying $H^\dagger = \eta H \eta^{-1}$ includes a positive-definite element.

(C2) H is Hermitian with respect to some positive-definite inner product $\langle \cdot, \cdot \rangle_+$ on $\mathcal{H}$ (which is generally different from its defining inner product $\langle \cdot | \cdot \rangle$). A specific choice for $\langle \cdot, \cdot \rangle_+$ is $\langle \cdot | \eta_+ \cdot \rangle$.

(C3) H may be mapped to a Hermitian Hamiltonian h by a similarity transformation, i.e., H is quasi-Hermitian [7, 8].

The framework provided in [1, 2] also explains the connection with PT-symmetry. It turns out that, under the same conditions, pseudo-Hermiticity of H is equivalent to the presence of an antilinear symmetry, PT-symmetry being the primary example [3, 9].

The condition that the Hamiltonian H must have a complete set of eigenvectors may be relaxed by extending the analysis of [1–3] to block-diagonalizable linear operators as discussed in [10, 11]. However, note that physically this condition is intertwined with the requirements of the quantum measurement theory. The failure to satisfy it is equivalent to allowing for the states that have zero overlap with all the energy eigenstates. As a result, the total probability of measuring any energy value for such a state is identically zero, i.e., one can never perform an energy measurement on such a state; it must not be possible to prepare it!

These physical considerations form the basis of a general framework, called pseudo-Hermitian quantum mechanics [12] that allows for formulating a quantum theory based on an eigenvalue problem for a linear operator H acting in a (complex) vector space V. A typical example is an eigenvalue (Sturm–Liouville) equation for a differential operator acting in a complex function space. Supposing that this eigenvalue problem has a solution, i.e., there are eigenvectors $\psi_n \in V$, one lets V_H be the span of ψ_n, endows V_H with an arbitrary positive-definite inner product, Cauchy completes [13] this inner product space to a Hilbert space $\mathcal{H}$, and views H as a (possibly densely defined) linear operator acting in $\mathcal{H}$. Then, by construction, H is a diagonalizable operator acting in $\mathcal{H}$, and the results of [1–3] apply.

As noted in [14], the equivalence of the reality of the spectrum of H and condition (C2) is the basic mathematical result underlying the construction of the so-called CPT-inner product for PT-symmetric quantum systems [15]. Also, as shown in [16], one can use condition (C3)

[1] An operator is called positive definite if it is Hermitian and has a strictly positive spectrum.

[2] For a discussion of this set, see [6].

to map H to a Hermitian Hamiltonian h acting in $\mathcal{H}$. If one identifies the physical Hilbert space $\mathcal{H}_{\rm phys}$ of the system with $\mathcal{H}$ endowed with the positive-definite inner product $\langle\cdot,\cdot\rangle_+$, then H and h are unitarily equivalent.

For models with a finite-dimensional Hilbert space the construction of the Hermitian Hamiltonian h is straightforward. In some cases h has a much simpler form than H [16]. The situation is quite different for systems with an infinite-dimensional Hilbert space, as almost nothing specific is known about the structure of h. It is nevertheless expected to be a generally complicated nonlocal (non-differential) operator [16].

The study of systems with an infinite-dimensional Hilbert space is particularly important, because it is for such systems that one can seek for an underlying classical system and attempt to formulate an associated quantization scheme. Obviously, a proper treatment of these issues requires a careful study of the notion of a physical observable in pseudo-Hermitian and, in particular, PT-symmetric quantum mechanics.

It has recently been shown [17] that the formulation of observables in PT-symmetric quantum mechanics as originally proposed in [15] and reiterated in [18] is inconsistent with its dynamical aspects and that enforcing the rules of the standard measurement theory restricts the choice of the observables O_α to linear operators that are Hermitian with respect to the inner product of the physical Hilbert space $\mathcal{H}_{\rm phys}$.[3] Accepting this definition for the observables, one can easily show that the unitary mapping that maps H to h also maps the observables O_α to the Hermitian operators o_α acting in $\mathcal{H}$. This in turn means that a physical system described by the Hilbert space $\mathcal{H}_{\rm phys}$, the PT-symmetric Hamiltonian H, and the observables O_α may be equivalently described by the Hilbert space $\mathcal{H}$, the Hermitian Hamiltonian h, and the observables o_α.

In this paper, we will introduce a canonical basis in which the construction of the Hermitian Hamiltonian h and the physical observables O_α simplifies considerably. This allows us to determine the underlying classical system and develop a pseudo-Hermitian quantization scheme. We will also introduce and construct the pseudo-Hermitian position operator, the corresponding position wavefunctions and the conserved probability density. As a concrete application of our general results we perform a thorough investigation of the PT-symmetric square well Hamiltonian, computing the corresponding Hermitian Hamiltonian h, the observables O_α (in particular the pseudo-Hermitian position operator), the probability density, the position expectation values and the localized states. We will also describe the effects of the non-Hermiticity of the Hamiltonian on the latter quantities and discuss the underlying classical Hamiltonian.

Throughout this paper, we will assume that H is diagonalizable and has a nondegenerate, real, discrete spectrum. The extension of the results to degenerate spectra may be easily achieved following the approach of [1–3, 14]. The presence of a continuous part of the spectrum does not lead to any serious complications either; see, for example, [21, 22].

2. Canonical metric basis

Let $\mathcal{H}$ be a Hilbert space and $H:\mathcal{H}\to\mathcal{H}$ be a diagonalizable linear (Hamiltonian) operator having a real, nondegenerate, discrete spectrum. Following [1–3, 14], we shall label the

[3] To resolve the inconsistency reported in [17], the authors of [15] have recently revised their definition of observables [19]. As noted in [20], when the contour defining the boundary conditions of the problem is the real line, the definition reduces to ours. But even in this case it is a more restrictive definition as it implies that the Hamiltonian must be (not only PT-symmetric but also) symmetric, i.e., in x-representation it is a symmetric (infinite) matrix. This leads to some undesirable consequences [20].

eigenvalues of H with E_n and let $\{|\psi_n\rangle\}$ denote a basis of $\mathcal{H}$ consisting of the eigenvectors $|\psi_n\rangle$ of H,

$$H|\psi_n\rangle = E_n|\psi_n\rangle. \tag{2}$$

Then one can construct another basis $\{|\phi_n\rangle\}$ of $\mathcal{H}$ that satisfies [3]

$$H^\dagger|\phi_n\rangle = E_n|\phi_n\rangle, \qquad \langle\phi_n|\psi_m\rangle = \delta_{mn}, \qquad \sum_n |\psi_n\rangle\langle\phi_n| = 1. \tag{3}$$

In particular, $\{|\psi_n\rangle, |\phi_n\rangle\}$ form a biorthonormal system [23], and

$$H = \sum_n E_n|\psi_n\rangle\langle\phi_n|, \qquad H^\dagger = \sum_n E_n|\phi_n\rangle\langle\psi_n|. \tag{4}$$

Here and throughout this paper, for any linear operator A acting in $\mathcal{H}$, $A^\dagger$ stands for the adjoint of A, i.e., the unique linear operator satisfying $\langle\cdot|A\cdot\rangle = \langle A^\dagger\cdot|\cdot\rangle$.

A central result of [1] is that the operator

$$\eta_+ = \sum_n |\phi_n\rangle\langle\phi_n| \tag{5}$$

satisfies (1). It is also manifestly positive definite, because it satisfies $\eta_+ = w^\dagger w$, where $w := \sum_n |n\rangle\langle\phi_n|$ and $\{|n\rangle\}$ is an orthonormal basis of $\mathcal{H}$, and that it is invertible, with the inverse given by

$$\eta_+^{-1} = \sum_n |\psi_n\rangle\langle\psi_n|. \tag{6}$$

We can use (5) to introduce the positive-definite inner product,

$$\langle\cdot,\cdot\rangle_+ := \langle\cdot|\eta_+\cdot\rangle, \tag{7}$$

and identify the physical Hilbert space $\mathcal{H}_{\rm phys}$ with the underlying vector space of $\mathcal{H}$ endowed with this inner product. This means that as complex vector spaces $\mathcal{H}$ and $\mathcal{H}_{\rm phys}$ are identical, but as Hilbert spaces they are not.

In view of (1), the Hermitian Hamiltonian h of condition (C3) has the form [16]

$$h = \rho H \rho^{-1}, \tag{8}$$

where $\rho := \sqrt{\eta_+}$ is the unique positive(-definite) square root of η_+. The transformation $H \to h$ corresponds to the linear mapping $|\psi\rangle \to \rho|\psi\rangle$. It is a simple exercise to check that, for any pair $|\psi\rangle, |\psi'\rangle$ of state vectors, $\langle\psi, \psi'\rangle_+ = \langle\psi|\eta_+\psi'\rangle = \langle\rho\psi|\rho\psi'\rangle$. Hence as a mapping of $\mathcal{H}_{\rm phys}$ onto $\mathcal{H}$, ρ is a unitary operator[4].

Now, consider a physical system S that is described by the Hilbert space $\mathcal{H}_{\rm phys}$, the Hamiltonian H and the observables O_α that are Hermitian operators acting in $\mathcal{H}_{\rm phys}$.[5] Because $\rho : \mathcal{H}_{\rm phys} \to \mathcal{H}$ is a unitary transformation, $O_\alpha : \mathcal{H}_{\rm phys} \to \mathcal{H}_{\rm phys}$ is Hermitian if and only if $o_\alpha := \rho O_\alpha \rho^{-1} : \mathcal{H} \to \mathcal{H}$ is Hermitian. This, in particular, means that the observables O_α may be constructed from the Hermitian operators o_α according to [17]

$$O_\alpha = \rho^{-1} o_\alpha \rho. \tag{9}$$

Consequently, we can also describe the physical system S using the original Hilbert space $\mathcal{H}$, the Hermitian Hamiltonian h and the observables o_α. The two descriptions are physically identical

[4] A linear map $U : \mathcal{H}_1 \to \mathcal{H}_2$ between two inner product (in particular Hilbert) spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ with inner products $\langle\cdot,\cdot\rangle_1$ and $\langle\cdot,\cdot\rangle_2$ is said to be a unitary operator if for all $\zeta, \chi \in \mathcal{H}_1$, we have $\langle U(\zeta), U(\chi)\rangle_2 = \langle\zeta, \chi\rangle_1$ [13]. U is unitary if and only if it is invertible (one-to-one and onto) and $U^{-1} = U^\dagger$.

[5] Being a Hermitian operator acting in $\mathcal{H}_{\rm phys}$, the Hamiltonian H is also an observable. But as operators acting in $\mathcal{H}$ neither H nor O_α are Hermitian.

as there is a one-to-one correspondence between the states and the observables used in these descriptions and more importantly the physical quantities such as the transition amplitudes or expectation values of the observables do not depend on the choice of the description.

The main ingredient of the above construction is the operator $\rho = \sqrt{\eta}_+$. It has three important properties:

(P1) As an operator mapping $\mathcal{H}_{\rm phys}$ to $\mathcal{H}$, it is a unitary operator.
(P2) As an operator mapping $\mathcal{H}$ to $\mathcal{H}$, it is a Hermitian operator.
(P3) As an operator mapping $\mathcal{H}_{\rm phys}$ to $\mathcal{H}_{\rm phys}$, it is also a Hermitian operator[6]. In particular, both ρ and $\eta_+ = \rho^2$ are physical observables.

Property (P2) suggests that a natural method for computing the operators h and O_α is to use an orthonormal basis $\{|\epsilon_n\rangle\}$ of $\mathcal{H}$ that consists of the eigenvectors[7] $|\epsilon_n\rangle$ of η_+. Denoting the eigenvalues of η_+ by ϵ_n, we have

$$\eta_+|\epsilon_n\rangle = \epsilon_n|\epsilon_n\rangle, \qquad \langle\epsilon_m|\epsilon_n\rangle = \delta_{mn}, \qquad \sum_n |\epsilon_n\rangle\langle\epsilon_n| = 1. \tag{10}$$

These in turn imply

$$\eta_+ = \sum_n \epsilon_n|\epsilon_n\rangle\langle\epsilon_n|, \qquad \rho = \sum_n \sqrt{\epsilon_n}|\epsilon_n\rangle\langle\epsilon_n|. \tag{11}$$

In the following, we shall refer to $\{|\epsilon_n\rangle\}$ as a *canonical metric basis*.

Let A be a linear operator acting in $\mathcal{H}$, we can uniquely identify A with its matrix representation (A_{mn}) in the basis $\{|\epsilon_n\rangle\}$, where

$$A_{mn} := \langle\epsilon_m|A|\epsilon_n\rangle. \tag{12}$$

Because $\{|\epsilon_n\rangle\}$ is an orthonormal basis of $\mathcal{H}$, the matrix elements of $A^\dagger$ are given by

$$A^\dagger_{mn} = A^*_{nm}. \tag{13}$$

In particular, A is Hermitian with respect to the defining inner product $\langle\cdot|\cdot\rangle$ of $\mathcal{H}$ if and only if (A_{mn}) is a Hermitian (possibly infinite) matrix, i.e., $A^*_{mn} = A_{nm}$.

The following important identities follow from (1), (5), (6) and (8):

$$\epsilon_n^{-1}\epsilon_m H_{mn} = H^\dagger_{mn} = H^*_{nm}, \tag{14}$$

$$\epsilon_n = \sum_m |\langle\phi_m|\epsilon_n\rangle|^2 = \left(\sum_m |\langle\psi_m|\epsilon_n\rangle|^2\right)^{-1}, \tag{15}$$

$$h_{mn} = \sqrt{\frac{\epsilon_m}{\epsilon_n}}H_{mn}. \tag{16}$$

Furthermore, let $o : \mathcal{H} \to \mathcal{H}$ be a Hermitian operator and $O := \rho^{-1}o\rho$, then

$$O_{mn} = \sqrt{\frac{\epsilon_n}{\epsilon_m}}o_{mn}. \tag{17}$$

Equations (16) and (17) provide the following expressions for the Hermitian Hamiltonian $h : \mathcal{H} \to \mathcal{H}$ and the observables $O : \mathcal{H}_{\rm phys} \to \mathcal{H}_{\rm phys}$:

$$h = \sum_{m,n} \sqrt{\frac{\epsilon_m}{\epsilon_n}}H_{mn}|\epsilon_m\rangle\langle\epsilon_n|, \tag{18}$$

$$O = \sum_{m,n} \sqrt{\frac{\epsilon_n}{\epsilon_m}}o_{mn}|\epsilon_m\rangle\langle\epsilon_n|. \tag{19}$$

[6] This can be easily checked: $\langle\cdot, \rho\cdot\rangle_+ = \langle\cdot, |\eta_+\rho\cdot\rangle = \langle\cdot|\rho\eta_+\cdot\rangle = \langle\rho\cdot\,|\,\eta_+\cdot\rangle = \langle\rho\cdot, \cdot\rangle_+$.

[7] Here we suppress the degeneracy labels for the eigenvectors $|\epsilon_n\rangle$ for simplicity. Note also that in view of the non-uniqueness [24, 14] of η_+ one can assume without loss of generality that the eigenvalues of η_+ are nondegenerate.

3. Classical system and its pseudo-Hermitian canonical quantization

For $\mathcal{H} = L^2(\mathbb{R})$, we can define the *$\eta_+$-pseudo-Hermitian position (X) and momentum (P) operators* according to

$$X := \sum_{m,n} \sqrt{\frac{\epsilon_n}{\epsilon_m}}\, x_{mn} |\epsilon_m\rangle\langle\epsilon_n|, \qquad P := \sum_{m,n} \sqrt{\frac{\epsilon_n}{\epsilon_m}}\, p_{mn} |\epsilon_m\rangle\langle\epsilon_n|, \tag{20}$$

where $x_{mn} := \langle\epsilon_m|x|\epsilon_n\rangle$, $p_{mn} := \langle\epsilon_m|p|\epsilon_n\rangle$, and x and p are the usual position and momentum operators acting in $\mathcal{H} = L^2(\mathbb{R})$.

Clearly, the η_+-pseudo-Hermitian position and momentum operators satisfy the canonical commutation relation

$$[X, P] = \mathrm{i}\hbar 1. \tag{21}$$

Indeed, together with the identity operator 1, they provide a unitary irreducible representation of the Weyl–Heisenberg algebra which has the physical Hilbert space $\mathcal{H}_{\rm phys}$ as the representation space. The fact that by construction this representation is unitarily equivalent to the standard representation of the Weyl–Heisenberg algebra (that has $\mathcal{H} = L^2(\mathbb{R})$ as the representation space) is a manifestation of von Neumann's celebrated uniqueness theorem[8].

Having introduced the η_+-pseudo-Hermitian position and momentum operators, we can also speak of the following *η_+-pseudo-Hermitian canonical quantization* of classical systems,

$$x_c \to X, \qquad p_c \to P, \qquad \{\cdot,\cdot\}_c \to -\mathrm{i}\hbar^{-1}[\cdot,\cdot], \tag{22}$$

where x_c, p_c and $\{\cdot,\cdot\}_c$ stand for classical position, momentum and Poisson bracket, respectively. For instance, η_+-pseudo-Hermitian quantization of the classical Hamiltonian for a free particle leads to the pseudo-Hermitian quantum Hamiltonian:

$$H_{\rm free} = \frac{P^2}{2m} = \rho^{-1}\left[\frac{p^2}{2m}\right]\rho, \tag{23}$$

which is a generally nonlocal (non-differential) operator.

Note that in general the Hamiltonian operator H, that is used to construct the metric operator η_+ and consequently define the above notion of pseudo-Hermitian quantization, does not have the standard form $P^2/(2m) + V(X)$. For example, a PT-symmetric Hamiltonian of the standard form [4] (with a complex-valued potential $v(x)$),

$$H = \frac{p^2}{2m} + v(x) = \rho\left[\frac{P^2}{2m} + v(X)\right]\rho^{-1}, \tag{24}$$

cannot generally be expressed in the form $P^2/2m + V(X)$ for any real-valued function V. Nevertheless, because (in light of property (P3)) ρ is also a physical observable, one can express ρ and ρ^{-1} and consequently the Hamiltonian (24) as certain power series in X and P (modulo commutation relations (21)). This in turn implies that the classical Hamiltonian H_c, whose η_+-pseudo-Hermitian quantization yields H, is not generally of the standard (kinetic+potential) type. Rather it is a complicated (non-polynomial) function of x_c and p_c.

The classical Hamiltonian H_c may also be obtained using the Hermitian Hamiltonian h which according to (8) and (24) takes the form

$$h = \rho\left[\frac{p^2}{2m} + v(x)\right]\rho^{-1}. \tag{25}$$

[8] This theorem states that up to unitary equivalence the Weyl–Heisenberg algebra has a unique unitary irreducible (projective) representation [13].

Again this is a nonlocal operator which can be expressed as a power series in p with x-dependent coefficients. This is because (according to property (P2)) ρ and ρ^{-1} are Hermitian operators acting in $\mathcal{H}$. The classical Hamiltonian may be obtained by replacing x and p in the expression for h by their classical counterparts x_c and p_c, respectively. Clearly, the resulting H_c is identical with that obtained from H.

Next, we wish to recall a simple procedure for associating a power series in x and p (i.e., a pseudo-differential operator) with a nonlocal linear operator $K : L^2(\mathbb{R}) \to L^2(\mathbb{R})$. Suppose that K may be expressed in terms of its kernel $\mathcal{K} : \mathbb{R}^2 \to \mathbb{C}$ according to

$$(K\psi)(x) = \int_{\mathbb{R}} \mathcal{K}(x, x')\psi(x')\,\mathrm{d}x'. \tag{26}$$

Then for real analytic wavefunctions, which form a dense subset of $L^2(\mathbb{R})$, we can expand $\psi(x')$ appearing on the right-hand side of (26) in Taylor series about x. Substituting the result in (26), we find $(K\psi)(x) = \hat{K}\psi(x)$ where

$$\hat{K} := \sum_{\ell=0}^{\infty} (-\mathrm{i}\hbar)^{\ell} a_{\ell}(x) \frac{\mathrm{d}^{\ell}}{\mathrm{d}x^{\ell}}, \tag{27}$$

$$a_{\ell}(x) = \frac{\mathrm{i}^{\ell}}{\ell!\hbar^{\ell}} \int_{\mathbb{R}} K(x, x')(x' - x)^{\ell}\,\mathrm{d}x'. \tag{28}$$

As a result, we have the following (densely defined) identity

$$K = \sum_{\ell=0}^{\infty} a_{\ell}(x)\, p^{\ell}. \tag{29}$$

If the operator K is Hermitian, we can express (29) in a manifestly Hermitian form, namely

$$K = \frac{1}{2} \sum_{\ell=0}^{\infty} [a_{\ell}(x)\, p^{\ell} + p^{\ell} a_{\ell}(x)^*]. \tag{30}$$

The classical counterpart of this operator is the following real-valued function of the phase space ($\mathbb{R}^2$),

$$K_c(x_c, p_c) := \sum_{\ell=0}^{\infty} \mathrm{Re}[a_{\ell}(x_c)] p_c^{\ell}, \qquad x_c, p_c \in \mathbb{R}, \tag{31}$$

where Re means 'real part of'.

The results reported in this section clearly generalize to the Hilbert spaces $\mathcal{H}(V)$ where V is $\mathbb{R}^n$ or a topologically equivalent subset of $\mathbb{R}^n$. Together with the results of the preceding section, they lead to the following prescription for determining the classical Hamiltonian for a pseudo-Hermitian (particularly PT-symmetric) quantum system:

(1) Given the Hamiltonian H, compute a metric operator η_+.
(2) Diagonalize η_+ and construct a corresponding canonical metric basis $\{|\epsilon_n\rangle\}$.
(3) Compute the matrix elements H_{mn} of H in this basis and use (18) to obtain the Hermitian Hamiltonian h.
(4) Apply the above-described method of associating a pseudo-differential operator with the operator h, express the latter in a manifestly Hermitian form $(h + h^{\dagger})/2$, and take $x \to x_c$ and $p \to p_c$ in the resulting expression. This yields a classical Hamiltonian H_c for the theory.

The Hamiltonian H_c obtained in this way generally involves $\hbar$. The strictly classical Hamiltonian will correspond to evaluating $\hbar \to 0$ limit of H_c. The latter is an admissible prescription only if this limit exists.

We end this section by making the last step of the above prescription more specific. Using (18), (28), (29) and (31), identifying the kernel of h with $\langle x|h|x'\rangle$, and denoting the normalized eigenfunctions of η_+ by ε_n, i.e.,

$$\varepsilon_n(x) = \langle x|\epsilon_n\rangle, \tag{32}$$

we have

$$h = \sum_{\ell=0}^{\infty} a_\ell(x)\, p^\ell, \qquad H_c = \sum_{\ell=0}^{\infty} \mathrm{Re}[a_\ell(x_c)]\, p_c^\ell, \tag{33}$$

$$a_\ell(x) = \frac{\mathrm{i}^\ell}{\ell!\hbar^\ell} \sum_{m,n} \sqrt{\frac{\epsilon_m}{\epsilon_n}}\, H_{mn}\varepsilon_m(x) \int_{\mathbb{R}} \varepsilon_n(x')^*(x'-x)^\ell \,\mathrm{d}x'. \tag{34}$$

Admittedly, the computation of h as outlined above is too complicated to be done exactly. In section 5, we study its application to a simple PT-symmetric model where a particularly useful approximation scheme allows for computing h with any desired accuracy. Finally, we should like to add that the above prescription for computing h may also be used to compute the pseudo-Hermitian observables such as the position operator X.

4. Localized states, position wavefunctions and the probability density

Having introduced the η_+-pseudo-Hermitian position operator X we can identify its (generalized [25]) eigenvectors $\xi^{(x)}$ with the localized states of the system. They are defined by

$$X\xi^{(x)} = x\xi^{(x)}, \qquad \text{for all} \quad x \in \mathbb{R}. \tag{35}$$

In view of the identity $X = \rho^{-1}x\rho$, we have

$$\xi^{(x)} = \rho^{-1}|x\rangle, \tag{36}$$

where $|x\rangle$ are the usual position kets satisfying, for all $x, x' \in \mathbb{R}$,

$$\langle x|x'\rangle = \delta(x-x'), \qquad \int_{\mathbb{R}} \mathrm{d}x\,|x\rangle\langle x| = 1. \tag{37}$$

Using these relations and the fact that $\rho : \mathcal{H}_{\rm phys} \to \mathcal{H}$ is a unitary mapping, we can establish the orthonormality and completeness relations for the localized states $\xi^{(x)}$:

$$\langle \xi^{(x)}, \xi^{(x')}\rangle_+ = \delta(x-x'), \qquad \int_{\mathbb{R}} \mathrm{d}x\, \Xi^{(x)} = 1, \tag{38}$$

where $\Xi^{(x)}$ denotes the projection operator defined by

$$\Xi^{(x)}\psi := \langle \xi^{(x)}, \psi\rangle_+ \xi^{(x)}, \qquad \text{for all} \quad \psi \in \mathcal{H}_{\rm phys}. \tag{39}$$

Next, consider a particle[9] whose state at a fixed time t_0 is described by the state vector $\psi \in \mathcal{H}_{\rm phys}$. We can introduce the *position wavefunction*,

$$\Psi(x) := \langle \xi^{(x)}, \psi\rangle_+ = \langle x|\rho|\psi\rangle, \tag{40}$$

and use (38) to expand the state vector ψ in the position basis $\{\xi^{(x)}\}$ according to

$$\psi = \int_{\mathbb{R}} \Psi(x)\xi^{(x)}\,\mathrm{d}x. \tag{41}$$

[9] Here by a particle we mean a quantum system having $\mathbb{R}$ as its classical configuration space.

As seen from (40), the position wavefunction $\Psi(x)$ is generally different from $\psi(x)$. This is a direct consequence of the fact that H as an operator acting in $\mathcal{H} = L^2(\mathbb{R})$ fails to be Hermitian. Furthermore, in view of (38) and (40),

$$\|\Psi\|^2 := \int_{\mathbb{R}} |\Psi(x)|^2 \, \mathrm{d}x = \int_{\mathbb{R}} |\langle \xi^{(x)}, \psi\rangle_+|^2 \, \mathrm{d}x = \int_{\mathbb{R}} \langle \psi, \Xi^{(x)}\psi\rangle_+ \, \mathrm{d}x = \langle \psi, \psi\rangle_+ < \infty.$$

Hence as a function mapping $\mathbb{R}$ to $\mathbb{C}$, the wavefunction Ψ belongs to $L^2(\mathbb{R})$.[10] The converse is also true in the sense that every square-integrable function Ψ defines a state vector $\psi \in \mathcal{H}_{\rm phys}$. Therefore, we may identify $L^2(\mathbb{R})$ with the vector space of position wavefunctions Ψ for the system. It is also a straightforward exercise to show that the assignment F of a wavefunction $\Psi =: F(\psi)$ to each state vector ψ, viewed as a map $F : \mathcal{H}_{\rm phys} \to L^2(\mathbb{R})$, is a unitary operator. In order to see this, let $\psi, \phi \in \mathcal{H}_{\rm phys}$ be arbitrary state vectors and $\Psi = F(\psi)$ and $\Phi = F(\psi)$, then

$$\begin{aligned}\langle F(\psi)|F(\phi)\rangle = \langle \Psi|\Phi\rangle &= \int_{\mathbb{R}} \Psi(x)^* \Phi(x) \, \mathrm{d}x = \int_{\mathbb{R}} \langle \psi, \xi^{(x)}\rangle_+ \langle \xi^{(x)}, \phi\rangle_+ \, \mathrm{d}x \\ &= \int_{\mathbb{R}} \langle \psi, \Xi^{(x)}\phi\rangle_+ \, \mathrm{d}x = \langle \psi, \phi\rangle_+.\end{aligned}$$

In the following, we will assume without loss of generality that ψ is normalized with respect to the inner product $\langle\cdot,\cdot\rangle_+$, i.e., set $\langle \psi, \psi\rangle_+ = \|\Psi\|^2 = 1$.

According to the standard quantum measurement theory, the probability of finding the particle in a region $V \subseteq \mathbb{R}$ at time t_0 is given by

$$\Pi_V(\psi) := \int_V |\langle \xi^{(x)}, \psi\rangle_+|^2 \, \mathrm{d}x. \tag{42}$$

Hence

$$\varrho(x) := |\langle \xi^{(x)}, \psi\rangle_+|^2 = |\Psi(x)|^2 \tag{43}$$

is the *probability density* of the localization of the particle in space.

Unlike the naive 'probability density' $\varrho^{(0)}(x) := |\psi(x)|^2$, $\varrho(x)$ defines a conserved total probability. This follows from the fact that H is Hermitian with respect to the inner product $\langle\cdot,\cdot\rangle_+$ of $\mathcal{H}_{\rm phys}$. It is instructive to demonstrate the conservation of total probability in the position representation. In order to do so, consider the time evolution of the state vector ψ as determined by the Schrödinger equation:

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = H\psi(t). \tag{44}$$

Computing the inner product of both sides of this equation with $\xi^{(x)}$ (using the inner product $\langle\cdot,\cdot\rangle_+$) and employing the completeness relation given in (38), we find

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}\Psi(x;t) = \hat{h}\Psi(x;t), \tag{45}$$

where $\Psi(x;t) := \langle \xi^{(x)}, \psi(t)\rangle_+$ and $\hat{h} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is defined by

$$\hat{h}\Psi(x;t) := \int_{\mathbb{R}} \mathcal{K}(x,y)\Psi(y;t) \, \mathrm{d}y, \qquad \mathcal{K}(x,y) := \langle \xi^{(x)}, H\xi^{(y)}\rangle_+. \tag{46}$$

Because, as an operator acting in $\mathcal{H}_{\rm phys}$, H is Hermitian,

$$\mathcal{K}(x,y)^* = \langle \xi^{(x)}, H\xi^{(y)}\rangle_+^* = \langle H\xi^{(x)}, \xi^{(y)}\rangle_+^* = \langle \xi^{(y)}, H\xi^{(x)}\rangle_+ = \hat{\mathcal{K}}(y,x).$$

[10] Here we view Ψ as an abstract vector belonging to $L^2(\mathbb{R})$. The state vector ψ also belongs to the Hilbert space $\mathcal{H}$ which coincides with $L^2(\mathbb{R})$. However, these two copies of $L^2(\mathbb{R})$ should not be confused.

This is sufficient to conclude that $\hat{h}$ is a Hermitian operator acting in $L^2(\mathbb{R})$. As a result, in the position representation the dynamics is determined by a Hermitian Hamiltonian; the time-evolution operator, $\mathrm{e}^{-\mathrm{i}(t-t_0)\hat{h}/\hbar}$, for the position wavefunctions is unitary; and the total probability

$$\Pi_{\mathbb{R}}(\psi(t)) = \int_{\mathbb{R}} |\Psi(x;t)|^2 \,\mathrm{d}x$$

is conserved.

The Hamiltonian operator $\hat{h}$ is directly related to the Hermitian Hamiltonian h. Substituting (36) in (46) and using (7) and (8), we have

$$\mathcal{K}(x,y) = \langle x|\rho^{-1}\eta_+ H\rho^{-1}|y\rangle = \langle x|h|y\rangle,$$
$$\hat{h}\Psi(x;t) = \int_{\mathbb{R}} \langle x|h|y\rangle\Psi(y;t)\,\mathrm{d}y = \int_{\mathbb{R}} \langle x|h|y\rangle\langle y|\rho\psi(t)\rangle\,\mathrm{d}y = \langle x|h\rho\psi(t)\rangle.$$

Hence, in light of (40), the Hamiltonian $\hat{h}$ is the usual position representation of the Hermitian Hamiltonian h, i.e.,

$$\langle x|h = \hat{h}\langle x|. \tag{47}$$

This relationship between the Hamiltonian operators $\hat{h}$ and h extends to all the physical observables. Given an observable O acting in $\mathcal{H}_{\mathrm{phys}}$ and the corresponding operator $o = \rho O\rho^{-1}$ acting in $\mathcal{H}$, we can define an associated Hermitian operator $\hat{o}$ acting in $L^2(\mathbb{R})$ that realizes the action of O on a state vector $\psi \in \mathcal{H}_{\mathrm{phys}}$ in terms of the corresponding position wavefunction Ψ according to

$$O\psi = \int_{\mathbb{R}} [\hat{o}\Psi(x)]\xi^{(x)}\,\mathrm{d}x. \tag{48}$$

The operator $\hat{o}$ is the position representation of the abstract operator o:

$$\langle x|o = \hat{o}\langle x|. \tag{49}$$

In view of (48), (49), (38) and (40), the expectation value of O in a state described by the normalized state vector ψ and position wavefunction Ψ is given by

$$\langle\psi, O\psi\rangle_+ = \int_{\mathbb{R}} \Psi(x)^*\hat{o}\Psi(x)\,\mathrm{d}x. \tag{50}$$

As shown in the preceding paragraphs, one can formulate both the dynamics and the kinematics of the theory using the position wavefunctions Ψ. In this formulation, the observables and in particular the Hamiltonian are Hermitian operators acting in $\mathcal{H}$ similarly to the conventional quantum mechanics. In order to use this formulation, however, one needs a more explicit expression for the wavefunction Ψ. We may derive such an expression using the canonical metric basis $\{|\epsilon_n\rangle\}$. In view of (10), (11), (32) and (40), we have

$$\Psi(x) = \sum_n f_n\varepsilon_n(x), \qquad f_n := \epsilon_n^{1/2}\int_{\mathbb{R}} \varepsilon_n(x')^*\psi(x')\,\mathrm{d}x'. \tag{51}$$

5. Application to the PT-symmetric square well

The PT-symmetric square well potential, originally introduced by Znojil in [26], provides a simple model with generic properties of general PT-symmetric potentials. Its Hamiltonian is given by

$$H = \frac{p^2}{2m} + v(x), \tag{52}$$

where

$$v(x) = \begin{cases} \infty & \text{for} \quad x \notin \left(-\frac{L}{2}, \frac{L}{2}\right) \\ \mathrm{i}\zeta & \text{for} \quad x \in \left(-\frac{L}{2}, 0\right) \\ -\mathrm{i}\zeta & \text{for} \quad x \in \left(0, \frac{L}{2}\right), \end{cases} \tag{53}$$

$L \in \mathbb{R}^+$ and $\zeta \in \mathbb{R}$. Usually, one employs units in which $L = 2$, $m = 1/2$ and $\hbar = 1$. This is equivalent to using the dimensionless variables

$$x \to \mathrm{x} := \left(\frac{2}{L}\right) x, \qquad p \to \mathrm{p} := \left(\frac{L}{2\hbar}\right) p, \qquad \zeta \to Z := \left(\frac{mL^2}{2\hbar^2}\right) \zeta, \tag{54}$$

and working with the dimensionless Hamiltonian,

$$\mathrm{H} := \left(\frac{mL^2}{2\hbar^2}\right) H = \mathrm{p}^2 + \mathrm{v}(\mathrm{x}), \tag{55}$$

where

$$\mathrm{v}(\mathrm{x}) = \begin{cases} \infty & \text{for} \quad \mathrm{x} \notin (-1, 1) \\ \mathrm{i}Z & \text{for} \quad \mathrm{x} \in (-1, 0) \\ -\mathrm{i}Z & \text{for} \quad \mathrm{x} \in (0, 1). \end{cases} \tag{56}$$

In the x-representation, the eigenvalue problem for H takes the form[11]

$$\left[-\frac{\mathrm{d}^2}{\mathrm{dx}^2} + \mathrm{v}(\mathrm{x}) - \mathrm{E}_n\right] \psi_n(\mathrm{x}) = 0. \tag{57}$$

The Hilbert space to which the eigenvectors ψ_n belong is[12]

$$\mathcal{H} = \{\psi \in L^2(\mathbb{R}) \mid \psi(x) = 0 \text{ for } |x| \geqslant 1\} = \{\psi \in L^2([-1, 1]) \mid \psi(\pm 1) = 0\}. \tag{58}$$

Clearly, H is not Hermitian with respect to the defining inner product $\langle\cdot|\cdot\rangle$ of $\mathcal{H}$. This is an indication that $\mathcal{H}$ is not the physical Hilbert space $\mathcal{H}_{\text{phys}}$. In order to specify the latter, we should determine an appropriate metric operator η_+. This in turn requires the solution of the eigenvalue equation (57).

The eigenvalue problem for the PT-symmetric square well admits an essentially explicit solution. A detailed discussion is provided in [26, 27]. If Z is below the critical value $Z_\star \approx 4.48$ the Hamiltonian has a real spectrum [26][13]. For these values of the 'non-Hermiticity' parameter Z, the Hilbert spaces $\mathcal{H}$ and $\mathcal{H}_{\text{phys}}$ are identical as complex vector spaces, i.e., they are obtained by endowing their common vector space with different inner products.

In this paper, we will only be concerned with the case $0 \leqslant Z < Z_\star$. For these values of Z, one obtains the following complete set of eigenfunctions of H,

$$\psi_n(\mathrm{x}) = \begin{cases} \psi_{n-}(\mathrm{x}) & \text{for} \quad \mathrm{x} \in [-1, 0] \\ \psi_{n+}(\mathrm{x}) & \text{for} \quad \mathrm{x} \in [0, 1], \end{cases} \tag{59}$$

$$\psi_{n\pm}(\mathrm{x}) := \frac{\alpha_n \sinh[\kappa_{n\pm}(1 \mp x)]}{\sinh(\kappa_{n\pm})}, \tag{60}$$

[11] The eigenvalues E_n of the Hamiltonian (52) are given by $2\hbar^2 \mathrm{E}_n/(mL^2)$.

[12] The Hilbert space associated with the unscaled Hamiltonian H is obtained by changing 1 in (58) to $L/2$.

[13] $Z = Z_\star$ marks an exceptional point [28] where two real eigenvalues cross in such a way that the Hamiltonian becomes non-diagonalizable. Once Z exceeds $Z_\star$, H regains its diagonalizability, but a pair of complex-conjugate eigenvalues appear in its spectrum [10, 6]. Increasing the value of Z indefinitely one encounters an infinite number of exceptional points passing each of which produces a complex-conjugate pair of eigenvalues.

where α_n are arbitrary nonzero real coefficients,

$$\kappa_{n\pm} = s_n \mp \mathrm{i}t_n, \tag{61}$$

$$s_n := \frac{Z}{2t_n}, \tag{62}$$

and t_n with $n \in \mathbb{Z}^+$ are the real solutions of the transcendental equation:

$$(Z/t_n)\sinh(Z/t_n) + 2t_n \sin(2t_n) = 0. \tag{63}$$

The eigenvalues E_n are given by

$$\mathrm{E}_n = -\left(\kappa_{n+}^2 + \mathrm{i}Z\right) = t_n^2 - s_n^2. \tag{64}$$

Usually, the coefficients α_n are fixed arbitrarily [26] or kept as unimportant free coefficients [27]. We will fix them in such a way that in the limit $Z \to 0$, the eigenfunctions ψ_n of (59) tend to the well-known normalized eigenfunctions $\psi_n^{(0)}$ of the conventional (Hermitian) square well Hamiltonian (the case $Z = 0$):

$$\lim_{Z\to 0} \psi_n = \psi_n^{(0)} := \psi_n|_{_{Z=0}}. \tag{65}$$

Because, by construction, ψ_n are also the eigenfunctions of the PT operator, the continuity requirement (65) constrains $\psi_n^{(0)}$ to be PT invariant. The normalized and PT-invariant eigenfunctions of the Hermitian infinite square well potential ($Z = 0$) are, up to a sign, given by

$$\psi_n^{(0)}(\mathrm{x}) = \mathrm{i}^{\mu_n} \sin\left[\frac{\pi n}{2}(\mathrm{x}+1)\right], \tag{66}$$

where

$$\mu_n := \frac{1+(-1)^n}{2}. \tag{67}$$

The eigenfunctions (66) form an orthonormal basis of the Hilbert space (58). We will denote the corresponding abstract basis vectors by $|n\rangle$, i.e.,

$$\langle \mathrm{x}|n\rangle := \psi_n^{(0)}(\mathrm{x}), \qquad \text{for all} \quad n \in \mathbb{Z}^+. \tag{68}$$

The continuity requirement (65) together with equation (66) restricts the coefficients α_n of the eigenfunctions (59). Specifically, if we only keep the leading-order term in powers of Z and neglect the higher order terms, we find

$$\alpha_n = (-1)^{\lfloor \frac{n}{2} \rfloor} \left(\frac{Z}{\pi n}\right)^{\mu_n}, \tag{69}$$

where $\lfloor \frac{n}{2} \rfloor$ stands for the integer part of $\frac{n}{2}$. Both the eigenvalues E_n and the eigenfunctions ψ_n are therefore determined once we obtain the solutions of (63). As shown in [26], this equation may be easily solved numerically for various values of Z. In this paper, we will solve this equation perturbatively by expanding the relevant quantities in powers of Z.

5.1. Perturbative calculation of ψ_n and E_n

Suppose that t_n admits a power series expansion about $Z = 0$,

$$t_n = \sum_{k=0}^{\infty} t_n^{(k)} Z^k, \tag{70}$$

where $t_n^{(k)} \in \mathbb{R}$ are to be determined. Substituting (70) in (63), expanding both sides of the resulting equation in powers of Z, solving it term by term for $t_n^{(k)}$, and using (70), (62) and (64), we find

$$t_n = \left(\frac{\pi n}{2}\right)\left\{1 - (-1)^n\nu^2 - \left[3 + \frac{(-1)^n\pi^2n^2}{6}\right]\nu^4 + \mathcal{O}(\nu^6)\right\}, \tag{71}$$

$$s_n = \left(\frac{\pi n\nu}{2}\right)\left\{1 + (-1)^n\nu^2 + \left[4 + \frac{(-1)^n\pi^2n^2}{6}\right]\nu^4 + \mathcal{O}(\nu^6)\right\}, \tag{72}$$

$$\mathrm{E}_n = \left(\frac{\pi n}{2}\right)^2\left\{1 - [1 + 2(-1)^n]\nu^2 - \left[5 + 2(-1)^n + \frac{(-1)^n\pi^2n^2}{3}\right]\nu^4 + \mathcal{O}(\nu^6)\right\}, \tag{73}$$

where

$$\nu := \frac{2Z}{(\pi n)^2}, \tag{74}$$

and $\mathcal{O}(\nu^k)$ stands for terms of order ν^k and higher.

Equations (71)–(73) reveal the curious fact that the effective perturbation parameter is $2Z/(\pi n)^2$.[14] This is a clear indication that the non-Hermiticity of the Hamiltonian H only affects the low-lying energy levels. This property of the PT-symmetric square well Hamiltonian—which has been previously known [26]—is particularly significant, for as we explain below it implies that within the confines of the perturbation theory all the infinite sums appearing in the expressions (5), (18) and (51) for the metric operator η_+, the Hermitian Hamiltonian h, and the position wavefunctions may be safely truncated. For example, for $Z = 1$, $\nu \approx 0.2/n^2$. Therefore, if we set $\mathrm{E}_n^{(0)} := \mathrm{E}_n|_{\nu=0} = (\pi n/2)^2$ and use $q_n := \left|\mathrm{E}_n/\mathrm{E}_n^{(0)} - 1\right|$ as a measure of the contribution of the non-Hermiticity of the Hamiltonian to the energy eigenvalues, we find for $n > 10$ $\nu < 2 \times 10^{-3}$ and $q_n < 1.3 \times 10^{-5}$.[15] More generally, we can ignore the effects of the non-Hermiticity parameter Z for all the computations involving the levels with $n > 10$ and still obtain results that are accurate at least up to three decimal places.

In the following, we will employ an approximation scheme that neglects the effects of the non-Hermiticity parameter Z for all levels with n greater than a given number N. In view of the above discussion, the results obtained using this approximation will have an accuracy of the order of

$$\nu_N = \frac{2Z}{(\pi N)^2}. \tag{75}$$

We will respectively refer to N and ν_N as the 'order' and the 'accuracy index' of our approximation scheme.

5.2. *Construction of a canonical metric basis*

Having obtained the expression for (71) and (72) for t_n and s_n, we can compute κ_n and use equations (59), (60) and (69) to determine the eigenfunctions ψ_n of the Hamiltonian H as a power series in ν.

[14] The condition that the above perturbative calculations would be unreliable for the ground state, i.e., $\nu \approx 1$, corresponds to $Z \approx 4.92$ which is slightly above the critical value $Z_\star = 4.48$.

[15] The value $Z = 1$, say for an electron ($m \approx 10^{-30}$ Kg) confined in a nanometre size well ($L \approx 10^{-9}$ m), corresponds to an energy scale $\zeta \approx 0.1$ eV for the potential (53). This is comparable with the ground state energy ($E_1 \approx 0.5$ eV) of the corresponding Hermitian infinite square well potential.

The computation of a metric operator η_+, however, involves the eigenfunctions ϕ_n of the adjoint $\mathrm{H}^\dagger$ of H. It is easy to see that $\mathrm{H}^\dagger = \mathrm{H}|_{Z\to -Z}$. This suggests that

$$\chi_n := \psi_n|_{Z\to -Z} \tag{76}$$

are eigenfunctions of $\mathrm{H}^\dagger$. The eigenfunctions ϕ_n, which together with ψ_n form a biorthonormal system for the Hilbert space $\mathcal{H}$, are obtained by properly normalizing χ_n. They are given by

$$\phi_n(\mathrm{x}) = N_n^{-1}\,\chi_n(\mathrm{x}), \tag{77}$$

where

$$\begin{aligned} N_n &:= \langle\psi_n|\chi_n\rangle = \int_{-1}^{1} \psi_n(\mathrm{x})^*\chi_n(\mathrm{x})\,\mathrm{dx} \\ &= \frac{2\alpha_{n+}\alpha_{n-}\big[1-\cos(2t_n)\cosh(2s_n)+\frac{t_n\sin(2t_n)[\cos(2t_n)-\cosh(2s_n)]}{s_n^2+t_n^2}\big]}{[\cos(2t_n)-\cosh(2s_n)]^2}, \end{aligned} \tag{78}$$

and

$$\alpha_{n+} := \alpha_n, \qquad \alpha_{n-} := \alpha_n|_{Z\to -Z}. \tag{79}$$

Next, we construct the metric operator (5) using the approximation scheme described in the preceding section and the orthonormal basis $\{|n\rangle\}$ consisting of the eigenvectors (68) of the ordinary Hermitian infinite square well.

In the Nth order approximation, we have

$$|\psi_n\rangle \overset{N}{\approx} |\phi_n\rangle \overset{N}{\approx} |n\rangle, \qquad \text{for all} \quad n > N, \tag{80}$$

where '$\overset{N}{\approx}$' stands for an equality that is valid up to terms of order ν_N. Combining (80) with (5) we have

$$\eta_+ \overset{N}{\approx} \sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n| + \sum_{n=N+1}^{\infty} |n\rangle\langle n| = 1 + \delta\eta_+^{(N)}, \tag{81}$$

$$\delta\eta_+^{(N)} := \sum_{n=1}^{N} (|\phi_n\rangle\langle\phi_n| - |n\rangle\langle n|). \tag{82}$$

This relation shows that the metric operator η_+ is essentially determined by its projection onto the span $\mathcal{H}_N$ of $|n\rangle$ with $n \leqslant N$. Indeed, at this order of approximation, $\mathcal{H}_N$ may also be identified with the span of ψ_n with $n \leqslant N$, or the span of ϕ_n with $n \leqslant N$.

Clearly, the Hilbert space $\mathcal{H}$ is the direct sum of $\mathcal{H}_N$ and its orthogonal complement $\mathcal{H}_N^\perp := \{\zeta \in \mathcal{H} | \langle\zeta|\psi\rangle = 0, \forall\psi \in \mathcal{H}_N\}$. As shown by (81) both of these are invariant subspaces [29] of η_+. Therefore, one can solve the eigenvalue problem for η_+ by restricting it onto $\mathcal{H}_N$ and $\mathcal{H}_N^\perp$ and diagonalize the resulting operators separately. The restriction of η_+ onto $\mathcal{H}_N^\perp$ coincides with that of the identity operator. In particular, it is diagonalized in the basis $\{|n\rangle : n > N\}$, and we have

$$|\epsilon_n\rangle \overset{N}{\approx} |n\rangle \quad \text{and} \quad \epsilon_n \overset{N}{\approx} 1, \qquad \text{for all} \quad n > N. \tag{83}$$

The restriction of η_+ onto $\mathcal{H}_N$ yields a Hermitian operator having a Hermitian matrix representation $\mathcal{E}$ in the basis $\{|n\rangle : n \leqslant N\}$. According to (81), the matrix elements of $\mathcal{E}$ are given by

$$\mathcal{E}_{mn} = \langle m|\eta_+|n\rangle = \sum_{k=1}^{N} \langle m|\phi_k\rangle\langle\phi_k|n\rangle, \tag{84}$$

which in view of (76)–(79), (59)–(62), (69), (71) and (72) can be computed explicitly. The computation of the metric basis vectors $|\epsilon_n\rangle$ with $n \leqslant N$ is equivalent to the diagonalization of the Hermitian matrix $\mathcal{E}$. The latter can be done both numerically and perturbatively.

Let $\{\vec{e}_n\}$ be a set of orthonormal eigenvectors of $\mathcal{E}$ so that $\mathcal{E}\vec{e}_n = e_n\vec{e}_n$. Then clearly, up to permutations of the labels, e_n coincide with ϵ_n for $n \leqslant N$. The canonical metric basis vectors $|\epsilon_n\rangle$, with $n \leqslant N$, are also related to the eigenvectors $\vec{e}_n$. To make this relation explicit, we introduce the unitary $N \times N$ matrix $\mathcal{U}$ whose columns coincide with the vectors $\vec{e}_n$. Then, in view of (11), it is a straightforward exercise to show that

$$|\epsilon_n\rangle \overset{N}{\approx} \sum_{m=1}^{N} \mathcal{U}_{mn}|m\rangle \quad \text{and} \quad \epsilon_n \overset{N}{\approx} e_n, \qquad \text{for all} \quad n \leqslant N. \tag{85}$$

Clearly, the above approximation scheme would be consistent only if in the above calculation of $\mathcal{E}_{mn}$, e_n and $\vec{e}_n$ one takes into account the contribution of the terms of order ν^ℓ for which $\nu^\ell \geqslant \nu_N$. We can use equations (74) and (75) to make this condition more explicit. A simple calculation shows that the negligible terms are those of order ν^ℓ with $\ell > \ell_n$, where

$$\ell_n := \frac{\ln(N) + r}{\ln n + r}, \qquad r := \ln\left(\frac{\pi}{\sqrt{2Z}}\right) \approx 0.789 - \frac{\ln Z}{2}. \tag{86}$$

Clearly, for smaller values of n one should include higher order corrections, the highest order term being of the order ν^{ℓ_1}. For example, for $Z \leqslant 1$ and $N \leqslant 25$, $\ell_1 \leqslant 5.03$ and one can safely ignore $\mathcal{O}(\nu^6)$. For the values $Z = 1$ and $N = 25$, the results will have a minimum accuracy of the order of $\nu_N \approx 3.2 \times 10^{-4}$. Similarly for $Z \leqslant 0.5$ and $N \leqslant 100$, $\ell_1 \leqslant 5.02$ and one can again ignore $\mathcal{O}(\nu^6)$. The minimum accuracy corresponding to the values $Z = 0.5$ and $N = 100$ is of the order of $\nu_N \approx 1.0 \times 10^{-5}$. Note that for all the above values of Z and N the terms given explicitly in equations (71)–(73) are sufficient to perform a consistent perturbative calculation. A direct check of the validity of this statement is to compare the exact value $\mathrm{E}_n^{\mathrm{exact}}$ of E_n obtained by an accurate numerical solution of (63) and the perturbative value $\mathrm{E}_n^{\mathrm{pert}}$ of E_n calculated using (73) and ignoring $\mathcal{O}(\nu^6)$. Clearly, the largest difference is for $n = 1$. If we express

$$\mathrm{E}_1^{\mathrm{exact}} = \frac{\pi^2}{4}\big(1 + \epsilon_1^{\mathrm{exact}}\big), \qquad \mathrm{E}_1^{\mathrm{pert}} = \frac{\pi^2}{4}\big(1 + \epsilon_1^{\mathrm{pert}}\big),$$

we find, for $Z = 1$, $\epsilon_1^{\mathrm{exact}} = 0.041\,5652$, $\epsilon_1^{\mathrm{pert}} = 0.041\,5527$. This is in complete agreement with our expectations, because the difference, $\epsilon_1^{\mathrm{exact}} - \epsilon_1^{\mathrm{pert}} = 1.244\,65 \times 10^{-5}$, is much smaller than the accuracy index $\nu_{N=25} \approx 3.2 \times 10^{-4}$.

Next, observe that our approximation, in particular (81), corresponds to $\eta_+ \overset{N}{\approx} \eta_+^{(N)}$ where

$$\eta_+^{(N)}\psi := \begin{cases} \eta_+\psi & \text{if} \quad \psi \in \mathcal{H}_N \\ \psi & \text{if} \quad \psi \in \mathcal{H}_N^{\perp}. \end{cases}$$

It is a reliable approximation, only if the distance between $\eta_+^{(N)}$ and the identity operator 1, as defined by

$$\sigma_N := \sqrt{\mathrm{trace}\big[\big(\eta_+^{(N)} - 1\big)^2\big]} = \sqrt{\mathrm{trace}\big[\big(\delta\eta_+^{(N)}\big)^2\big]}, \tag{87}$$

has a finite large N-limit. This makes σ_N a useful measure of the validity of the above approximate calculation of the canonical metric basis $\{|\epsilon_n\rangle\}$. Clearly, σ_N is just the Frobenius or Euclidean distance [30] between $\mathcal{E}$ and the $N \times N$ identity matrix I:

$$\sigma_N = \|\mathcal{E} - I\|_2 = \sqrt{\mathrm{trace}[(\mathcal{E} - I)^2]} = \left[\sum_{n=1}^{N}(\epsilon_n - 1)^2\right]^{1/2}, \tag{88}$$

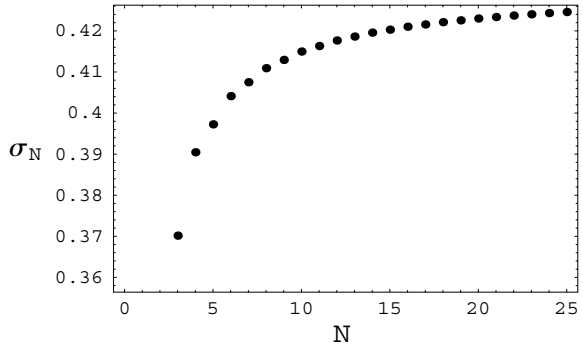

Figure 1. Graph of σ_N as a function of N, for $Z = 1$.

where $\|\cdot\|_2$ stands for the Frobenius (Euclidean) norm [30], defined for every square matrix M by

$$\|M\|_2 := \sqrt{\text{trace}(M^\dagger M)}. \tag{89}$$

Figure 1 shows a plot of σ_N for $Z = 1$ and $N \leqslant 25$ for which we can neglect $\mathcal{O}(\nu^6)$ in our calculations while retaining the consistency of our approximation scheme. The graph of σ_N clearly shows the desired behaviour even for $N \approx 20$. The effective slope $\sigma_N - \sigma_{N-1}$ of the graph has the values 4.4×10^{-4} and 2.5×10^{-4} for $N = 20$ and $N = 25$, respectively.

Next, we describe another way of checking the reliability of our approximation scheme. In view of (80) and (4), the matrix elements

$$\mathrm{H}^{(0)}_{mn} := \langle m|\mathrm{H}|n\rangle \tag{90}$$

may be approximated as

$$\mathrm{H}^{(0)}_{mn} \overset{N}{\approx} \begin{cases} \mathcal{X}^{(N)}_{mn} & \text{for} \quad m, n \leqslant N \\ \frac{1}{4}\pi^2 n^2 \delta_{mn} & \text{for} \quad m, n > N, \end{cases} \tag{91}$$

where

$$\mathcal{X}^{(N)}_{mn} := \sum_{k=1}^{N} \mathrm{E}_k \langle m|\psi_k\rangle\langle\phi_k|n\rangle \tag{92}$$

are computed by substituting (71) and (72) in (61) and using (60), (73) and (77).

Consider the $N \times N$ matrix $\mathcal{X}^{(N)}$ with entries (92) and let $\mathcal{Y}^{(N)}$ be the $N \times N$ matrix with entries $\mathcal{Y}^{(N)}_{mn} := \mathrm{H}^{(0)}_{mn}$ for all $m, n \leqslant N$. Then $\mathcal{Y}^{(N)}$ may be computed exactly using (55), (66), (68) and (90), whereas the calculation of $\mathcal{X}^{(N)}$ uses our approximation scheme. In order to compare $\mathcal{X}^{(N)}$ and $\mathcal{Y}^{(N)}$, we will first introduce the normalized matrices,

$$\hat{\mathcal{X}}^{(N)} := \frac{\mathcal{X}^{(N)}}{\|\mathcal{X}^{(N)}\|_2}, \qquad \hat{\mathcal{Y}}^{(N)} := \frac{\mathcal{Y}^{(N)}}{\|\mathcal{Y}^{(N)}\|_2},$$

and use the Euclidean distance between the matrices $\hat{\mathcal{X}}^{(N)}$ and $\hat{\mathcal{Y}}^{(N)}$, namely

$$\Sigma_N := \|\hat{\mathcal{X}}^{(N)} - \hat{\mathcal{Y}}^{(N)}\|_2, \tag{93}$$

as a measure of the accuracy of our approximation. A reliable approximation corresponds to a vanishing large N-limit of Σ_N.[16] Figure 2 shows the plot of Σ_N for $N \leqslant 25$ and $Z = 1$.

[16] Our use of the normalized matrices $\hat{\mathcal{X}}^{(N)}$ and $\hat{\mathcal{Y}}^{(N)}$ stems from the fact that H is not a bounded operator. It allows for the interpretation of the term 'a vanishing large N-limit' as '$\Sigma_N \ll 1$ for sufficiently large N'. In practice this means $\Sigma_N \leqslant \nu_N$.

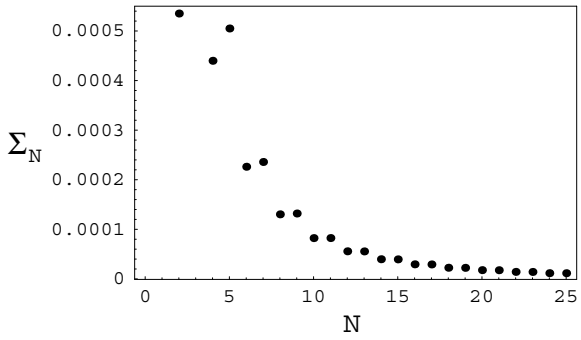

Figure 2. Graph of Σ_N of equation (93) as a function of N, for $Z = 1$. Note that $\Sigma_{25} \approx 1.1 \times 10^{-5}$.

Table 1. Values of Σ_N of equation (93), S_n of equation (101), and the accuracy index $\nu_N = 2Z/(\pi N)^2$ for $Z = 1$ and various relevant values of N.

N	Σ_N	S_N	ν_N
10	8.2×10^{-5}	1.7×10^{-5}	2.0×10^{-3}
15	3.9×10^{-5}	9.0×10^{-6}	9.0×10^{-4}
20	1.7×10^{-5}	3.4×10^{-6}	5.1×10^{-4}
25	1.1×10^{-5}	2.4×10^{-6}	3.2×10^{-4}

Table 1 lists the values of Σ_N for various values of N and the corresponding values for the accuracy index ν_N. The results indicate that even for $N = 10$ we have a highly reliable approximation.

5.3. Construction of the Hermitian Hamiltonian h

We can use the above approximation scheme to compute the Hermitian Hamiltonian $\mathrm{h} := \rho \mathrm{H} \rho^{-1}$ (respectively $h = \rho H \rho^{-1} = 2\hbar^2 \mathrm{h}/(mL^2)$) that is associated with the PT-symmetric square well Hamiltonian H (respectively H). In order to do this we first use (18), (80), (83), (85), to express h in the form

$$\mathrm{h} \overset{N}{\approx} \sum_{m,n=1}^{N} \sqrt{\frac{\epsilon_m}{\epsilon_n}} \mathrm{H}_{mn} |\epsilon_m\rangle\langle\epsilon_n| + \sum_{m,n=N+1}^{\infty} \mathrm{H}^{(0)}_{mn} |m\rangle\langle n| + \sum_{m=1}^{N} \sum_{n=N+1}^{\infty} \left[\sqrt{\epsilon}_m H_{mn} |\epsilon_m\rangle\langle n| + \frac{1}{\sqrt{\epsilon}_m} H_{nm} |n\rangle\langle\epsilon_m| \right] = \mathrm{H} + \delta\mathrm{H}, \tag{94}$$

where $\mathrm{H}^{(0)}_{mn}$ is given by (90),

$$\mathrm{H}_{mn} = \langle\epsilon_m|\mathrm{H}|\epsilon_n\rangle \overset{N}{\approx} \begin{cases} \sum_{j,k=1}^{N} \mathcal{U}^{\dagger}_{mj} \mathrm{H}^{(0)}_{jk} \mathcal{U}_{kn} & \forall m, n \leqslant N, \\ \langle\epsilon_m|\mathrm{H}|n\rangle \overset{N}{\approx} \langle\epsilon_m|\mathrm{H}|\psi_n\rangle = \mathrm{E}_n \langle\epsilon_m|n\rangle \overset{N}{\approx} 0 & \forall m \leqslant N, \quad n > N, \end{cases} \tag{95}$$

$$\delta\mathrm{H} := \sum_{m,n=1}^{N} \left(\sqrt{\frac{\epsilon_m}{\epsilon_n}} \mathrm{H}_{mn} |\epsilon_m\rangle\langle\epsilon_n| - \mathrm{H}^{(0)}_{mn} |m\rangle\langle n| \right). \tag{96}$$

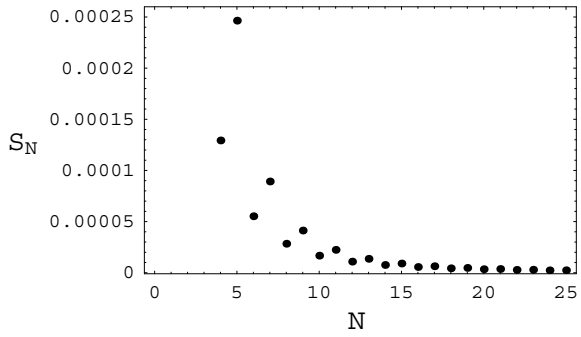

Figure 3. Graph of S_N of equation (101) as a function of N, for $Z = 1$. Note that $S_{25} = 2.4 \times 10^{-6}$.

Substituting (95) in (96) and using (85) and

$$\mathcal{E}_{jk}^{\pm 1/2} = \sum_{m=1}^{N} \mathcal{U}_{jm}\, \epsilon_m^{\pm 1/2}\, \mathcal{U}_{mk}^{\dagger}, \tag{97}$$

we find

$$\delta \mathrm{H} = \sum_{m,n=1}^{N} \delta \mathrm{H}_{mn}^{(0)} |m\rangle\langle n|, \tag{98}$$

where, for all $m, n \in \{1, 2, \ldots, N\}$,

$$\delta \mathrm{H}_{mn}^{(0)} := \sum_{j,k=1}^{N} \mathcal{E}_{mj}^{1/2} \mathrm{H}_{jk}^{(0)} \mathcal{E}_{kn}^{-1/2} - \mathrm{H}_{mn}^{(0)}. \tag{99}$$

To confirm the consistency of our approximate calculation of h, we check its Hermiticity. To do this we compare the $N \times N$ matrices $\mathcal{Q}^{(N)}$ and $\mathcal{Q}^{(N)\dagger}$ defined in terms of their entries according to $\mathcal{Q}_{mn}^{(N)} := \langle m|\mathrm{h}|n\rangle$ and $\mathcal{Q}_{mn}^{(N)\dagger} := \mathcal{Q}_{nm}^{(N)*} = \langle n|\mathrm{h}|m\rangle^*$. Clearly, the condition $\mathrm{h}^\dagger = \mathrm{h}$ is equivalent to

$$\mathcal{Q}^{(N)\dagger} \to \mathcal{Q}^{(N)} \qquad \text{as} \quad N \to \infty. \tag{100}$$

Noting that H is not a bounded operator, we follow the method of the preceding section and define the normalized matrix $\hat{\mathcal{Q}}^{(N)} := \mathcal{Q}^{(N)}/\|\mathcal{Q}^{(N)}\|_2$. This allows us to identify the Hermiticity condition (100) with

$$S_N := \|\hat{\mathcal{Q}}^{(N)} - \hat{\mathcal{Q}}^{(N)\dagger}\|_2 \leqslant \nu_N. \tag{101}$$

Figure 3 shows the plot of S_N for $N \leqslant 25$ and $Z = 1$. Table 1 shows some typical values of S_N. The results depicted in figure 3 and table 1 are in complete agreement with (101).

Having obtained the matrix elements of δH in the basis $\{|n\rangle\}$, we can compute its integral kernel,

$$\mathcal{K}_{\delta \mathrm{H}}(\mathrm{x}, \mathrm{x}') := \langle \mathrm{x}|\delta \mathrm{H}|\mathrm{x}'\rangle, \tag{102}$$

and the corresponding pseudo-differential operator in the x-representation. In view of (66), (68) and (98),

$$\begin{aligned} \mathcal{K}_{\delta \mathrm{H}}(\mathrm{x}, \mathrm{x}') &= \sum_{m,n=1}^{N} \delta \mathrm{H}_{mn}^{(0)} \psi_m^{(0)}(\mathrm{x}) \psi_n^{(0)}(\mathrm{x}')^* \\ &= \sum_{m,n=1}^{N} \Delta_{mn} \sin\left[\frac{\pi m}{2}(\mathrm{x}+1)\right] \sin\left[\frac{\pi n}{2}(\mathrm{x}'+1)\right], \end{aligned} \tag{103}$$

where

$$\Delta_{mn} := \mathrm{i}^{\mu_m-\mu_n}\delta \mathrm{H}^{(0)}_{mn}. \tag{104}$$

Next, we follow the derivation of equations (27)–(29) to express $\delta\mathrm{H}$ as a series in powers of the momentum operator p. This yields

$$\delta\mathrm{H} = \sum_{\ell=0}^{\infty} \delta_\ell(\mathrm{x})\mathrm{p}^\ell, \tag{105}$$

where

$$\delta_\ell(\mathrm{x}) := \mathrm{i}^\ell \tilde{\delta}_\ell(\mathrm{x}), \tag{106}$$

$$\tilde{\delta}_\ell(\mathrm{x}) := \frac{1}{\ell!}\int_{-1}^{1} \mathcal{K}_{\delta\mathrm{H}}(\mathrm{x},\mathrm{x}')(\mathrm{x}'-\mathrm{x})^\ell\,\mathrm{d}\mathrm{x}' = \sum_{m,n=1}^{N} \Delta_{mn}\sin\Big[\frac{\pi m}{2}(\mathrm{x}+1)\Big]\mathcal{P}_{n\ell}(\mathrm{x}), \tag{107}$$

$$\mathcal{P}_{n\ell}(\mathrm{x}) := \frac{1}{\ell!}\int_{-1}^{1} \sin\Big[\frac{\pi n}{2}(\mathrm{x}'+1)\Big](\mathrm{x}'-\mathrm{x})^\ell\,\mathrm{d}\mathrm{x}'. \tag{108}$$

Using (52)–(56) and (94) we then obtain

$$\mathrm{h} \overset{N}{\approx} \mathrm{H} + \sum_{\ell=0}^{\infty}\delta_\ell(\mathrm{x})\mathrm{p}^\ell = \mathrm{p}^2 + \mathrm{v}(\mathrm{x}) + \sum_{\ell=0}^{\infty}\delta_\ell(\mathrm{x})\mathrm{p}^\ell. \tag{109}$$

The analogous expression for the Hermitian Hamiltonian h associated with the unscaled Hamiltonian H is

$$h \overset{N}{\approx} \frac{p^2}{2m} + v(x) + \sum_{\ell=0}^{\infty}\gamma_\ell(x)\,p^\ell, \tag{110}$$

where

$$\gamma_\ell(x) := \frac{L^{\ell-2}\delta_\ell(2x/L)}{m2^{\ell-1}\hbar^{\ell-2}}. \tag{111}$$

The integral in (108) may be evaluated analytically. A simple change of variable reduces it to an integral of the form $\int_0^\pi y^m \sin(ny)\,\mathrm{d}y$ that may be looked up in [31]. Substituting the value of this integral in (108) and doing the necessary algebra, we find

$$\mathcal{P}_{n\ell}(\mathrm{x}) = \sum_{j=0}^{\ell} a_{nj\ell}(\mathrm{x}+1)^{\ell-j}, \tag{112}$$

where

$$a_{nj\ell} := \frac{(-1)^\ell 2^{j+1}}{(\ell-j)!}\left\{\sum_{k=0}^{\lfloor\frac{j}{2}\rfloor}\frac{(-1)^{j+n+k+1}}{(\pi n)^{2k+1}(j-2k)!} + \frac{(-1)^{\lfloor\frac{j}{2}\rfloor}[1+(-1)^j]}{2(\pi n)^{j+1}}\right\}, \tag{113}$$

and $\lfloor\frac{j}{2}\rfloor$ denotes the integer part of $\frac{j}{2}$. As seen from (112), $\mathcal{P}_{n\ell}$ is a polynomial of degree ℓ.

Using (112) we can obtain a more explicit expression for the coefficient functions δ_ℓ appearing in (109) and (111). Substituting (112) in (107) and introducing

$$b_{mk\ell} := \sum_{n=1}^{N}\Delta_{mn}a_{nk\ell}, \tag{114}$$

we have

$$\tilde{\delta}_\ell(\mathrm{x}) = \sum_{k=0}^{\ell}\sum_{m=1}^{N} b_{mk\ell}\sin\Big[\frac{\pi m}{2}(\mathrm{x}+1)\Big](\mathrm{x}+1)^{\ell-k}. \tag{115}$$

This relation together with (106) yields the desired expression for $\delta_\ell(\mathrm{x})$.

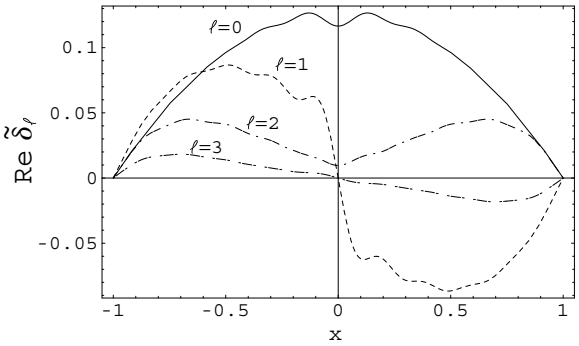

Figure 4. Plot of $\mathrm{Re}[\tilde{\delta}_\ell]$ for $\ell = 0, 1, 2, 3$, $Z = 1$ and $N = 20$.

Next, we recall that the standard calculation (50) of the energy expectation value for a state vector $\psi \in \mathcal{H}_{\rm phys}$, which uses the position wavefunction Ψ introduced in section 4, involves the representation $\hat{\mathrm{h}}$ of the Hermitian Hamiltonian h:

$$\langle \psi, H\psi\rangle_+ = \frac{2\hbar^2}{mL^2}\,\langle \psi, \mathrm{H}\psi\rangle_+ = \frac{2}{mL^2}\int_{-1}^{1} \Psi(\mathrm{x})^*\,\hat{\mathrm{h}}\Psi(\mathrm{x})\,\mathrm{dx}.$$

Using $\langle \mathrm{x}|\mathrm{h} = \hat{\mathrm{h}}\langle \mathrm{x}|$, the identity

$$\langle \mathrm{x}|\mathrm{p} = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{dx}}\langle \mathrm{x}|, \tag{116}$$

and equations (106), (109), (115) and (114), we have

$$\hat{\mathrm{h}} \overset{N}{\approx} -\frac{\mathrm{d}^2}{\mathrm{dx}^2} + \mathrm{v}(\mathrm{x}) + \sum_{\ell=0}^{\infty} \tilde{\delta}_\ell(\mathrm{x})\frac{\mathrm{d}^\ell}{\mathrm{dx}^\ell}. \tag{117}$$

Figures 4 and 5 show the plots of the real and imaginary parts of $\tilde{\delta}_\ell(\mathrm{x})$ for $\ell = 0, 1, 2, 3$, $Z = 1$ and $N = 20$. As seen from figure 5, the graph of $\mathrm{Im}(\tilde{\delta}_0)$ is reminiscent of the approximation of a step function, namely iv, with the first few terms in its Fourier series expansion. In the appendix we offer an explanation for this observation. Furthermore, these figures suggest that $\delta_\ell(\mathrm{x})$ and consequently $\tilde{\delta}_\ell(\mathrm{x})$ have a vanishing large ℓ-limit. This can be established analytically. Using (106)–(108) and the fact that for all $\mathrm{x}, \mathrm{x}' \in [-1, 1]$ both $(\mathrm{x} - \mathrm{x}')/2$ and $\sin[\pi m(\mathrm{x}' + 1)/2]$ are bounded by 1, we can easily conclude that

$$|\tilde{\delta}_\ell(\mathrm{x})| \leqslant \frac{M2^\ell}{\ell!}, \tag{118}$$

where M is a positive number depending on Δ_{mn}. This shows that, for all $\mathrm{x} \in [-1, 1]$, $\lim_{\ell\to\infty} \tilde{\delta}_\ell(\mathrm{x}) = 0$.

5.4. The classical Hamiltonian

Having obtained the Hermitian Hamiltonian h for the PT-symmetric square well, we can use the prescription described in section 3 to obtain the following expression for an underlying classical Hamiltonian,

$$H_c(x_c, p_c) \overset{N}{\approx} \frac{p_c^2}{2m} + \sum_{\ell=0}^{\infty} \mathrm{Re}[\gamma_\ell(x_c)]p_c^\ell, \tag{119}$$

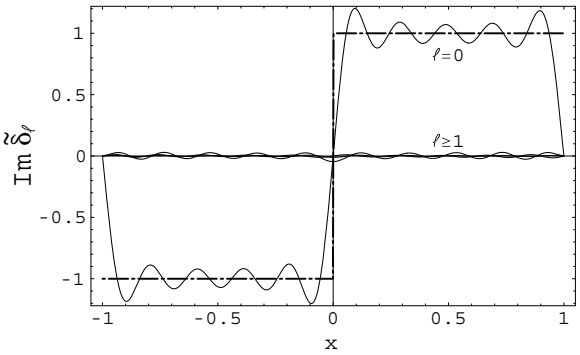

Figure 5. Plot of $\mathrm{Im}[\tilde{\delta}_\ell]$ for $\ell = 0, 1, 2, 3$, $Z = 1$ and $N = 20$. The dashed curve is the graph of iv. The resemblance of the graphs of $\mathrm{Im}[\tilde{\delta}_0]$ and iv is described in the appendix. The difference between $\mathrm{Im}[\tilde{\delta}_\ell]$ with $\ell \geqslant 1$ is too small to be distinguished in the energy scale determined by the potential which is unity in the units used.

where $x_c \in [-L/2, L/2]$ and $p_c \in \mathbb{R}$. Equation (119) is a meaningful relation, only if the series on its right-hand side converges. In view of (106) and (111), the latter is equivalent to the convergence of

$$\sum_{\ell-0}^{\infty} \mathrm{Re}[\delta_\ell(\mathrm{x}_c)]\mathrm{p}_c^\ell, \tag{120}$$

where $\mathrm{x}_c \in [-1, 1]$ and $\mathrm{p}_c \in \mathbb{R}$. According to (118), for all $\mathrm{x}_c \in [-1, 1]$, $|\mathrm{Re}[\delta_\ell(\mathrm{x}_c)]| \leqslant M2^\ell/\ell!$. Using this relation (and performing the comparison and ratio tests [32]) we can easily show that the series (120) converges (absolutely) for all values of $\mathrm{p}_c \in \mathbb{R}$ and $\mathrm{x}_c \in [-1, 1]$. Hence (119) is a meaningful expression yielding a well-defined classical Hamiltonian.

Note that H_c as given by (119) is not the classical Hamiltonian in the strict sense that it would not involve $\hbar$. This is simply because we have not evaluated the $\hbar \to 0$ limit. Indeed, for the PT-symmetric square well Hamiltonian (52), the assumption that this limit exists has drastic implications. This is simply because, according to (54), if we assume that the coupling constant ζ appearing in (53) does not depend on $\hbar$, then taking the limit $\hbar \to 0$ corresponds to $Z \to \infty$. This implies the occurrence of an infinite number of complex eigenvalues which in turn indicates that the system does not admit a unitary quantum mechanical description [6]. The only way in which one can retain such a description and at the same time be allowed to take the limit $\hbar \to 0$ is to assume that ζ depends on $\hbar$ and is at least of order $\hbar^2$.

We can reach the same conclusion by noting that the condition $Z < Z_\star \approx 4.48$, for the possibility of formulating a unitary quantum theory for PT-symmetric square well, is equivalent to $\zeta < 8.96\hbar^2/(mL^2) < 2E_1 < E_2$, where E_1 and E_2 are respectively the ground state and first excited states of the system. For a light molecule, say O_2, with mass $m \approx 30$ GeV, confined in a micrometre size well—which should allow for a classical description—we find $\zeta < 1.3 \times 10^{-28}$ eV. This corresponds to the classical molecule moving with a speed $v < 4.7 \times 10^{-20}$ m s^{-1} and a temperature of $T < 1.6 \times 10^{-24}$ K. These numbers provide a conclusive evidence that non-Hermiticity effects quantified with the coupling constant ζ are quantum mechanical in nature and have no classical counterpart.

Furthermore, recall that the classical limit $\hbar \to 0$ is meaningful if it is accompanied with taking $n \to \infty$ in such a way that $\hbar n$ stays constant[17]. But as we explained in section 5.1, in

[17] This follows from (73) and the requirement that in the classical limit not all the energy levels collapse to zero.

the limit $n \to \infty$ the effects of the non-Hermiticity of the Hamiltonian disappear. Therefore, the classical limit of all the theories with different allowed values of $Z < Z_\star$ coincides with that of the Hermitian infinite square well ($Z = 0$).

The above discussion of the classical limit of the PT-symmetric square well Hamiltonian is based on the requirement that the corresponding quantum theory has a $\hbar \to 0$ limit. This is the conventional way of defining the classical limit of a quantum system. Yet we can consider the $\hbar$-dependent classical observable H_c and view it as a classical Hamiltonian with the property that its pseudo-Hermitian quantization with appropriate (symmetric) factor ordering yields the Hermitian Hamiltonian h.

There is also another approach for determining a classical Hamiltonian for PT-symmetric quantum systems [5, 33]. It involves a direct replacement of the operators x and p, which appear in the expression for the quantum Hamiltonian operator H, by the classical position x_c and momentum p_c and letting the latter take complex values. If one applies this prescription to the PT-symmetric square well and enforces the condition of the existence of a proper $\hbar \to 0$ limit, then again the condition $Z < Z_\star$ implies $\zeta \to 0$, and one recovers the classical Hamiltonian for a free particle confined in an infinite (real) square well. However, if one does not identity the substitution $p \to p_c$ and $x \to x_c$ with taking $\hbar \to 0$ in (52), then one obtains a complex-valued 'classical Hamiltonian', namely

$$H'_c = \frac{p_c^2}{2m} + v(x_c). \tag{121}$$

It is the classical Hamiltonian dynamical system defined by such complex 'classical Hamiltonians' that are studied in [5, 33]. Although we acknowledge the interesting mathematical consequences of this study and its relevance to the use of complex WKB approximation in calculating the energy levels of various PT-symmetric models [34], we are inclined to adopt the standard definition of a classical observable which requires the latter to be real valued [36][18]. The PT-symmetric quantum mechanics also makes an implicit use of this definition in insisting that the eigenvalues of the observables, in particular the Hamiltonian, be real [15, 35]. According to this definition, the observables x_c and p_c assume real values, and H'_c, which is a complex-valued function of x_c and p_c, is not a physical observable. In particular, it cannot serve as a physical classical Hamiltonian (for a system with a one-dimensional configuration space).

5.5. *Construction of the observables*

The construction of the observables $O : \mathcal{H}_{\rm phys} \to \mathcal{H}_{\rm phys}$ for the PT-symmetric square well mimics that of the Hermitian Hamiltonian h. We begin our calculation of O by employing our approximation scheme to express (19) in the form

$$\begin{aligned} O \overset{N}{\approx} & \sum_{m,n=1}^{N} \sqrt{\frac{\epsilon_n}{\epsilon_m}}\, o_{mn} |\epsilon_m\rangle\langle\epsilon_n| + \sum_{m,n=N+1}^{\infty} o^{(0)}_{mn} |m\rangle\langle n| \\ & + \sum_{m=1}^{N} \sum_{n=N+1}^{\infty} \left[\frac{1}{\sqrt{\epsilon_m}}\, o_{mn} |\epsilon_m\rangle\langle n| + \sqrt{\epsilon}_m o_{nm} |n\rangle\langle\epsilon_m| \right] \overset{N}{\approx} o + \delta o, \end{aligned} \tag{122}$$

where $o : \mathcal{H} \to \mathcal{H}$ is a Hermitian operator,

$$o_{mn} := \langle\epsilon_m|o|\epsilon_n\rangle \overset{N}{\approx} \begin{cases} \sum_{j,k=1}^{N} \mathcal{U}^\dagger_{mj} o^{(0)}_{jk} \mathcal{U}_{kn} & \text{for} \quad m, n \leqslant N, \\ \langle\epsilon_m|o|n\rangle \overset{N}{\approx} \sum_{k=1}^{N} \mathcal{U}^\dagger_{mk} o^{(0)}_{kn} & \text{for} \quad m \leqslant N, n > N, \end{cases} \tag{123}$$

[18] This is because we are not aware of any other precise definition of a classical observable.

$$o^{(0)}_{mn} := \langle m|o|n\rangle, \tag{124}$$

$$\delta o := \sum_{m,n=1}^{N} A_{mn}|m\rangle\langle n| + \sum_{m=1}^{N}\sum_{n=N+1}^{\infty}\left(B_{mn}|m\rangle\langle n| + C_{nm}|n\rangle\langle m|\right), \tag{125}$$

$$A_{mn} := \sum_{j,k=1}^{N} \mathcal{E}^{-1/2}_{mj} o^{(0)}_{jk} \mathcal{E}^{1/2}_{kn} - o^{(0)}_{mn}, \tag{126}$$

$$B_{mn} := \sum_{k=1}^{N} \left(\mathcal{E}^{-1/2}_{mk} - \delta_{mk}\right) o^{(0)}_{kn}, \tag{127}$$

$$C_{nm} := \sum_{k=1}^{N} o^{(0)}_{nk} \left(\mathcal{E}^{1/2}_{km} - \delta_{km}\right). \tag{128}$$

Here δ_{mk} stands for the Kronecker δ-function, and we have used (83), (85) and (97).

We can express δo and consequently O as power series in p with x-dependent coefficients similarly to our derivation of (110). Note, however, that in this case we have to deal with the infinite sum appearing in (125). The presence of this sum is a manifestation of the fact that (unlike the Hamiltonian) a general observable will mix the state vectors $|n\rangle$ with $n \leqslant N$ with those with $n > N$.

The power series expansion of O in powers of p has the form

$$O \overset{N}{\approx} o + \sum_{\ell=0}^{\infty} \omega_\ell(\mathrm{x})\, \mathrm{p}^\ell, \qquad \omega_\ell(\mathrm{x}) = \mathrm{i}^\ell \tilde{\omega}_\ell(\mathrm{x}), \tag{129}$$

$$\tilde{\omega}_\ell(\mathrm{x}) := \sum_{k=0}^{\ell}\sum_{m=1}^{\infty} c_{mk\ell} \sin\left[\frac{\pi m}{2}(\mathrm{x}+1)\right](\mathrm{x}+1)^{\ell-k}, \tag{130}$$

$$c_{mk\ell} := \begin{cases} \sum_{n=1}^{N} \mathrm{i}^{\mu_m-\mu_n} A_{mn} a_{nk\ell} + \sum_{n=N+1}^{\infty} \mathrm{i}^{\mu_m-\mu_n} B_{mn} a_{nk\ell} & \text{for} \quad m \leqslant N \\ \sum_{n=1}^{N} \mathrm{i}^{\mu_m-\mu_n} C_{mn} a_{nk\ell} & \text{for} \quad m > N, \end{cases} \tag{131}$$

where $a_{nk\ell}$ are the coefficients given in (113). Again in calculating the expectation value of O for a normalized state vector $\psi \in \mathcal{H}_{\text{phys}}$ with position wavefunction Ψ, we use the position representation $\hat{o}$ of o (defined by $\langle \mathrm{x}|o = \hat{o}\langle \mathrm{x}|$):

$$\langle \psi, O\psi\rangle_+ = \int_{-1}^{1} \Psi(\mathrm{x})^*\, \hat{o}\Psi(\mathrm{x})\, \mathrm{dx}. \tag{132}$$

Note also that by replacing $(o, \mathrm{x}, \mathrm{p})$ in (129) with the corresponding classical quantities $(o_c, \mathrm{x}_c, \mathrm{p}_c)$, we obtain a generally complex-valued function $\Omega_c(\mathrm{x}_c, \mathrm{p}_c)$ (provided that the corresponding infinite series appearing in (130) and (131) converge). Clearly, taking $o = h$, we have $\Omega_c = H'_c$, where H'_c is the complex Hamiltonian (121).

In order to compare the operators o and O we represent them in the ordinary position representation, i.e., compare $\hat{o}$ with $\hat{O}$. The latter is defined by $\langle \mathrm{x}|O = \hat{O}\langle \mathrm{x}|$. Using (130), (131) and (116), we have

$$\hat{O} = \hat{o} + \sum_{\ell=0}^{\infty} \tilde{\omega}_\ell(\mathrm{x})\, \frac{\mathrm{d}^\ell}{\mathrm{dx}^\ell}. \tag{133}$$

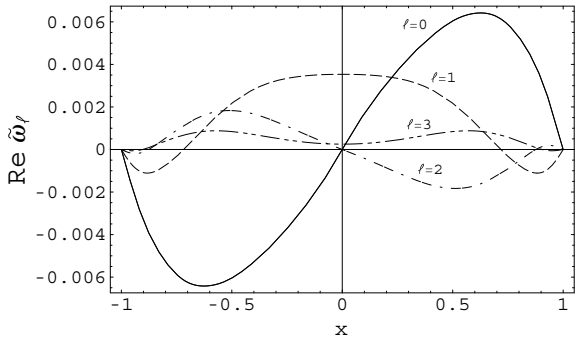

Figure 6. Graph of $\mathrm{Re}[\tilde{\omega}_\ell^{(X)}]$ for $\ell = 0, 1, 2, 3$, $Z = 1$ and $N = 20$.

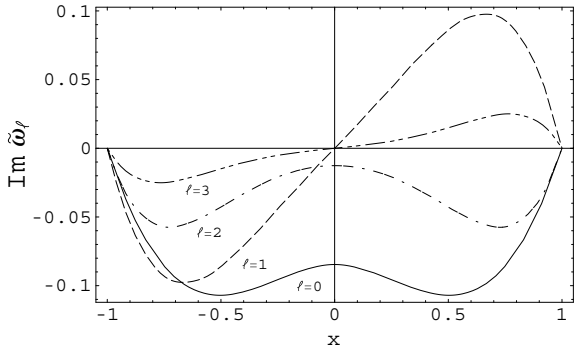

Figure 7. Graph of $\mathrm{Im}[\tilde{\omega}_\ell^{(X)}]$ for $\ell = 0, 1, 2, 3$, $Z = 1$ and $N = 20$.

A concrete example is the dimensionless position operator $\mathrm{X} := 2X/L$: letting $o = \mathrm{x}$, we find

$$\mathrm{X} = \mathrm{x} + \sum_{\ell=0}^{\infty} \omega_\ell^{(X)}(\mathrm{x})\, \mathrm{p}^\ell, \tag{134}$$

where $\omega_\ell^{(X)}(\mathrm{x})$ denote the value of $\omega_\ell(\mathrm{x})$ obtained by setting $o = \mathrm{x}$ in (124). The x-representation of X has the form

$$\hat{\mathrm{X}} = \mathrm{x} + \sum_{\ell=0}^{\infty} \tilde{\omega}_\ell^{(X)}(\mathrm{x})\, \frac{\mathrm{d}^\ell}{\mathrm{dx}^\ell}, \tag{135}$$

where $\tilde{\omega}_\ell^{(X)}(\mathrm{x})$ is the value of $\tilde{\omega}_\ell(\mathrm{x})$ for $o = \mathrm{x}$. Note that the infinite series in (131) that defines $\tilde{\omega}_\ell(\mathrm{x})$ converges quite rapidly. This allows us to obtain an approximate value for this series (for any value of ℓ) by summing just the first few terms. We can include enough terms in this series so that the approximation error becomes smaller than our accuracy index ν_N. Figures 6 and 7 illustrate the plots of the real and imaginary parts of $\tilde{\omega}_\ell^{(x)}$, for $\ell = 0, 1, 2, 3$, $Z = 1$, and $N = 20$, that we have obtained in this way.

5.6. Probability density, position measurements and localized states

According to (43), the probability density for the localization in space is given by the modulus square of the position wavefunction Ψ. We can employ our approximation scheme to reduce

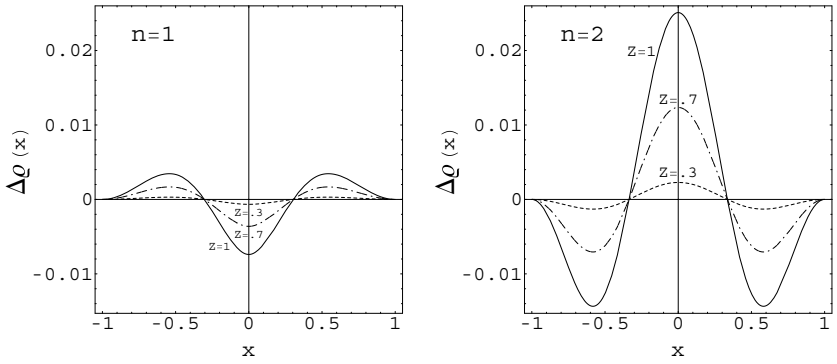

Figure 8. Graph of $\Delta\varrho = \varrho - \varrho_0$ for $\psi(\mathrm{x}) = \mathcal{N}_n \sin[n\pi(\mathrm{x}+1)/2]$ with $n = 1, 2$, $N = 20$ and $Z = 0.3, 0.7, 1$, where ϱ is the probability density and ϱ_0 is its value for $Z = 0$ and $\mathcal{N}_n$ are normalization constants.

the expansion (51) of Ψ into the finite sum

$$\Psi(\mathrm{x}) \overset{N}{\approx} \psi(\mathrm{x}) + \sum_{n=1}^{N} a_n \sin\left[\frac{\pi n}{2}(\mathrm{x}+1)\right], \tag{136}$$

where

$$a_n = \mathrm{i}^{\mu_n}\left(\sum_{m=1}^{N} \mathcal{E}_{nm}^{1/2} f_m^{(0)} - f_n^{(0)}\right), \tag{137}$$

$$f_m^{(0)} = \langle m|\psi\rangle = \mathrm{i}^{-\mu_m}\int_{-1}^{1} \sin\left[\frac{\pi m}{2}(\mathrm{x}'+1)\right]\psi(\mathrm{x}')\,\mathrm{d}\mathrm{x}', \tag{138}$$

and we have made use of (66)–(68), (83), (85), (51) and (97).

Having obtained the general expression for the position wavefunction, we can compute the probability density $\varrho(\mathrm{x}) := |\Psi(\mathrm{x})|^2$. Note, however, that the latter expression is valid for the normalized wavefunctions. Figure 8 shows the plots of the difference $\Delta\varrho$ of the probability density ϱ for $\psi(\mathrm{x}) = \mathcal{N}_n \sin[n\pi(\mathrm{x}+1)/2]$, with $n = 1, 2$, for $N = 20$ and $Z = 0.3, 0.7, 1$ with that (ϱ_0) for $Z = 0$. Figure 9 gives the plots of the probability density difference $\Delta\varrho$ for $\psi(\mathrm{x}) = \mathcal{N}_n \sin[n\pi(\mathrm{x}+1)/2]$ with $n = 3, 4, \ldots, 8$, $N = 20$, and $Z = 1$.[19]

We can also use expression (136) for the position wavefunction to compute the position expectation value,

$$\langle\psi, \mathrm{X}\psi\rangle_+ = \int_{-1}^{1} \mathrm{x}|\Psi(\mathrm{x})|^2\,\mathrm{d}\mathrm{x}. \tag{139}$$

and the uncertainty in position

$$\Delta\mathrm{x} = \sqrt{\langle\psi, \mathrm{X}^2\psi\rangle_+ - \langle\psi, \mathrm{X}\psi\rangle_+^2}. \tag{140}$$

Table 2 gives $\Delta\mathrm{x}$ for $\psi(\mathrm{x}) = N_n \sin[n\pi(\mathrm{x}+1)/2]$ with $n = 1, 2, \ldots, 7$, $Z = 0, 0.5, 1$ and $N = 20$. It turns out that the calculation of the same quantities using $N = 10$ yields results that differ from those listed in table 2 by numbers that are smaller than 10^{-6}. This is another

[19] Here $\mathcal{N}_n$ are appropriate normalization constants.

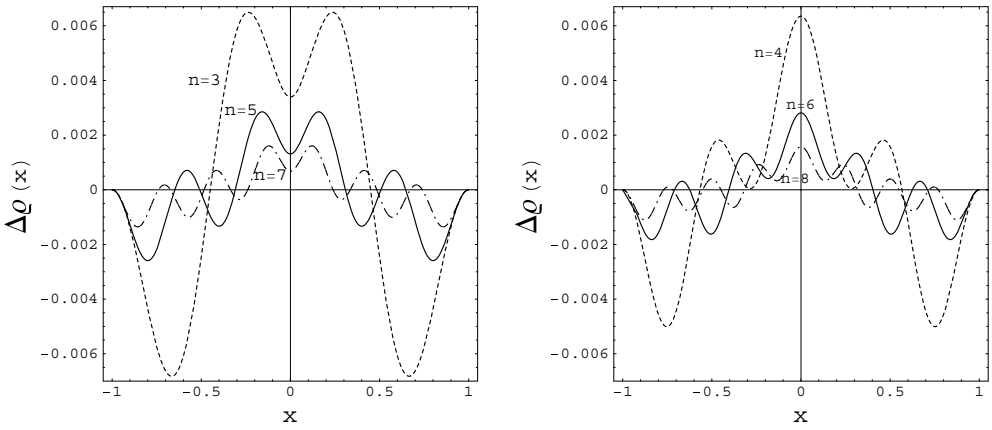

Figure 9. Graphs of $\Delta\varrho = \varrho - \varrho_0$ for $\psi(\mathrm{x}) = \mathcal{N}_n \sin[n\pi(\mathrm{x}+1)/2]$ for $n = 3, 4, \ldots, 8$, $N = 20$ and $Z = 1$, where ϱ is the probability density and ϱ_0 is its value for $Z = 0$ and $\mathcal{N}_n$ are normalization constants.

Table 2. The position uncertainty $\Delta\mathrm{x}$ for $\psi(\mathrm{x}) = N_n \sin[n\pi(\mathrm{x}+1)/2]$ with $n = 1, 2, \ldots, 7$, $Z = 0, 0.5, 1$, and $N = 20$. Note that for $n = 6$ and 7 the difference between values of $\Delta\mathrm{x}$ for $Z = 1$ and $Z = 0$ is smaller than the accuracy index $\nu_{20} = 0.0005$.

n	$Z = 0$	$Z = 0.5$	$Z = 1$	$\Delta\mathrm{x}\|_{Z=1} - \Delta\mathrm{x}\|_{Z=0}$
1	0.3615	0.3618	0.3628	0.0013
2	0.5317	0.5308	0.5280	−0.0037
3	0.5575	0.5571	0.5559	−0.0016
4	0.5663	0.5660	0.5652	−0.0011
5	0.5704	0.5702	0.5697	−0.0006
6	0.5725	0.5724	0.5721	−0.0004
7	0.5738	0.5737	0.5735	−0.0003

confirmation of the consistency of our approximation scheme. Furthermore, note that as we expect the effect of the non-Hermiticity of the initial Hamiltonian (52) diminishes as n increases. Already for $n = 6$, its contribution to position uncertainty is smaller than the accuracy index $\nu_{20} = 0.0005$.

As seen from (134), in the x-representation the position operator X is a pseudo-differential operator. This in particular means that the expectation value of X in a state described by the state vector ψ depends on all the derivatives of ψ. In this sense unlike the usual position operator, X is a nonlocal operator. Note, however, that this nonlocal character of X manifests itself only if one insists on using the usual position representation $\psi(x)$ of the state vectors ψ. This is not a reasonable choice, because being a non-Hermitian operator acting in $\mathcal{H}_{\rm phys}$ the usual position operator x is not a physical observable.

Probably the best demonstration of the nonlocal nature of X is provided by the shape of the position state vector $\xi^{(y)}$ that is localized at $y \in (-L, L)$. As a function belonging to $\mathcal{H}$, it has the form

$$\xi^{(y)}(x) = \langle x|\xi^{(y)}\rangle = \langle x|\rho^{-1}|y\rangle = \sum_{n=1}^{\infty} \epsilon_n^{-1/2} \varepsilon_n(x)\varepsilon_n(y)^*,$$

where we have employed (36), (11) and (32). Using the same method as that leading to (136) we can express this relation as

$$\xi^{(y)}(x) \overset{N}{\approx} \delta(x-y) + \mathcal{F}(x,y), \tag{141}$$

where

$$\mathcal{F}(x,y) := \sum_{m,n=1}^{N} \mathrm{i}^{\mu_m-\mu_n}\big(\mathcal{E}^{-1/2}_{mn} - \delta_{mn}\big) \sin\left[\frac{\pi m}{L}\left(x+\frac{L}{2}\right)\right] \sin\left[\frac{\pi n}{L}\left(y+\frac{L}{2}\right)\right],$$

and we have used (97).

Figure 10 shows the real and imaginary parts of $\xi^{(y)}(x)$ for $L = 2, N = 20, Z = 1$ and $y = -1/2, 0, 1/2$. Figure 11 shows the real and imaginary parts of $\xi^{(1/3)}(x)$ for $L = 2, N = 20$, and various values of Z. As expected the spreading of the localized state $\xi^{(1/3)}$ is an increasing function of the non-Hermiticity parameter Z.

5.7. Dynamical consequences of non-Hermiticity

In the preceding subsection, we discussed the computation of the observables and the associated physical quantities. These provide information on the kinematical content of the PT-symmetric square well. In this subsection, we investigate its dynamical content.

The time evolution of an initial state vector $\psi(t_0) \in \mathcal{H}_{\text{phys}}$ is given by

$$\psi(t) = \mathrm{e}^{-\mathrm{i}(t-t_0)H/\hbar}\psi(t_0), \qquad \text{for all} \quad t \in \mathbb{R}. \tag{142}$$

Alternatively, in terms of the dimensionless time parameter,

$$\tau := \left(\frac{2\hbar}{mL^2}\right) t, \tag{143}$$

we have

$$\psi(\tau) = \mathrm{e}^{-\mathrm{i}(\tau-\tau_0)\mathrm{H}}\psi(\tau_0), \tag{144}$$

where $\tau_0 = 2\hbar t_0/(mL^2)$.

Expanding $\psi(\tau)$ in the basis $\{\psi_n\}$, we can express (144) in the form

$$\psi(\tau) = \sum_{n=1}^{\infty} c_n\, \mathrm{e}^{-\mathrm{i}(\tau-\tau_0)\mathrm{E}_n}\psi_n, \qquad c_n := \langle\phi_n|\psi(\tau_0)\rangle. \tag{145}$$

Next, we employ our Nth order approximation scheme. Using (80), we have

$$\psi(\tau) \overset{N}{\approx} \sum_{n=1}^{N} c_n\, \mathrm{e}^{-\mathrm{i}(\tau-\tau_0)\mathrm{E}_n}\psi_n + \sum_{n=N+1}^{\infty} c^{(0)}_n\, \mathrm{e}^{-\mathrm{i}\pi^2n^2(\tau-\tau_0)/4}\psi^{(0)}_n, \tag{146}$$

where

$$c^{(0)}_n := \big\langle\psi^{(0)}_n\big|\psi(\tau_0)\big\rangle, \tag{147}$$

and we have used $\mathrm{E}_n \overset{N}{\approx} \mathrm{E}^{(0)}_n := \pi^2n^2/4$ for $n > N$.

To explore the dynamical effects of the non-Hermiticity of the Hamiltonian (for $Z \neq 0$) we compute the position expectation value for the evolving state vectors $\psi(\tau)$ having the initial value,

$$\psi(\tau_0) = \mathcal{N}_j\psi^{(0)}_j \qquad \text{with} \quad j \leqslant N, \tag{148}$$

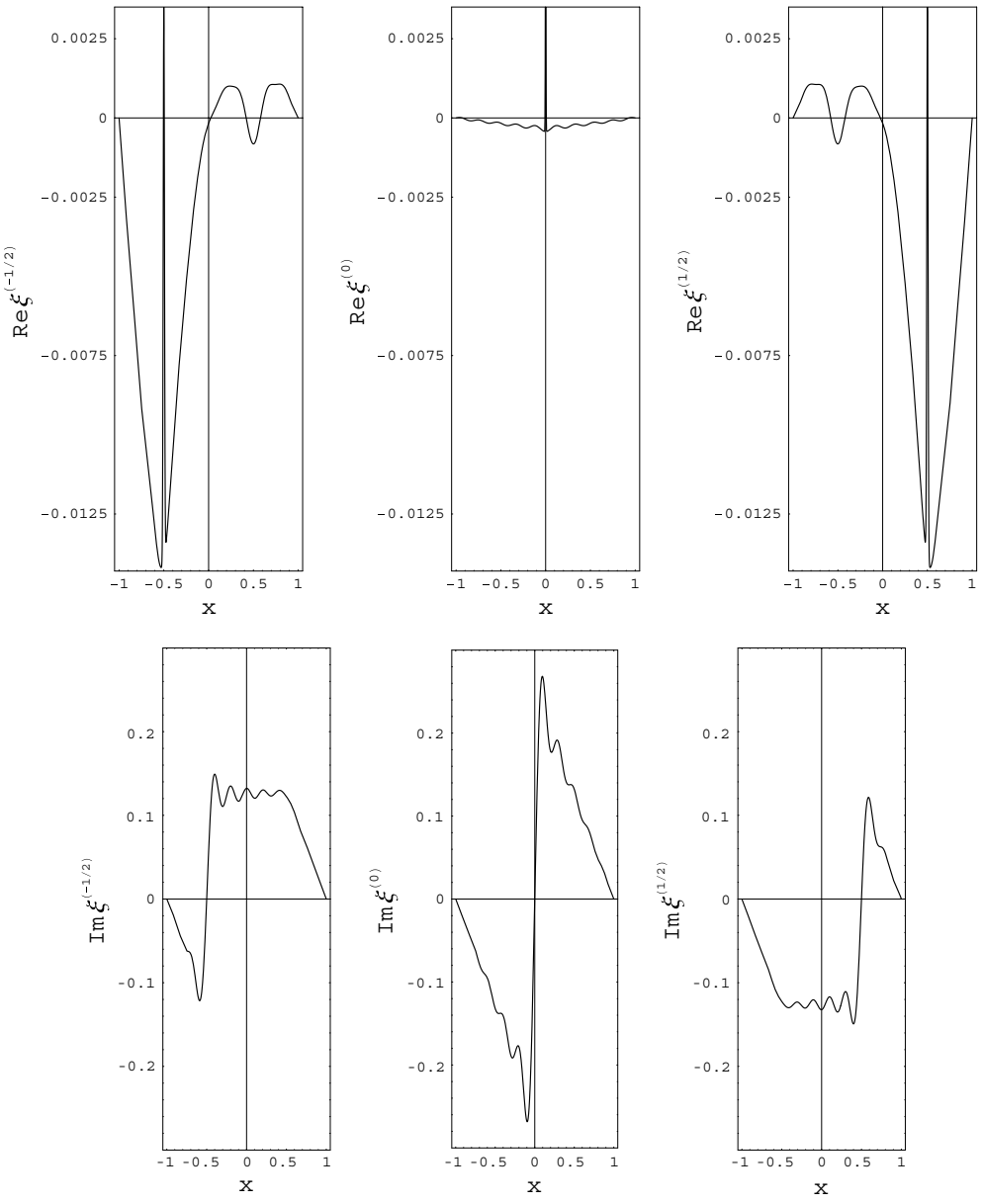

Figure 10. Graph of $\mathrm{Re}[\xi^{(y)}]$ and $\mathrm{Im}[\xi^{(y)}]$ for $L = 2$, $N = 20$, $Z = 1$ and $y = -1/2, 0, 1/2$. Note that $\mathrm{Re}[\xi^{(y)}]$ has a δ-function singularity at y and that except for this singularity the scale of variations of $\mathrm{Im}[\xi^{(y)}]$ is much greater than that of $\mathrm{Re}[\xi^{(y)}]$.

and $\mathcal{N}_j := \langle \psi_j^{(0)}, \psi_j^{(0)} \rangle_+^{-1/2}$. For these choices of the initial state vector, $c_n^{(0)} = 0$ for $n > N$ and (146) simplifies as

$$\psi(\tau) \approx \sum_{n=1}^{N} c_n \, \mathrm{e}^{-\mathrm{i}(\tau-\tau_0)\mathrm{E}_n} \psi_n. \tag{149}$$

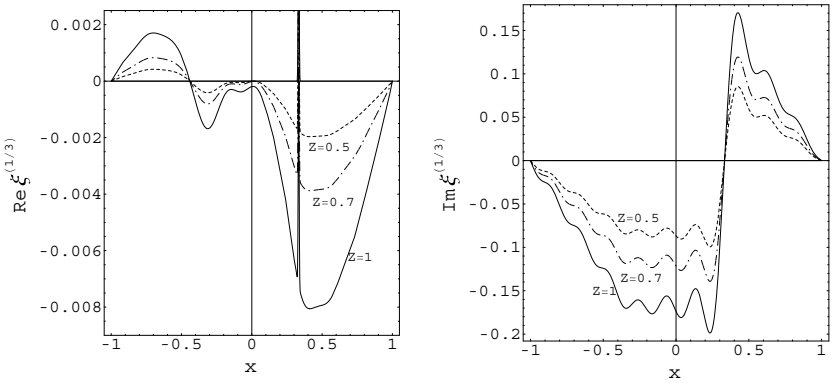

Figure 11. Graph of $\mathrm{Re}[\xi^{(1/3)}]$ and $\mathrm{Im}[\xi^{(1/3)}]$ for $L = 2$, $N = 20$ and $Z = 0, 0.5, 0.7, 1$.

Furthermore, for $Z = 0$, $\psi(\tau_0)$ corresponds to a stationary state with a vanishing position expectation value for all $\tau \in \mathbb{R}$. For $Z > 0$, $\psi(\tau_0)$ does not represent a stationary state and the position expectation value is a nonconstant function of time. To determine this function, we use the position representation of the state.

Let $\Psi(\mathrm{x};\tau) := \langle \xi^{(\mathrm{x})}, \psi(\tau)\rangle_+ = \langle \mathrm{x}|\rho|\psi(\tau)\rangle$ be the position wavefunction for the state vector $\psi(\tau)$. Then, in light of (83), (85), (97) and (149), we have

$$\Psi(\mathrm{x};\tau) \overset{N}{\approx} \sum_{n=1}^{N} c_n\, \mathrm{e}^{-\mathrm{i}(\tau-\tau_0)\mathrm{E}_n}\Gamma_n(\mathrm{x}), \tag{150}$$

where for all $n \leqslant N$

$$\Gamma_n(\mathrm{x}) := \langle \mathrm{x}|\rho|\psi_n\rangle \overset{N}{\approx} \sum_{q,k=1}^{N} \mathrm{i}^{\mu_q}\mathcal{E}_{qk}^{1/2}\langle k|\psi_n\rangle \sin\Big[\frac{\pi q}{2}(\mathrm{x}+1)\Big]. \tag{151}$$

Next, we employ (139) to compute the position expectation value for $\psi(\tau)$. In view of (150),

$$\langle \psi(\tau), \mathrm{X}\psi(\tau)\rangle_+ = \int_{-1}^{1} \mathrm{x}|\Psi(\mathrm{x};\tau)|^2\,\mathrm{dx} \overset{N}{\approx} \sum_{m,n=1}^{N} \Theta_{mn}\,\mathrm{e}^{-\mathrm{i}(\tau-\tau_0)(\mathrm{E}_n-\mathrm{E}_m)}, \tag{152}$$

where

$$\begin{aligned}\Theta_{mn} &:= c_m^* c_n \int_{-1}^{1} \mathrm{x}\Gamma_m(\mathrm{x})^*\Gamma_n(\mathrm{x})\,\mathrm{dx}\\ &= c_m^* c_n \sum_{k,q,v=1}^{N}\sum_{\substack{u=1\\ u\neq q}}^{N}\left(\frac{8qu[(-1)^{q+u}-1]}{\pi^2(q^2-u^2)^2}\right)\mathrm{i}^{\mu_u-\mu_q}\mathcal{E}_{kq}^{1/2}\mathcal{E}_{uv}^{1/2}\langle\psi_m|k\rangle\langle v|\psi_n\rangle.\end{aligned} \tag{153}$$

Figures 12 and 13 show the trajectories traced by the position expectation value (152) in time, for the initial state vector (148) with $j = 1, 2, \ldots, 7$, $Z = 1$ and $N = 10$.

6. Discussion and conclusion

In this paper, we have outlined a general formulation of PT-symmetric (and more generally pseudo-Hermitian) quantum mechanics paying attention to the physical aspects of the theory. This formulation, is consistent with the requirements of quantum measurement theory and allows for the determination of the physical observables. In fact, to the best of our knowledge,

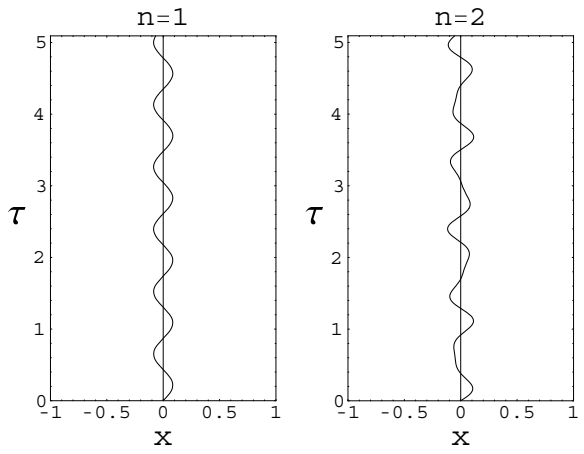

Figure 12. Graph of the trajectory traced by the position expectation value in time for the initial state vector $\psi(0) = \mathcal{N}_j\psi_j^{(0)}$ with $j = 1, 2$, where $Z = 1, N = 10, \tau_0 = 0, \tau \in [0, 16/\pi]$. The horizontal and vertical axes, respectively, represent $\langle\psi(\tau), \mathrm{X}\psi(\tau)\rangle_+$ and τ. The τ-axis also corresponds to the trajectory for the Hermitian case ($Z = 0$). Note that $16/\pi \approx 5.1$ is twice the characteristic period $2\pi/\mathrm{E}_1^{(0)}$ for the ground state of the corresponding Hermitian square well.

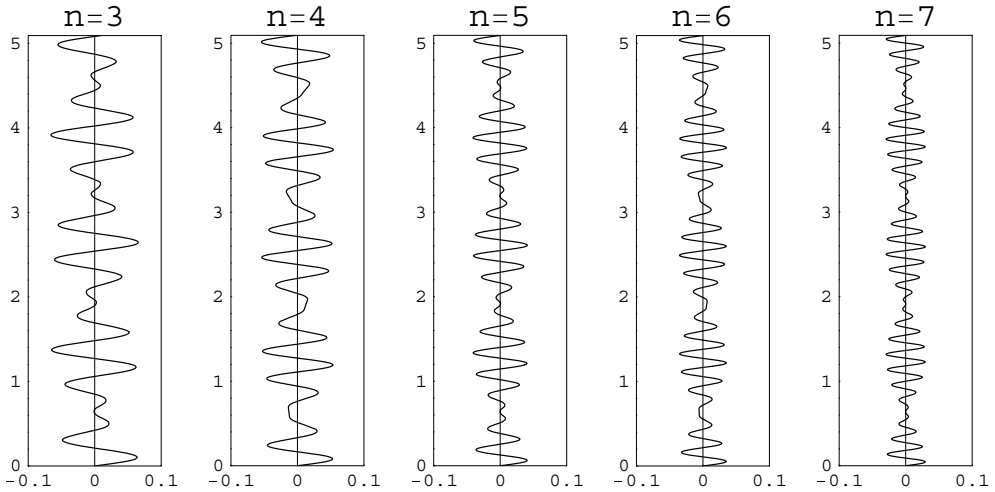

Figure 13. Graph of the trajectory traced by $\langle\psi(\tau), \mathrm{X}\psi(\tau)\rangle_+$ for $\psi(0) = \mathcal{N}_j\psi_j^{(0)}$ with $j = 3, 4, \ldots, 7$ and the same parameters and conventions as in figure 12. Note that the range of values of the horizontal axis is reduced to amplify the behaviour of the trajectories. The envelops seem to have the same period as that of $E_1^{(0)}$, i.e., $2\pi/\mathrm{E}_1^{(0)} \approx 8/\pi$.

this paper is the first to offer an explicit calculation of observables and concrete physical quantities for a PT-symmetric system with an infinite-dimensional Hilbert space. Perhaps more importantly, it proposes a method to identify an underlying classical Hamiltonian that satisfies the usual postulates of classical mechanics and a quantization scheme that relates the latter to the defining Hamiltonian of the theory. We view this as a necessary step towards a clearer understanding of the potential physical applications of PT-symmetric quantum mechanics.

Another important outcome of our investigation is that we are now able to consider the addition of the interaction terms to a PT-symmetric Hamiltonian H without disturbing the structure of its Hilbert space. This is simply done by selecting the additional interaction terms from among physical observables.

Our investigation of the PT-symmetric square well revealed the fact that the underlying classical Hamiltonian for this system coincides with that of the ordinary Hermitian infinite square well. In other words, the non-Hermiticity effects are quantum mechanical in nature. This can be traced back to the simple observation that the non-Hermiticity of the Hamiltonian (52) only affects the low-lying energy levels[20].

Our general results confirm the assertion that as a fundamental theory PT-symmetric quantum mechanics is both mathematically and physically equivalent to conventional quantum mechanics [17]. In fact, it is this very equivalence that allows for the computation of the physical observables. This in turn leads to the natural question of whether there is any valid motivation for further development of PT-symmetric and pseudo-Hermitian quantum mechanics. Our answer to this question is in the affirmative. It is supported by the following observations.

(1) As we showed for any PT-symmetric Hamiltonian H, there is a corresponding Hermitian Hamiltonian. But the latter is a generically nonlocal (pseudo-differential) operator. Therefore, if one is interested in calculating physical quantities that make explicit use of the Hamiltonian one is naturally inclined to make use of the original Hamiltonian H and the inner product $\langle\cdot,\cdot\rangle_+$. However, if one wishes to compute quantities involving the position and momentum of the system, then one is essentially forced to use the Hermitian picture. In summary, developing PT-symmetric quantum mechanics opens up the possibility of treating quantum systems with certain nonlocal Hermitian Hamiltonians. The classical Hamiltonian for such a system is a real analytic function of x and p that involves arbitrarily high powers of p. The pseudo-Hermitian quantization scheme introduced in this paper provides a description of the quantum systems associated with these complicated Hamiltonians. It yields a PT-symmetric quantum Hamiltonian operator that is a local (differential) operator. In a sense, the use of the PT-symmetric quantum mechanics is equivalent to trading a complicated nonlocal Hermitian Hamiltonian with a local PT-symmetric Hamiltonian[21].

(2) The basic ideas so far developed within the framework of pseudo-Hermitian quantum mechanics to assess the structure of PT-symmetric quantum mechanics have some remarkable applications in relativistic quantum mechanics [21, 22, 37], quantum cosmology [21, 38], statistical mechanics [39] and magnetohydrodynamics [40]. This strengthens the belief that the study of PT-symmetric quantum mechanics may lead to some concrete advances in other research areas. It is needless to mention the possibility that the field theoretical extension of such a study may actually turn out to achieve some of the ambitious goals described in [18].

Next, we wish to elucidate the relationship between our approach and the formulation of the PT-symmetric quantum mechanics based on the so-called charge-conjugation operator C as outlined in [15]. See also [41]. In our approach, the metric operator η_+ plays the same role

[20] We do not claim that this is a common feature of all the PT-symmetric quantum Hamiltonians. In general, we expect the non-Hermiticity of the quantum Hamiltonian to affect the underlying classical Hamiltonian. We leave a more detailed study of this issue for a future publication.

[21] The characterization of all the nonlocal Hermitian Hamiltonians that may be mapped to PT-symmetric or pseudo-Hermitian Hamiltonians of the standard (kinetic+potential) form is a difficult open problem.

as the operator C. In fact as shown in [14], C may be expressed in terms of η_+ according to

$$C = \eta_+^{-1} P. \tag{154}$$

Although both η_+ and C determine the inner product of the physical Hilbert space, the expression of the latter in terms of η_+ is slightly simpler. It also agrees with the standard mathematical approach used in dealing with different inner products on the same vector space. Furthermore, the recent attempts [42] at approximate calculations of C for PT-symmetric potentials of the form $\mu^2 x^2 - \lambda^2(\mathrm{i}x)^N$, with $\mu, \lambda \in \mathbb{R}$, have revealed the remarkable fact that these calculations simplify enormously provided that one first computes η_+ and then uses (154) to determine C.[22] This provides a practical justification for the assertion that η_+ is a more basic ingredient of the theory than C. The construction of the observables provides a much more concrete evidence for the validity of this assertion. Note also that the formulation of the theory that uses C and avoids any explicit mention of η_+ leads to the same general conclusions such as the physical equivalence of the PT-symmetric and conventional quantum mechanics. A mathematically rigorous proof of this statement is given in [35].

Finally, we wish to comment on whether one can apply the general scheme offered by pseudo-Hermitian quantum mechanics to PT-symmetric systems defined on a complex contour. The negative attitude expressed by some of the workers on this issue is based on the argument that for these systems the eigenfunctions of the Hamiltonian do not belong to the Hilbert space $L^2(\mathbb{R})$ and hence one cannot define a metric operator η_+ and apply the results of the theory of pseudo-Hermitian operators. The problem with this argument is that nowhere in the formulation of the pseudo-Hermitian quantum mechanics [12] does one assume that the initial Hilbert space $\mathcal{H}$ is $L^2(\mathbb{R})$. As explained in section 2, $\mathcal{H}$ is constructed in two steps: (i) one takes the span V_H of the eigenvectors ψ_n of H (that is assumed to have a real and discrete spectrum) and endows it with some arbitrary (positive-definite) inner product; (ii) one performs the Cauchy completion of this inner product space to obtain the Hilbert space $\mathcal{H}$. The only important condition to be checked is whether $\mathcal{H}$ is separable. This follows from the following simple argument (see also [35]). The set $\{\psi_n\}$ of the eigenvectors spans V_H, and as $\mathcal{H}$ is the Cauchy completion of V_H, V_H is dense in $\mathcal{H}$. This implies that $\mathcal{H}$ is the closure of the span of $\{\psi_n\}$. Being eigenvectors with different eigenvalues, ψ_n are also linearly independent. Hence $\{\psi_n\}$ is a countable basis of $\mathcal{H}$. In particular, performing Gram–Schmidt orthonormalization on $\{\psi_n\}$, one can construct a countable orthonormal basis of $\mathcal{H}$. This is equivalent to the statement that $\mathcal{H}$ is a separable Hilbert space [13]. This general argument shows that indeed there is no obstruction to employ pseudo-Hermitian quantum mechanics to systems defined on a complex contour. The practical difference with systems defined on the real axis is that one cannot make a direct use of the familiar L^2-inner product. It turns out that this does not lead to any insurmountable difficulty either. In contrast, the use of the machinery of pseudo-Hermitian quantum mechanics in describing PT-symmetric systems defined on a complex contour has both practical and conceptual advantages [43].

Acknowledgments

This work has been supported by the Turkish Academy of Sciences in the framework of the Young Researcher Award Program (EA-TÜBA-GEBİP/2001-1-1). AM wishes to thank Tekin Dereli and Ali Ülger for fruitful discussions.

[22] What authors of [42] do is to express η_+ as e^{-Q}, calculate Q approximately, and express C as $C = \mathrm{e}^{Q} P$. Note that this equation is identical with equation (154) that was initially derived in [14]. The calculation of Q makes use of the fact that C is a symmetry generator. The observation that operators of the form $\eta_1^{-1}\eta_2$ generate symmetries of a Hamiltonian that is both η_1- and η_2-pseudo-Hermitian was initially reported in [1].

Appendix

In this appendix, we present a general method for checking the Hermiticity of the Hamiltonian h using its power series expansion (109). This provides an interesting explanation for the resemblance of the graph of the function $\mathrm{Im}[\tilde{\delta}_0(\mathrm{x})]$ to that of the $\mathrm{iv}(\mathrm{x})$ as shown in figure 5.

Using (109) and the fact that $\mathrm{v}(\mathrm{x})$ is imaginary, we have

$$\mathrm{h}^\dagger \overset{N}{\approx} \mathrm{p}^2 - \mathrm{v}(\mathrm{x}) + \sum_{\ell=0}^{\infty} \mathrm{p}^\ell \delta_\ell(\mathrm{x})^*. \tag{A.1}$$

Substituting (109) and (A.1), in $\mathrm{h}^\dagger = \mathrm{h}$, we then find

$$\mathrm{v}(\mathrm{x}) + \frac{1}{2}\sum_{\ell=0}^{\infty}[\delta_\ell(\mathrm{x})\mathrm{p}^\ell - \mathrm{p}^\ell \delta_\ell(\mathrm{x})^*] \overset{N}{\approx} 0. \tag{A.2}$$

Our purpose is to express the left-hand side of this relation as a power series in p with all x-dependent coefficient appearing to the left of powers of p, i.e., obtain a set of functions f_ℓ such that

$$\sum_{\ell=0}^{\infty} f_\ell(\mathrm{x})\mathrm{p}^\ell = \mathrm{v}(\mathrm{x}) + \frac{1}{2}\sum_{\ell=0}^{\infty}[\delta_\ell(\mathrm{x})\mathrm{p}^\ell - \mathrm{p}^\ell \delta_\ell(\mathrm{x})^*] = \mathrm{v}(\mathrm{x}) + \frac{1}{2}\sum_{\ell=0}^{\infty}\mathrm{i}^\ell[\tilde{\delta}_\ell(\mathrm{x})\mathrm{p}^\ell - \mathrm{p}^\ell \tilde{\delta}_\ell(\mathrm{x})^*]. \tag{A.3}$$

Then the condition (A.2) takes the form

$$f_\ell(\mathrm{x}) \overset{N}{\approx} 0 \qquad \text{for all} \quad \ell \in \{0, 1, 2, \ldots\}. \tag{A.4}$$

In order to compute f_ℓ, we use the following useful identity which may be proven by induction on ℓ and use of $[\mathrm{x}, \mathrm{p}] = \mathrm{i}$,

$$\mathrm{p}^\ell f(\mathrm{x}) = \sum_{k=0}^{\ell}\binom{\ell}{k}(-\mathrm{i})^k \frac{\mathrm{d}^k f(\mathrm{x})}{\mathrm{dx}^k}\mathrm{p}^{\ell-k}, \tag{A.5}$$

where $f : \mathbb{R} \to \mathbb{R}$ is an ℓ-times differentiable function and $\binom{\ell}{k} := \frac{\ell!}{k!(\ell-k)!}$.

Using (A.5), (A.3), and the fact that $\mathrm{v}(\mathrm{x})$ is imaginary, we can express the condition (A.4), after some rather lengthy algebra, as follows:

- For $\ell = 0$, $f_0 \overset{N}{\approx} 0$ yields

$$u_0(\mathrm{x}) \overset{N}{\approx} 0, \qquad w_0(\mathrm{x}) \overset{N}{\approx} \mathrm{iv}(\mathrm{x}), \tag{A.6}$$

where

$$u_0(\mathrm{x}) := \sum_{k=1}^{\infty}(-1)^k \frac{\mathrm{d}^k}{\mathrm{dx}^k}\,\mathrm{Re}[\tilde{\delta}_k(\mathrm{x})], \tag{A.7}$$

$$w_0(\mathrm{x}) := \mathrm{Im}[\tilde{\delta}_0(\mathrm{x})] + \frac{1}{2}\sum_{k=1}^{\infty}(-1)^k \frac{\mathrm{d}^k}{\mathrm{dx}^k}\,\mathrm{Im}[\tilde{\delta}_k(\mathrm{x})]. \tag{A.8}$$

- For odd values of ℓ, $f_\ell \overset{N}{\approx} 0$ yields

$$u_{\ell-}(\mathrm{x}) \overset{N}{\approx} \mathrm{Re}[\tilde{\delta}_\ell(\mathrm{x})], \qquad w_{\ell-}(\mathrm{x}) \overset{N}{\approx} 0, \qquad \text{for all} \quad \ell \in \{1, 3, 5, \ldots\}, \tag{A.9}$$

where

$$u_{\ell-}(\mathrm{x}) := \frac{1}{2}\sum_{k=1}^{\infty}(-1)^{\ell+k}\left[\frac{(\ell+k)!}{\ell!\,k!}\right]\frac{\mathrm{d}^k}{\mathrm{dx}^k}\,\mathrm{Re}[\tilde{\delta}_{\ell+k}(\mathrm{x})], \tag{A.10}$$

$$w_{\ell-}(\mathrm{x}) := \sum_{k=1}^{\infty}(-1)^{\ell+k}\left[\frac{(\ell+k)!}{\ell!\,k!}\right]\frac{\mathrm{d}^k}{\mathrm{dx}^k}\,\mathrm{Im}[\tilde{\delta}_{\ell+k}(\mathrm{x})]. \tag{A.11}$$

- For positive even values of ℓ, $f_\ell \overset{N}{\approx} 0$ yields

$$u_{\ell+}(\mathrm{x}) \overset{N}{\approx} 0, \qquad w_{\ell+}(\mathrm{x}) \overset{N}{\approx} \mathrm{Im}[\tilde{\delta}_\ell(\mathrm{x})], \qquad \text{for all} \quad \ell \in \{2, 4, 5, \ldots\}, \tag{A.12}$$

where

$$u_{\ell+}(\mathrm{x}) := \sum_{k=1}^{\infty}(-1)^{\ell+k}\left[\frac{(\ell+k)!}{\ell!\,k!}\right]\frac{\mathrm{d}^k}{\mathrm{dx}^k}\,\mathrm{Re}[\tilde{\delta}_{\ell+k}(\mathrm{x})], \tag{A.13}$$

$$w_{\ell+}(\mathrm{x}) := -\frac{1}{2}\sum_{k=1}^{\infty}(-1)^{\ell+k}\left[\frac{(\ell+k)!}{\ell!\,k!}\right]\frac{\mathrm{d}^k}{\mathrm{dx}^k}\,\mathrm{Im}[\tilde{\delta}_{\ell+k}(\mathrm{x})]. \tag{A.14}$$

Unfortunately, the infinite series appearing in the above relations involve arbitrarily high order derivatives of $\tilde{\delta}_\ell$. This reduces their convergence rate appreciably (compared to the series expansion (109) for h) and amplifies the approximation errors considerably, thus rendering a numerical verification of (A.6), (A.12) and (A.9) intractable. However, the second condition in (A.6) provides an interesting explanation for the particular shape of $\mathrm{Im}[\tilde{\delta}_0]$: neglecting all the terms involving $\mathrm{Im}[\tilde{\delta}_\ell]$ with $\ell > 0$, this condition reads,

$$\mathrm{Im}[\tilde{\delta}_0(\mathrm{x})] \approx \mathrm{iv}(\mathrm{x}) = \begin{cases} -Z & \text{for} \quad -1 < \mathrm{x} < 0 \\ Z & \text{for} \quad 0 < \mathrm{x} < 1. \end{cases}$$

This is in remarkable good agreement with the graph of $\mathrm{Im}[\tilde{\delta}_0(\mathrm{x})]$ as depicted in figure 5.

References

[1] Mostafazadeh A 2002 *J. Math. Phys.* **43** 205
[2] Mostafazadeh A 2002 *J. Math. Phys.* **43** 2814
[3] Mostafazadeh A 2002 *J. Math. Phys.* **43** 3944
[4] Bender C M and Boettcher S 1998 *Phys. Rev. Lett.* **80** 5243
[5] Bender C M, Boettcher S and Meisenger P N 1999 *J. Math. Phys.* **40** 2201
[6] Mostafazadeh A 2004 *J. Math. Phys.* **45** 932
[7] Scholtz F G, Geyer H B and Hahne F J W 1992 *Ann. Phys.* **213** 74
[8] Kretschmer R and Szymanowski L 2004 *Phys. Lett.* A **325** 112
[9] Solombrino L 2002 *J. Math. Phys.* **43** 5439
[10] Mostafazadeh A 2002 *J. Math. Phys.* **43** 6343
Mostafazadeh A 2003 *J. Math. Phys.* **44** 943 (erratum)
[11] Scolarici G and Solombrino L 2003 *J. Math. Phys.* **44** 4450
[12] Mostafazadeh A 2003 *Czech J. Phys.* **53** 1079
[13] Reed M and Simon B 1980 *Functional Analysis* vol 1 (San Diego, CA: Academic)
[14] Mostafazadeh A 2003 *J. Math. Phys.* **44** 974
[15] Bender C M, Brody D C and Jones H F 2002 *Phys. Rev. Lett.* **89** 270401
[16] Mostafazadeh A 2003 *J. Phys. A: Math. Gen.* **36** 7081
[17] Mostafazadeh A 2003 *Preprint* quant-ph/0310164
[18] Bender C M, Brody D C and Jones H F 2003 *Am. J. Phys.* **71** 1095
[19] Bender C M, Brody D C and Jones H F 2004 *Phys. Rev. Lett.* **92** 119902

[20] Mostafazadeh A 2004 *Preprint* quant-ph/0407070
[21] Mostafazadeh A 2003 *Class. Quantum Grav.* **20** 155
[22] Mostafazadeh A 2003 *Preprint* quant-ph/0307059
[23] Wong J 1967 *J. Math. Phys.* **8** 2039
Faisal F H M and Moloney J V 1981 *J. Phys. B: At. Mol. Phys.* **14** 3603
[24] Mostafazadeh A 2002 *Nucl. Phys.* B **640** 419
[25] Bohm A 1993 *Quantum Mechanics: Foundations and Applications* 3rd edn (Berlin: Springer)
[26] Znojil M 2001 *Phys. Lett.* A **285** 7
[27] Bagchi B, Mallik S and Quesne C 2002 *Mod. Phys. Lett* A **17** 1651
[28] Dembowski C, Gräf H D, Harney H L, Heine A A, Heiss W D, Rehfeld H and Richter A 2001 *Phys. Rev. Lett.* **86** 787
Heiss W D and Harney H L 2001 *Eur. Phys. J.* D **17** 149
[29] Gelfand I M 1989 *Lectures on Linear Algebra* (New York: Dover)
[30] Horn R A and Johnson C R 1985 *Matrix Analysis* (Cambridge: Cambridge University Press)
[31] Gradshteyn I S and Ruzhik I M 1980 *Table of Integrals, Series, and Products* (San Diego, CA: Academic)
[32] Lang S 1998 *A First Course in Calculus* (New York: Springer)
[33] Nanayakkara A 2004 *J. Phys. A: Math. Gen.* **37** 4321
[34] Bender C M, Berry M, Meisinger P N, Savage V M and Simsek M 2001 *J. Phys. A: Math. Gen.* **34** L31
See also Delabaere E and Pham F 1998 *Phys. Lett.* A **250** 25
Delabaere E and Trinh D T 2000 *J. Phys. A: Math. Gen.* **33** 8771
[35] Mostafazadeh A 2004 *Preprint* quant-ph/0407213 (*Czech. J. Phys.* at press)
[36] Isham C J 1995 *Lectures on Quantum Theory* (London: Imperial College Press)
[37] Mostafazadeh A and Zamani F 2003 *Preprint* quant-ph/0312078
[38] Mostafazadeh A 2004 *Ann. Phys., NY* **309** 1
[39] Ahmed Z and Jain S R 2003 *Phys. Rev.* E **67** 045106
Ahmed Z and Jain S R 2003 *J. Phys. A: Math. Gen.* **36** 3349
[40] Günther U and Stefani F 2003 *J. Math. Phys.* **44** 3097
[41] Weigert S 2003 *Phys. Rev.* A **68** 062111
[42] Bender C M, Brody D C and Jones H F 2004 *Preprint* hep-th/0402183 and hep-th/0402011
Bender C M and Jones H F 2004 *Preprint* hep-th/0405113
[43] Mostafazadeh A 2004 *Preprint* quant-ph/0410012