AIP | Journal of Mathematical Physics

Application of pseudo-Hermitian quantum mechanics to a P T -symmetric Hamiltonian with a continuum of scattering states

Ali Mostafazadeh

Citation: Journal of Mathematical Physics **46**, 102108 (2005); doi: 10.1063/1.2063168
View online: http://dx.doi.org/10.1063/1.2063168
View Table of Contents: http://scitation.aip.org/content/aip/journal/jmp/46/10?ver=pdfcov
Published by the AIP Publishing

Application of pseudo-Hermitian quantum mechanics to a $\mathcal{PT}$-symmetric Hamiltonian with a continuum of scattering states

Ali Mostafazadeh[a)]
Department of Mathematics, Koç University, 34450 Sariyer, Istanbul, Turkey

(Received 20 May 2005; accepted 23 August 2005; published online 21 October 2005)

We extend the application of the techniques developed within the framework of the pseudo-Hermitian quantum mechanics to study a unitary quantum system described by an imaginary $\mathcal{PT}$-symmetric potential $v(x)$ having a continuous real spectrum. For this potential that has recently been used, in the context of optical potentials, for modeling the propagation of electromagnetic waves traveling in a waveguide half and half filled with gain and absorbing media, we give a perturbative construction of the physical Hilbert space, observables, localized states, and the equivalent Hermitian Hamiltonian. Ignoring terms of order three or higher in the non-Hermiticity parameter ζ, we show that the equivalent Hermitian Hamiltonian has the form $p^2/2m+(\zeta^2/2)\Sigma_{n=0}^{\infty}\{\alpha_n(x),p^{2n}\}$ with $\alpha_n(x)$ vanishing outside an interval that is three times larger than the support of $v(x)$, i.e., in 2/3 of the physical interaction region the potential $v(x)$ vanishes identically. We provide a physical interpretation for this unusual behavior and comment on the classical limit of the system. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2063168]

I. INTRODUCTION

During the past seven years there have appeared over 200 research papers on $\mathcal{PT}$-symmetric quantum systems. This was initially triggered by the surprising observation of Bessis and Zinn-Justin and its subsequent numerical verification by Bender and his co-workers[1] that certain non-Hermitian but $\mathcal{PT}$-symmetric Hamiltonians, such as

$$H = p^2 + x^2 + i\epsilon x^3 \text{ with } \epsilon \in \mathbb{R}^+, \tag{1}$$

have a purely real spectrum. This observation suggested the possibility to use these Hamiltonians in the description of certain quantum systems. Since the $\mathcal{PT}$-symmetry of a non-Hermitian Hamiltonian H, i.e., the condition $[H,\mathcal{PT}]=0$, did not ensure the reality of its spectrum, a crucial task was to seek the necessary and sufficient conditions for the reality of the spectrum of a given non-Hermitian Hamiltonian H. This was achieved in Ref. 2 where it was shown, under the assumptions of the diagonalizability of H and discreteness of its spectrum, that the reality of the spectrum was equivalent to the existence of a positive-definite inner product $\langle\cdot,\cdot\rangle_+$ that rendered the Hamiltonian self-adjoint, i.e., for any pair (ψ,ϕ) of state vectors $\langle\psi,H\phi\rangle_+=\langle H\psi,\phi\rangle_+$.

Another condition that is equivalent to the reality of the spectrum of H is that it can be mapped to a Hermitian Hamiltonian h via a similarity transformation;[2,3] there is an invertible Hermitian operator ρ such that

$$H = \rho^{-1} h \rho. \tag{2}$$

The positive-definite inner product $\langle\cdot,\cdot\rangle_+$ and the operator ρ entering (2) are determined by a positive-definite operator η_+ according to[2,3]

[a)]Electronic mail: amostafazadeh@ku.edu.tr

$$\langle\cdot,\cdot\rangle_+ := \langle\cdot|\eta_+\cdot\rangle, \tag{3}$$

$$\rho = \sqrt{\eta_+}, \tag{4}$$

and the Hamiltonian satisfies the η_+-pseudo-Hermiticity condition:[4]

$$H^\dagger = \eta_+ H \eta_+^{-1}. \tag{5}$$

Here $\langle\cdot|\cdot\rangle$ stands for the standard (L^2) inner product that determines the (reference) Hilbert space $\mathcal{H}$ as well as the adjoint $H^\dagger$ of H.[5] (The adjoint $A^\dagger$ of an operator A is the unique operator satisfying, for all $\psi,\phi\in\mathcal{H}$, $\langle\psi|A^\dagger\phi\rangle=\langle A\psi|\phi\rangle$. A is called Hermitian if $A^\dagger=A$.)

It is this, so-called metric operator, η_+ that determines the kinematic structure (the physical Hilbert space and the observables) of the desired quantum system. Note however that η_+ is not unique[6–8] (it is only unique up to symmetries of the Hamiltonian[7]). In Ref. 2 we have not only established the existence of a positive definite metric operator η_+ and the corresponding positive-definite inner product $\langle\cdot,\cdot\rangle_+$ for a diagonalizable Hamiltonian with a discrete real spectrum, but we have also explained the role of antilinear symmetries such as $\mathcal{PT}$ and offered a method for computing the most general η_+. [For a treatment of nondiagonalizable pseudo-Hermitian Hamiltonians see Refs. 9–11. Note that diagonalizability of the Hamiltonian is a necessary condition for applicability of the standard quantum measurement theory.[5] It is also necessary for the unitarity of the time-evolution, for a nondiagonalizable Hamiltonian is never Hermitian (its evolution operator is never unitary[11]) with respect to a positive-definite inner product.[9,10]] An alternative approach that yields a positive-definite inner product for a class of $\mathcal{PT}$-symmetric models is that of Ref. 12. As shown in Refs. 7 and 13, the $\mathcal{CPT}$-inner product proposed in Ref. 12 is identical to the inner product $\langle\cdot,\cdot\rangle_+=\langle\cdot|\eta_+\cdot\rangle$ for a particular choice of η_+.

Under the above-mentioned conditions every Hamiltonian having a real spectrum determines a set $\mathcal{U}_{H+}$ of positive-definite metric operators. To formulate a consistent unitary quantum theory having H as its Hamiltonian, one needs to choose an element η_+ of $\mathcal{U}_{H+}$. (Alternatively one may choose sufficiently many operators with real spectrum to construct a so-called irreducible set of observables which subsequently fixes a metric operator η_+.[14]) Each choice fixes a positive-definite inner product $\langle\cdot,\cdot\rangle_+$ and defines the physical Hilbert space $\mathcal{H}_{\rm phys}$ and the observables. The latter are by definition[15] the operators O that are self-adjoint with respect to $\langle\cdot,\cdot\rangle_+$, alternatively they are η_+-pseudo-Hermitian. These can be constructed from Hermitian operators o acting in $\mathcal{H}$ according to[5]

$$O = \rho^{-1} o \rho. \tag{6}$$

In particular, one can define η_+-pseudo-Hermitian position X and momentum P operators,[5,15] express H as a function of X and P, and determine the underlying classical Hamiltonian for the system by letting $\hbar\to 0$ in the latter expression.[5,16] Alternatively, one may calculate the equivalent Hermitian Hamiltonian h and obtain its classical limit (again by letting $\hbar\to 0$).

Another application of the η_+-pseudo-Hermitian position operator X is in the construction of the physical localized states:

$$|\xi^{(x)}\rangle := \rho^{-1}|x\rangle. \tag{7}$$

These in turn define the physical position wave function, $\Psi(x):=\langle\xi^{(x)},\psi\rangle_+=\langle x|\rho|\psi\rangle$, and the invariant probability density,

$$\varrho(x) := \frac{|\Psi(x)|^2}{\int_{-\infty}^{\infty}|\Psi(x)|^2 dx} = \frac{|\langle x|\rho|\psi\rangle|^2}{\langle\psi,\psi\rangle_+}, \tag{8}$$

for a given state vector $|\psi\rangle$.[5,16]

The above-mentioned prescription for treating $\mathcal{PT}$-symmetric and more generally pseudo-Hermitian Hamiltonians with a real spectrum has been successfully applied in the study of the $\mathcal{PT}$-symmetric square well in Ref. 5 and the cubic anharmonic oscillator (1) in Ref. 16—See also Ref. 17. Both these systems have a discrete nondegenerate energy spectrum, and the results of Refs. 4 and 2 are known to apply to them. The aim of the present paper is to seek whether these results (in particular the construction method for η_+) may be used for treating a system with a continuous spectrum. (The question whether the theory of pseudo-Hermitian operators as outlined in Refs. 4 and 2 is capable of treating a system having scattering states was posed to the author by Zafar Ahmed during the second International Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics, held in Prague, 14–16 June, 2004.) This question is motivated by the desire to understand field-theoretical analogues of $\mathcal{PT}$-symmetric systems which should admit an S-matrix formulation. Furthermore, there are some basic questions related to the nonlocal nature of the Hermitian Hamiltonian h and the pseudo-Hermitian observables such as X and P especially for $\mathcal{PT}$-symmetric potentials with a compact support (i.e., potentials vanishing outside a compact region).

To achieve this aim we will focus our attention on a simple toy model recently considered as an effective model arising in the treatment of the electromagnetic waves traveling in a planar slab waveguide that is half and half filled with gain and absorbing media.[18] This model has a standard Hamiltonian,

$$H = \frac{p^2}{2m} + v(x), \tag{9}$$

and a $\mathcal{PT}$-symmetric imaginary potential,

$$v(x) := i\zeta\left[\theta\left(x+\frac{L}{2}\right) + \theta\left(x-\frac{L}{2}\right) - 2\theta(x)\right] = \begin{cases} 0 & \text{for} \quad |x| \geqslant \dfrac{L}{2} \text{ or } x=0 \\ i\zeta & \text{for} \quad x \in \left(-\dfrac{L}{2},0\right) \\ -i\zeta & \text{for} \quad x \in \left(0,\dfrac{L}{2}\right), \end{cases} \tag{10}$$

where $L \in (0,\infty)$ is a length scale, $\zeta \in [0,\infty)$ determines the degree of non-Hermiticity of the system, and θ is the step function:

$$\theta(x) := \begin{cases} 0 & \text{for} \quad x<0 \\ \dfrac{1}{2} & \text{for} \quad x=0 \\ 1 & \text{for} \quad x>0. \end{cases} \tag{11}$$

The Hamiltonian (9) differs from a free particle Hamiltonian only within $(-L/2, L/2)$ where it coincides with the Hamiltonian for the $\mathcal{PT}$-symmetric square well.[5,19]

It is important to note that unlike in Ref. 18 we will consider the potential (10) as defining a fundamental (noneffective) quantum system having a unitary time-evolution (and S-matrix). Therefore our approach will be completely different from that pursued in Ref. 18 and the earlier studies of effective (optical) non-Hermitian Hamiltonians.[20]

Among the main reasons for our consideration of the potential (10) is that its eigenvalue problem can be solved exactly and analytically. However, the computation of the metric operator and consequently that of physical observables, localized states, associated Hermitian Hamiltonian, etc., are extremely involved, and we could only carry them out using first-order perturbation theory.

To the best of the author's knowledge, the only other non-Hermitian Hamiltonian with a continuous (and doubly degenerate) spectrum that is shown to admit a similar treatment is the one arising in the two-component formulation of the free Klein-Gordon equation.[21,22] Compared to (9), this Hamiltonian defines a technically much simpler system to handle, because it is essentially a tensor product of an ordinary Hermitian Hamiltonian and a 2×2 matrix pseudo-Hermitian Hamiltonian.

II. METRIC OPERATOR

The essential ingredient of our approach is the metric operator η_+. For a diagonalizable Hamiltonian with a discrete spectrum it can be expressed as

$$\eta_+ = \sum_n \sum_{a=1}^{d_a} |\phi_n,a\rangle\langle\phi_n,a|, \tag{12}$$

where n, a, and d_n are a spectral label, a degeneracy label, and the multiplicity (degree of degeneracy) for the eigenvalue E_n of H, respectively, and $\{|\phi_n,a\rangle\}$ is a complete set of eigenvectors of $H^\dagger$ that together with the eigenvectors $|\psi_n,a\rangle$ of H form a biorthonormal system.[4,2]

Now, consider a diagonalizable Hamiltonian with a purely continuous doubly degenerate real spectrum $\{E_k\}$, where $k\in(0,\infty)$. We will extend the application of (12) to this Hamiltonian by changing $\Sigma_n\cdots$ to $\int dk\cdots$. This yields

$$\eta_+ = \int_0^\infty dk(|\phi_k,+\rangle\langle\phi_k,+| + |\phi_k,-\rangle\langle\phi_k,-|), \tag{13}$$

where we have used $\pm$ as the values of the degeneracy label a.[22] The biorthonormal system $\{|\psi_k,a\rangle,|\phi_k,a\rangle\}$ satisfies

$$H|\psi_k,a\rangle = E_k|\psi_k,a\rangle, \quad H^\dagger|\phi_k,a\rangle = E_k|\phi_k,a\rangle, \tag{14}$$

$$\langle\phi_k,a|\psi_\ell,b\rangle = \delta_{ab}\delta(k-\ell), \quad \int_0^\infty (|\psi_k,+\rangle\langle\phi_k,+| + |\psi_k,-\rangle\langle\phi_k,-|)\mathrm{d}k = 1, \tag{15}$$

where δ_{ab} and $\delta(k)$ stand for the Kronecker and Dirac delta functions, respectively, $k\in(0,\infty)$, and $a,b\in\{-,+\}$,

We define the eigenvalue problem for the Hamiltonian (9) using the oscillating (plane wave) boundary conditions at $x=\pm\infty$ similar to the free particle case which corresponds to $\zeta=0$. To simplify the calculation of the eigenvectors we first introduce the following dimensionless quantities:

$$\mathrm{x} := \left(\frac{2}{L}\right)x, \quad \mathrm{p} := \left(\frac{L}{2\hbar}\right)p, \quad Z := \left(\frac{mL^2}{2\hbar^2}\right)\zeta, \quad \mathrm{H} := \left(\frac{mL^2}{2\hbar^2}\right)H = \mathrm{p}^2 + \mathrm{v}(\mathrm{x}), \tag{16}$$

$$\mathrm{v}(\mathrm{x}) := iZ[\theta(\mathrm{x}+1) + \theta(\mathrm{x}-1) - 2\theta(\mathrm{x})] = \begin{cases} 0 & \text{for } |\mathrm{x}| \geqslant 1 \text{ or } \mathrm{x}=0 \\ iZ & \text{for } \mathrm{x}\in(-1,0) \\ -iZ & \text{for } \mathrm{x}\in(0,1). \end{cases} \tag{17}$$

The eigenvalue problem for the scaled Hamiltonian H corresponds to the solution of the differential equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{dx}^2} + \mathrm{v}(\mathrm{x}) - \mathrm{E}_k\right]\psi(\mathrm{x}) = 0, \tag{18}$$

that is subject to the condition that ψ is a differentiable function at the discontinuities $\mathrm{x}=-1,0,1$ of v. Introducing $\psi_1:(-\infty,-1]\to\mathbb{C}$, $\psi_-:[-1,0]\to\mathbb{C}$, $\psi_+:[0,1]\to\mathbb{C}$, and $\psi_2:[1,\infty)\to\mathbb{C}$ according to

$$\psi(\mathrm{x}) =: \begin{cases} \psi_1(\mathrm{x}) & \text{for } \mathrm{x} \in (-\infty,-1] \\ \psi_-(\mathrm{x}) & \text{for } \mathrm{x} \in [-1,0] \\ \psi_+(\mathrm{x}) & \text{for } \mathrm{x} \in [0,1] \\ \psi_2(\mathrm{x}) & \text{for } \mathrm{x} \in [1,\infty), \end{cases} \tag{19}$$

we have

$$\psi_1(-1) = \psi_-(-1), \quad \psi_1'(-1) = \psi_-'(-1), \tag{20}$$

$$\psi_-(0) = \psi_+(0), \quad \psi_-'(0) = \psi_+'(0), \tag{21}$$

$$\psi_+(1) = \psi_2(1), \quad \psi_+'(1) = \psi_2'(1). \tag{22}$$

Now, imposing the plane-wave boundary condition at $\mathrm{x}=\pm\infty$ and demanding that the eigenfunctions ψ be $\mathcal{PT}$-invariant, which implies

$$\psi_-(0) = \psi_+(0)^*, \quad \psi_-'(0) = -\psi_+'(0)^*, \tag{23}$$

we find $E_k=k^2$, i.e., the spectrum is real positive and continuous, and

$$\psi_1(\mathrm{x}) = A_1 e^{ik\mathrm{x}} + B_1 e^{-ik\mathrm{x}}, \quad \psi_2(\mathrm{x}) = A_2 e^{ik\mathrm{x}} + B_2 e^{-ik\mathrm{x}}, \quad \psi_\pm(\mathrm{x}) = A_\pm e^{ik_\pm \mathrm{x}} + B_\pm e^{-ik_\pm \mathrm{x}}, \tag{24}$$

where

$$k_\pm := \sqrt{k^2 \pm iZ}, \tag{25}$$

$$A_1 = A_2^* = \frac{e^{ik}}{\sqrt{2\pi}}[L_-(k)u + K_-(k)v], \quad B_1 = B_2^* = \frac{e^{-ik}}{\sqrt{2\pi}}[L_-(-k)u + K_-(-k)v], \tag{26}$$

$$L_-(k) := \frac{1}{2}\left(\cos k_- - \frac{ik_- \sin k_-}{k}\right), \quad K_-(k) := \frac{1}{2}\sqrt{\frac{k_+}{k_-}}\left(\frac{k_- \cos k_-}{k} - i \sin k_-\right), \tag{27}$$

$$A_\pm = \frac{1}{\sqrt{8\pi}}\left[u + \left(\frac{k_+}{k_-}\right)^{\mp 1/2} v\right], \quad B_\pm = \frac{1}{\sqrt{8\pi}}\left[u - \left(\frac{k_+}{k_-}\right)^{\mp 1/2} v\right], \tag{28}$$

and $u, v \in \mathbb{R}$ are arbitrary constants (possibly depending on k and/or Z and not both vanishing).

The presence of the free parameters u and v is an indication of a double degeneracy of the eigenvalues $E_k=k^2$. We will select u and v in such a way as to ensure that in the limit $Z\to 0$ we recover the plane-wave solutions of the free particle Hamiltonian, i.e., we demand $\lim_{Z\to 0} \psi(x) = e^{\pm ik\mathrm{x}}/\sqrt{2\pi}$. This condition is satisfied if we set

$$u = 1, \quad v = \pm 1. \tag{29}$$

In the following we use the superscript $\pm$ to identify the value of a quantity obtained by setting $u=1$ and $v=\pm 1$. In this way we introduce $A_1^\pm$, $B_1^\pm$, $A_2^\pm$, $B_2^\pm$, $A_\pm^\pm$, $B_\pm^\pm$, and $\psi^\pm$. The latter define the basis (generalized[23]) eigenvectors $|\psi_k,\pm\rangle$ by $\langle \mathrm{x}|\psi_k,\pm\rangle := \psi^\pm(\mathrm{x})$.

The next step is to obtain $|\phi_k,\pm\rangle$. In view of the identity $\mathrm{H}^\dagger = \mathrm{H}|_{Z\to -Z}$, we can easily obtain the expression for the eigenfunctions ϕ of $H^\dagger$. Introducing

$$\phi(\mathrm{x}) =: \begin{cases} \phi_1(\mathrm{x}) & \text{for } \mathrm{x} \in (-\infty,-1] \\ \phi_-(\mathrm{x}) & \text{for } \mathrm{x} \in [-1,0] \\ \phi_+(\mathrm{x}) & \text{for } \mathrm{x} \in [0,1] \\ \phi_2(\mathrm{x}) & \text{for } \mathrm{x} \in [1,\infty), \end{cases} \tag{30}$$

we have

$$\phi_1(\mathrm{x}) = C_1 e^{ik\mathrm{x}} + D_1 e^{-ik\mathrm{x}}, \quad \phi_2(\mathrm{x}) = C_2 e^{ik\mathrm{x}} + D_2 e^{-ik\mathrm{x}}, \quad \phi_\pm(\mathrm{x}) = C_\pm e^{ik_\mp \mathrm{x}} + D_\pm e^{-ik_\mp \mathrm{x}}, \tag{31}$$

where

$$C_1 = C_2^* = \frac{e^{ik}}{\sqrt{2\pi}}[L_+(k)r + K_+(k)s], \quad D_1 = D_2^* = \frac{e^{-ik}}{\sqrt{2\pi}}[L_+(-k)r + K_+(-k)s], \tag{32}$$

$$L_+(k) := L_-(-k)^*, \quad K_+(k) := -K_-(-k)^*, \tag{33}$$

$$C_\pm = \frac{1}{\sqrt{8\pi}}\left[r + \left(\frac{k_+}{k_-}\right)^{\pm 1/2} s\right], \quad D_\pm = \frac{1}{\sqrt{8\pi}}\left[r - \left(\frac{k_+}{k_-}\right)^{\pm 1/2} s\right], \tag{34}$$

and $r,s \in \mathbb{R}$ are (possibly k- and/or Z-dependent) parameters that are to be fixed by imposing the biorthonormality condition (15). The latter is equivalent to a set of four (complex) equations [corresponding to the four possible choices for the pair of indices (a,b) in the first equation in (15)] which are to be solved for the two real unknowns r and s. This together with the presence of the delta function in two of these equations make the existence of a solution quite nontrivial.

We checked these equations by expanding all the quantities in powers of the non-Hermiticity parameter Z up to (but not including) terms of order two and found after a long and tedious calculation (partly done using MATHEMATICA) that indeed all four of these equations are satisfied, if we set $r=u=1$ and $s=v=\pm 1$. Again we will refer to this choice using superscript $\pm$. In particular, we have $\phi^\pm = \psi^\pm|_{Z\to -Z}$ and $\langle \mathrm{x}|\phi_k,\pm\rangle := \phi^\pm(\mathrm{x})$.

Having obtained $|\phi_k,\pm\rangle$ we are in a position to calculate the metric operator (13). We carried out this calculation using first-order perturbation theory in Z. It involved expanding the $\phi_1^\pm(\mathrm{x})$, $\psi_2^\pm(\mathrm{x})$, and $\psi_\pm^\pm(\mathrm{x})$ in powers of Z, substituting the result in

$$\langle \mathrm{x}|\eta_+|\mathrm{y}\rangle = \int_0^\infty [\phi^+(\mathrm{y})^* \phi^+(\mathrm{x}) + \phi^-(\mathrm{y})^* \phi^-(\mathrm{x})]dk \tag{35}$$

which follows from (13), and using the identities:

$$\int_{-\infty}^{\infty} e^{iak}dk = 2\pi\delta(a), \quad \int_{-\infty}^{\infty} \frac{e^{iak}}{k}dk = i\pi\,\mathrm{sign}(a), \quad \int_{-\infty}^{\infty} \frac{e^{iak}-e^{ibk}}{k^2}dk = \pi(|b|-|a|) \tag{36}$$

[where $a,b \in \mathbb{R}$ and $\mathrm{sign}(a) := \theta(a) - \theta(-a)$] to perform the integral over k for all 16 possibilities for the range of values of the pair of independent variables (x,y) in (35). This is an extremely lengthy calculation whose detail we will not include here. It is absolutely remarkable that the expressions for $\langle \mathrm{x}|\eta_+|\mathrm{y}\rangle$ that we obtain for these 16 possibilities may be combined to yield a single formula that is valid for all $\mathrm{x},\mathrm{y} \in \mathbb{R}$, namely

$$\langle \mathrm{x}|\eta_+|\mathrm{y}\rangle = \delta(\mathrm{x}-\mathrm{y}) + \frac{i}{8}(4 + 2|\mathrm{x}+\mathrm{y}| - |\mathrm{x}+\mathrm{y}+2| - |\mathrm{x}+\mathrm{y}-2|)\mathrm{sign}(\mathrm{x}-\mathrm{y})Z + \mathcal{O}(Z^2), \tag{37}$$

where $\mathcal{O}(Z^2)$ stands for terms of order two and higher in powers of Z. Note that $\langle \mathrm{x}|\eta_+|\mathrm{y}\rangle^* = \langle \mathrm{y}|\eta_+|\mathrm{x}\rangle$, which is consistent with the Hermiticity of η_+.

III. PHYSICAL OBSERVABLES AND LOCALIZED STATES

The physical observables of the system described by the Hamiltonian (9) are obtained from the Hermitian operators acting in $\mathcal{H}=L^2(\mathbb{R})$ by the similarity transformation (6). This equation involves the positive square root ρ of η_+ which takes the form[16]

$$\rho^{\pm 1} = e^{\mp Q/2}, \tag{38}$$

if we express η in the exponential form

$$\eta_+ = e^{-Q}. \tag{39}$$

In view of (38) and the Backer-Campbell-Hausdorff identity,

$$e^{-A}Be^{A} = B + [B,A] + \frac{1}{2!}[[B,A],A] + \dots \tag{40}$$

(where A and B are linear operators), physical observables (6) satisfy[16]

$$O = o - \tfrac{1}{2}[o,Q] + \tfrac{1}{8}[[o,Q],Q] + \ \dots . \tag{41}$$

If we expand η_+ and Q in powers of Z,

$$\eta_+ = 1 + \sum_{\ell=1}^{\infty} \eta_{+_\ell} Z^{\ell}, \quad Q = \sum_{\ell=1}^{\infty} Q_{\ell} Z^{\ell}, \tag{42}$$

where η_{+_ℓ} and Q_ℓ are Z-independent Hermitian operators, we find using (39) that

$$Q_1 = -\eta_{+_1}, \quad Q_2 = -\eta_{+_2} + \tfrac{1}{2}\eta_{+_1}^2. \tag{43}$$

Combining this relation with (41), we have

$$O = o - \tfrac{1}{2}[o,Q_1]Z + \tfrac{1}{8}(-4[o,Q_2] + [[o,Q_1],Q_1])Z^2 + \mathcal{O}(Z^3). \tag{44}$$

In the following we calculate the η_+-pseudo-Hermitian position (X) and momentum (P) operators,[16] up to (but not including) terms of order Z^2. This is because so far we have only calculated η_{+_1} which in view of (37) satisfies

$$\langle \mathrm{x}|\eta_{+_1}|\mathrm{y}\rangle = \tfrac{i}{8}(4 + 2|\mathrm{x}+\mathrm{y}| - |\mathrm{x}+\mathrm{y}+2| - |\mathrm{x}+\mathrm{y}-2|)\mathrm{sign}(\mathrm{x}-\mathrm{y}), \quad \forall\, \mathrm{x},\mathrm{y} \in \mathbb{R}. \tag{45}$$

Substituting the scaled position (x) and momentum (p) operator for o in (44), using (45), and doing the necessary algebra, we find

$$\langle \mathrm{x}|\mathrm{X}|\mathrm{y}\rangle = \mathrm{x}\,\delta(\mathrm{x}-\mathrm{y}) + \frac{i}{16}(4 + 2|\mathrm{x}+\mathrm{y}| - |\mathrm{x}+\mathrm{y}+2| - |\mathrm{x}+\mathrm{y}-2|)|\mathrm{x}-\mathrm{y}|Z + \mathcal{O}(Z^2), \tag{46}$$

$$\langle \mathrm{x}|\mathrm{P}|\mathrm{y}\rangle = -i\partial_{\mathrm{x}}\delta(\mathrm{x}-\mathrm{y}) + \tfrac{1}{8}[2\ \mathrm{sign}(\mathrm{x}+\mathrm{y}) - \mathrm{sign}(\mathrm{x}+\mathrm{y}+2) - \mathrm{sign}(\mathrm{x}+\mathrm{y}-2)]\mathrm{sign}(\mathrm{x}-\mathrm{x})Z + \mathcal{O}(Z^2), \tag{47}$$

where $\mathrm{X} := 2X/L$ and $\mathrm{P} := LP/(2\hbar)$ are dimensionless η_+-pseudo-Hermitian position and momentum operators, respectively.

As seen from (46), both X and P are manifestly nonlocal and non-Hermitian (but pseudo-Hermitian) operators. If we scale back the relevant quantities in (46) and (47) according to (16), we find

$$\langle x|X|y\rangle = x\,\delta(x-y) + \frac{im}{4\hbar^2}(2L + 2|x+y| - |x+y+L| - |x+y-L|)|x-y|\zeta + \mathcal{O}(\zeta^2), \tag{48}$$

$$\langle x|P|y\rangle = -i\hbar\partial_x\delta(x-y) + \frac{m}{4\hbar}[2\,\mathrm{sign}(x+y) - \mathrm{sign}(x+y+L) - \mathrm{sign}(x+y-L)]\mathrm{sign}(x-y)\zeta + \mathcal{O}(\zeta^2). \tag{49}$$

Note that the contributions of order ζ to P vanish, if both x and y take values outside $[-L/2, L/2]$.

Next, we compute the localized states $\xi^{(x)}$ of the system. The corresponding state vectors are defined by (7). Using this equation as well as (38), (42), (43), (45), and (16) we have the following expression for the x-representation of a localized state $\xi^{(y)}$ centered at $y \in \mathbb{R}$:

$$\langle x|\xi^{(y)}\rangle = \delta(x-y) - \frac{im\zeta}{8\hbar^2}(2L + 2|x+y| - |x+y+L| - |x+y-1|)\mathrm{sign}(x-y) + \mathcal{O}(\zeta^2). \tag{50}$$

Because the linear term in ζ is imaginary, the presence of a weak non-Hermiticity only modifies the usual (Hermitian) localized states by making them complex (nonreal) while keeping their real part intact. Note however that for a fixed y the imaginary part of $\langle x|\xi^{(y)}\rangle$ does not tend to zero as $|x-y| \to \infty$. This observation which seems to be in conflict with the usual notion of localizability has a simple explanation. Because the usual x operator is no longer an observable, it does not describe the position of the particle. This is done by the pseudo-Hermitian position operator X; it is the physical position wave function $\Psi(x) := \langle \xi^{(x)}, \psi\rangle_+$ that defines the probability density of localization in space (8). The physical position wave function for the localized state $\xi^{(y)}$ is given by $\langle \xi^{(x)}, \xi^{(y)}\rangle_+ = \langle x|y\rangle = \delta(x-y)$ which is the expected result.

IV. EQUIVALENT HERMITIAN HAMILTONIAN AND CLASSICAL LIMIT

The calculation of the equivalent Hermitian Hamiltonian h for the Hamiltonian (9) is similar to that of the physical observables. In view of (2), (38), (40), and (42), and the last equation in (16) which we express as

$$\mathrm{H} = \mathrm{p}^2 + i\nu(\mathrm{x})Z \text{ with } \nu(\mathrm{x}) := \theta(\mathrm{x}+1) + \theta(\mathrm{x}-1) - 2\theta(\mathrm{x}), \tag{51}$$

we have

$$\mathrm{h} = \mathrm{p}^2 + h_1 Z + h_2 Z^2 + \mathcal{O}(Z^3), \tag{52}$$

$$\mathrm{h}_1 := i\nu(\mathrm{x}) + \tfrac{1}{2}[\mathrm{p}^2, Q_1], \tag{53}$$

$$\mathrm{h}_2 := \tfrac{1}{8}\{4[\mathrm{p}^2, Q_2] + 4i[\nu(\mathrm{x}), Q_1] + [[\mathrm{p}^2, Q_1], Q_1]\}. \tag{54}$$

where

$$\mathrm{h} := \rho \mathrm{H} \rho^{-1} = mL^2 h/(2\hbar^2) \tag{55}$$

is the dimensionless Hermitian Hamiltonian associated with H.

Next, we substitute (43) and (45) in the identity $\langle \mathrm{x}|[\mathrm{p}^2, Q_1]|\mathrm{v}\rangle = (\partial_{\mathrm{y}}^2 - \partial_{\mathrm{x}}^2)\langle \mathrm{x}|Q_1|\mathrm{y}\rangle$, and perform the necessary algebra. We then find $\langle \mathrm{x}|[\mathrm{p}^2, Q_1]|\mathrm{v}\rangle = -2i\nu(\mathrm{x})\delta(\mathrm{x}-\mathrm{y})$. Therefore,

$$[\mathrm{p}^2, Q_1] = -2i\nu(\mathrm{x}), \tag{56}$$

and in view of (53)

$$\mathrm{h}_1 = 0. \tag{57}$$

This was actually to be expected, for both the operators appearing on the right-hand side of (53) are anti-Hermitian, while its left-hand side is Hermitian. The fact that an explicit calculation of the right-hand side of (53) yields the desired result, namely (57), is an important check on the validity of our calculation of η_{+_1}. It may also be viewed as an indication of the consistency and general applicability of our method, that was initially formulated for systems with a discrete spectrum.[5,16]

According to (57),

$$\mathrm{h} = \mathrm{p}^2 + \mathrm{h}_2 Z^2 + \mathcal{O}(Z^3). \tag{58}$$

Hence, in order to obtain a better understanding of the nature of the system described by the Hamiltonian H, we need to calculate h_2. As we will next show, the knowledge of $\langle \mathrm{x}|\eta_{+_1}|\mathrm{y}\rangle$ turns out to be sufficient for the calculation of h_2. To see this we first employ (56) to express h_2 in the form

$$\mathrm{h}_2 = \tfrac{1}{4}(2[\mathrm{p}^2, Q_2] + i[\nu(\mathrm{x}), Q_1]). \tag{59}$$

Now, we recall that p^2, Q_2, $\nu(\mathrm{x})$, and Q_1 are all Hermitian operators. Therefore $[\mathrm{p}^2, Q_2]$ and $i[\nu(\mathrm{x}), Q_1]$ are, respectively, anti-Hermitian and Hermitian. In view of (59) and the Hermiticity of h_2, this implies that

$$[\mathrm{p}^2, Q_2] = 0. \tag{60}$$

Hence,

$$\mathrm{h}_2 = \frac{i}{4}[\nu(\mathrm{x}), Q_1] = \frac{i}{4}[\eta_{+1}, \nu(\mathrm{x})], \tag{61}$$

where we have also made use of the first equation in (43). We should also mention that the identities (56) and (60) can be directly obtained from the pseudo-Hermiticity condition (5) by substituting (39) in (5) and using (40) and (42).

We can easily use (45) and (61) to yield the expression for the integral kernel of h_2, namely

$$\langle \mathrm{x}|\mathrm{h}_2|\mathrm{y}\rangle = \tfrac{1}{32}(4 + 2|\mathrm{x}+\mathrm{y}| - |\mathrm{x}+\mathrm{y}+2| - |\mathrm{x}+\mathrm{y}-2|)\mathrm{sign}(\mathrm{x}-\mathrm{y})[\nu(\mathrm{x}) - \nu(\mathrm{y})], \quad \forall\, \mathrm{x},\mathrm{y} \in \mathbb{R}. \tag{62}$$

As seen from this equation, $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{y}\rangle = 0$, if $\mathrm{x} \notin [-1,1]$ and $\mathrm{y} \notin [-1,1]$.

We can express h_2 as a function of x and p by performing a Fourier transformation on the y variable appearing in (62), i.e., computing

$$\langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle \coloneqq (2\pi)^{-1/2}\int_{-\infty}^{\infty} \langle \mathrm{x}|\mathrm{h}_2|\mathrm{y}\rangle e^{i\mathrm{py}} d\mathrm{y}. \tag{63}$$

This yields h_2 as a function of x and p, if we order the factors by placing x's to the left of p's. We can easily do this by expanding $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle$ in powers of p. Denoting the x-dependent coefficients by ω_n, we then have

$$\mathrm{h}_2 = \sum_{n=0}^{\infty} \omega_n(\mathrm{x})\mathrm{p}^n, \tag{64}$$

where we have made the implicit assumption that $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle$ is a real-analytic function of p.

The Fourier transform of $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{y}\rangle$ can be performed explicitly. [One way of doing this is to use the integral representations of the absolute value and sign function, as given in (36), to perform the y-integrations in (63) and use the identities

$$\int_{-\infty}^{\infty} \frac{e^{iau}du}{u(u-k)} = \frac{i\pi}{k}(e^{iak} - 1)\mathrm{sign}(a),$$

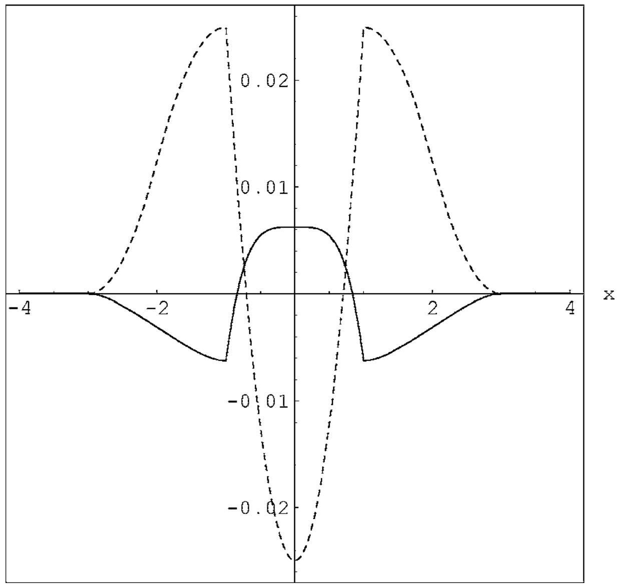

FIG. 1. Graph of the real part of ω_0 (dashed curve) and ω_2 (full curve).

$$\int_{-\infty}^{\infty}\frac{e^{iau}du}{u(u-k)^2}=\frac{i\pi}{k^2}[1+(iak-1)e^{iak}]\mathrm{sign}(a), \quad \forall\, a,k\in\mathbb{R},$$

to evaluate the remaining two integrals. The resulting expression is too lengthy and complicated to be presented here.] We have instead used MATHEMATICA to calculate $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle$ and found the coefficients ω_n for $n\leqslant 5$. It turns out that indeed $\langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle$ does not have a singularity at $\mathrm{p}=0$, and that $\omega_0,\omega_2,\omega_4$ are real and vanish outside $(-3,3)$ while $\omega_1,\omega_3,\omega_5$ are imaginary and proportional to $\theta(\mathrm{x})-1/2$ outside $(-3,3)$. As we will explain momentarily these properties are necessary to ensure the Hermiticity of h.

Figures 1, 2, and 3 show the plots of real part of ω_n for $n=0,2,4$ and the imaginary part of ω_n

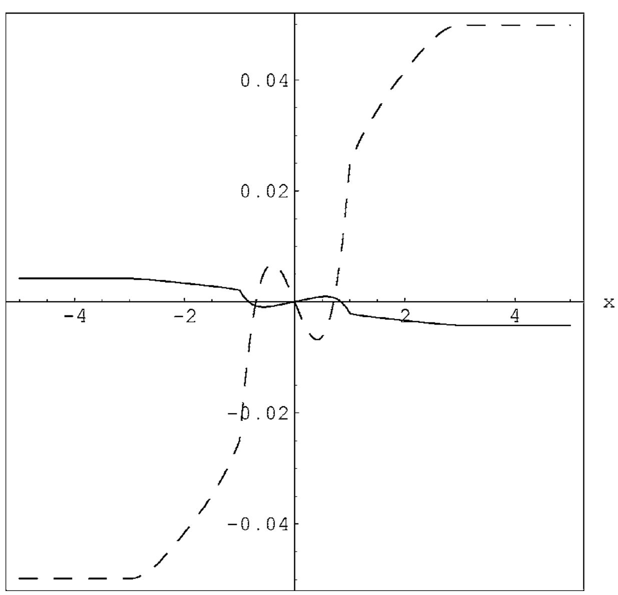

FIG. 2. Graph of the imaginary part of ω_1 (dashed curve) and ω_3 (full curve).

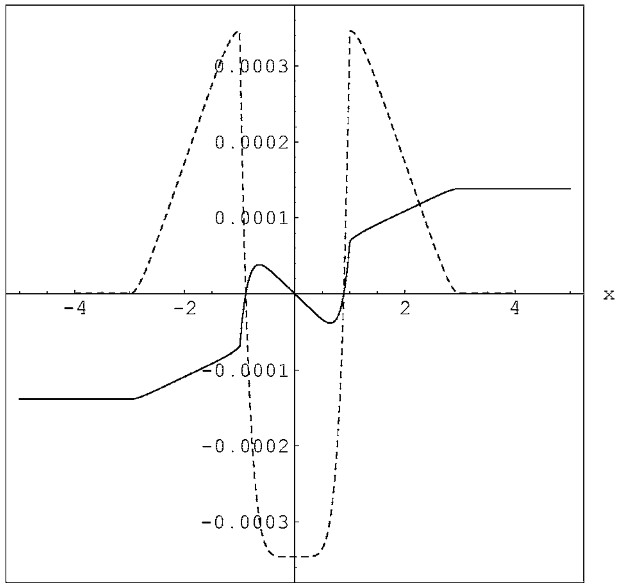

FIG. 3. Graph of the real part of ω_4 (dashed curve) and the imaginary part of ω_5 (full curve).

for $n=1,3,5$. As seen from these figures (the absolute value of) ω_n sharply decreases with n, which suggests that a truncation of (64) yields a good approximation for the action of h_2 on the wave functions with bounded and sufficiently small x-derivatives.

If we use $\langle \mathrm{p}|\mathrm{h}_2|\mathrm{x}\rangle = \langle \mathrm{x}|\mathrm{h}_2|\mathrm{p}\rangle^*$ to determine the form of h_2 and suppose that $\omega_{2n}(\mathrm{x})$ are real and $\omega_{2n+1}(\mathrm{x})$ are imaginary for all $n=0,1,2,3,\ldots$, we find

$$\mathrm{h}_2 = \sum_{n=0}^{\infty} \mathrm{p}^n \omega_n(\mathrm{x})^* = \sum_{n=0}^{\infty} [\mathrm{p}^{2n}\omega_{2n}(\mathrm{x}) - \mathrm{p}^{2n+1}\omega_{2n+1}(\mathrm{x})].$$

Adding both sides of this relation to those of (64) and diving by two, we obtain

$$\mathrm{h}_2 = \frac{1}{2}\sum_{n=0}^{\infty} \{a_n(\mathrm{x}),\mathrm{p}^{2n}\}, \quad a_n(\mathrm{x}) := \omega_{2n}(\mathrm{x}) + i\omega'_{2n+1}(\mathrm{x}), \tag{65}$$

where $\{\cdot,\cdot\}$ stands for the anticommutator, a prime denotes a derivative, and we have made use of the identity: $[f(\mathrm{x}),\mathrm{p}^m] = \{if'(\mathrm{x}),\mathrm{p}^{m-1}\}$. It is important to note that because $\omega_{2n}(\mathrm{x})$ are real and $\omega_{2n+1}(\mathrm{x})$ are imaginary, $a_n(\mathrm{x})$ are real. Moreover, outside $(-3,3)$, $\omega_{2n}(\mathrm{x})$, $\omega'_{2n+1}(\mathrm{x})$, and consequently a_n vanish. Therefore, we can express h_2 in the manifestly Hermitian form (65) with all the x-dependent coefficient functions vanishing outside $(-3,3)$. Figure 4 shows the plots of a_n for $n=0,1,2$. They are all even functions of x with an amplitude of variations that decreases rapidly as n increases.

Next, we scale back the relevant quantities and use (16), (55), (58), and (65) to obtain

$$h = \frac{p^2}{2m} + \frac{\zeta^2}{2}\sum_{n=0}^{\infty} \{\alpha_n(x),p^{2n}\} + \mathcal{O}(\zeta^3), \quad \alpha_n(x) := 2m\left(\frac{L}{2\hbar}\right)^{2(n+1)} a_n\left(\frac{2x}{L}\right). \tag{66}$$

In view of the fact that a_n and α_n are real-valued even functions, h is a manifestly Hermitian $\mathcal{P}$- and $\mathcal{T}$-symmetric Hamiltonian. We can also express it in the form

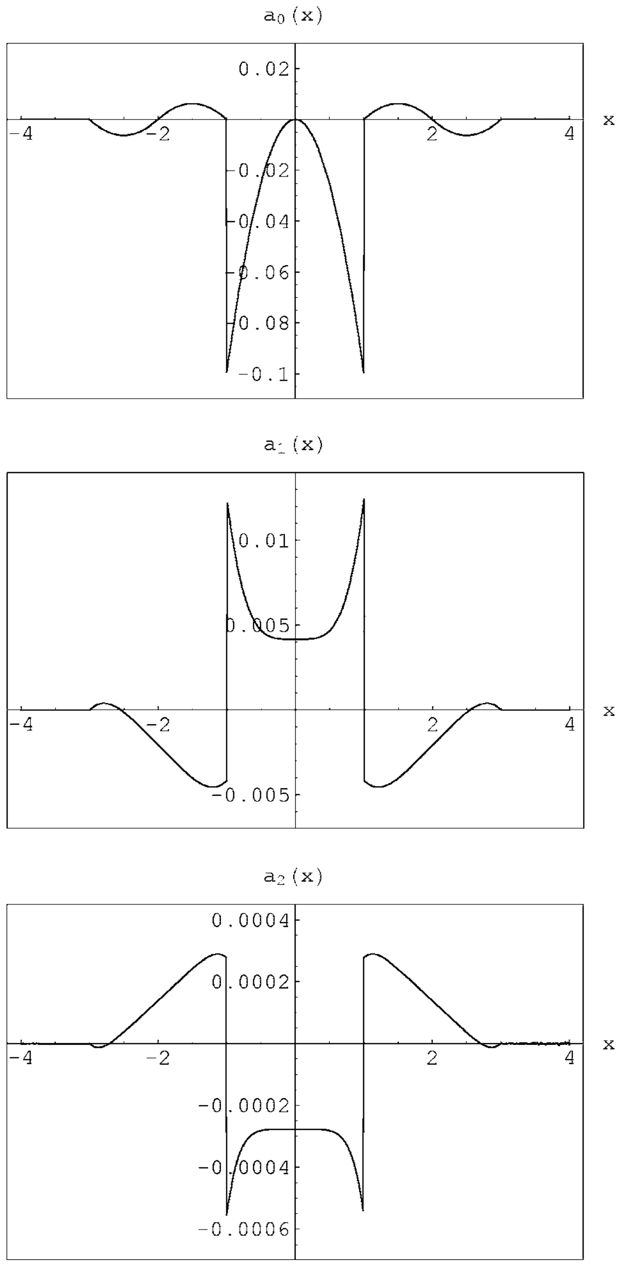

FIG. 4. Graph of a_0, a_1, and a_2.

$$h = \frac{1}{4}\{m_{\text{eff}}^{-1}(x), p^2\} + w(x) + \frac{\zeta^2}{2}\sum_{n=2}^{\infty}\{\alpha_n(x), p^{2n}\} + \mathcal{O}(\zeta^3), \tag{67}$$

where

$$m_{\text{eff}}(x) := \frac{m}{1 + 2m\zeta^2\alpha_1(x)}, \quad w(x) := \zeta^2\alpha_0(x).$$

Therefore, for low energy particles where one may neglect terms involving fourth and higher powers of p, the Hamiltonian h and consequently H describe motion of a particle with an effective position dependent mass $m_{\text{eff}}(x)$ that interacts with the potential $w(x)$. Figure 5 shows a graph of

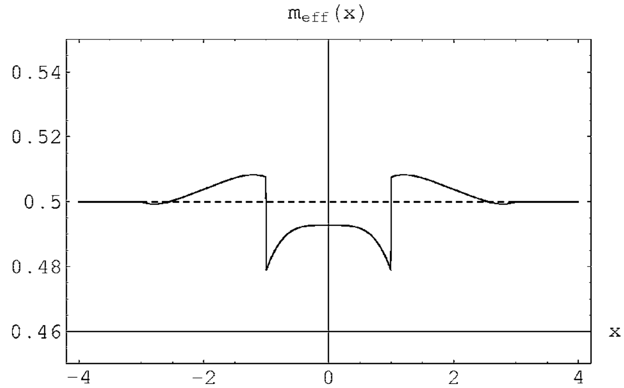

FIG. 5. Graph of the effective mass $m_{\rm eff}$ (full curve) for $m=\frac{1}{2}$, $\hbar=1$, $L=2$, and $\zeta=\frac{1}{3}$. The dashed curve represents $m=\frac{1}{2}$.

$m_{\rm eff}(x)$ for $m=1/2$, $\hbar=1$, $L=2$, and $\zeta=1/3$. For the same values of these parameters, $w(x)=a_0(x)/9$. See Fig. 4 for a graph of a_0.

If we replace (x,p) of (66) and (67) with their classical counterparts (x_c,p_c), we obtain the "classical" Hamiltonian:

$$\tilde{H}_c=\frac{p_c^2}{2m}+\frac{\zeta^2}{2}\sum_{n=0}^{\infty}\alpha_n(x_c)p_c^{2n}+\mathcal{O}(\zeta^3)=\frac{p_c^2}{2m_{\rm eff}(x_c)}+w(x_c)+\frac{\zeta^2}{2}\sum_{n=2}^{\infty}\alpha_n(x_c)p_c^{2n}+\mathcal{O}(\zeta^3), \qquad (68)$$

which coincides with the free particle Hamiltonian outside the *physical interaction region*, i.e., $(-3L/2,3L/2)$. The fact that this region is three times larger than the support $(-L/2,L/2)$ of the potential $v(x)$ is quite surprising. Note also that $\tilde{H}_c$ is an even function of both the position x_c and momentum p_c variables.

Figure 6 shows the phase space trajectories associated with the Hamiltonian $\tilde{H}_c$ for $L=2$, $\hbar=1$, $m=1/2$, $\zeta=Z=1/3$. For large values of the momentum the trajectories are open curves describing the scattering of a particle due to an interaction that takes place within the physical interaction region, $(-3,3)$. For sufficiently small values of the momentum closed trajectories are

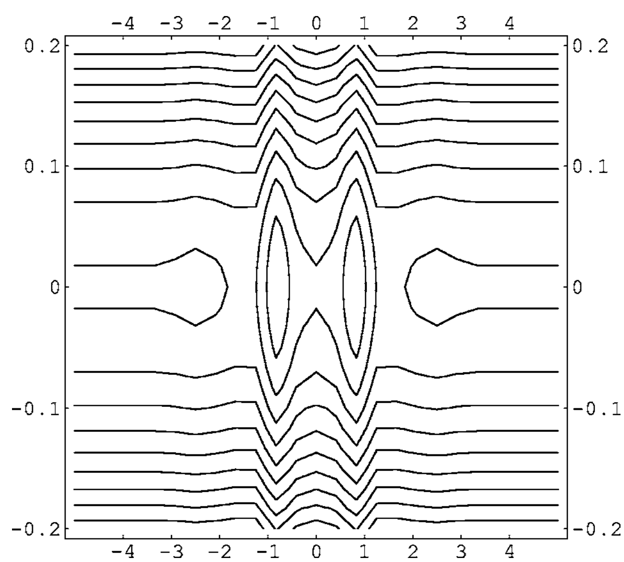

FIG. 6. Phase space trajectories of the Hamiltonian $\tilde{H}_c(x_c,p_c)$ for $m=\frac{1}{2}$, $\hbar=1$, $L=2$, and $\zeta=\frac{1}{3}$. The horizontal and vertical axes are, respectively, those of x_c and p_c.

generated. These describe a particle that is trapped inside the physical interaction region. This is consistent with the fact that for small p_c, $\widetilde{H}_c$ is dominated by the potential term $w(x_c)$ which in view of its relation to $a_0(x)$ and Fig. 4 can trap the particle.

We wish to emphasize that because we have not yet taken the $\hbar \to 0$ limit of $\widetilde{H}_c$, we cannot identify it with the the true classical Hamiltonian H_c for the quantum Hamiltonian h and consequently H. Given the limitations of our perturbative calculation of $\widetilde{H}_c$, we are unable to determine this limit. (This is in contrast with both the $\mathcal{PT}$-symmetric square well and the $\mathcal{PT}$-symmetric cubic anharmonic oscillator studied in Refs. 5 and 16, respectively. In the former system the presence of an exceptional spectral point imposes the condition that ζ must be of order $\hbar^2$ or higher and consequently the classical system is the same as that of the Hermitian infinite square well.[5] In the latter system, the $\hbar \to 0$ limit of the associated Hermitian Hamiltonian can be easily evaluated and classical Hamiltonian obtained.[16]) Therefore, we cannot view the presence of closed phase space trajectories for $\widetilde{H}_c$ as evidence for the existence of bound states of h and H. This is especially because these trajectories are associated with very low momentum values where the quantum effects are expected to be dominant.

V. CONCLUSION

In this paper we explored for the first time the utility of the methods of pseudo-Hermitian quantum mechanics in dealing with a non-Hermitian $\mathcal{PT}$-symmetric potential $v(x)$ that has a continuous spectrum. We were able to solve the eigenvalue problem for this potential exactly and obtain the explicit form of the metric operator, the pseudo-Hermitian position and momentum operators, the localized states, and the equivalent Hermitian Hamiltonian perturbatively.

Our analysis revealed the surprising fact that the physical interaction region for this model is three times larger than the support of the potential, i.e., there is a region of the configuration space in which $v(x)$ vanishes but the interaction does not seize.

A simple interpretation for this peculiar property is that the argument x of the potential $v(x)$ is not a physical observable and the support $(-L/2, L/2)$ of $v(x)$ being a range of eigenvalues of x does not have a direct physical meaning. This observation underlines the importance of the Hermitian representation of non-Hermitian (inparticular $\mathcal{PT}$-symmetric) Hamiltonians having a real spectrum.

The Hermitian representation involves a nonlocal Hamiltonian that is not suitable for the computation of the energy spectrum or the S-matrix of the theory. Yet it provides invaluable insight in the physical meaning and potential applications of pseudo-Hermitian and $\mathcal{PT}$-symmetric Hamiltonians and is indispensable for the determination of the other observables of the corresponding quantum systems.

[1] C. M. Bender and S. Boettcher, Phys. Rev. Lett. **80**, 5243 (1998); C. M. Bender, S. Boettcher, and P. N. Meisenger, J. Math. Phys. **40**, 2201 (1999).
[2] A. Mostafazadeh, J. Math. Phys. **43**, 2814 (2002); **43**, 3944 (2002).
[3] A. Mostafazadeh, J. Phys. A **36**, 7081 (2003).
[4] A. Mostafazadeh, J. Math. Phys. **43**, 205 (2002).
[5] A. Mostafazadeh and A. Batal, J. Phys. A **37**, 11645 (2004).
[6] A. Mostafazadeh, Nucl. Phys. B **640**, 419 (2002).
[7] A. Mostafazadeh, J. Math. Phys. **44**, 974 (2003).
[8] H. B. Geyer, F. G. Scholtz, and I. Snyman, Czech. J. Phys. **54**, 1069 (2004).
[9] A. Mostafazadeh, J. Math. Phys. **43**, 6343 (2002); **44**, 943 (2003).
[10] G. Scolarici and L. Solombrino, J. Math. Phys. **44**, 4450 (2003).
[11] A. Mostafazadeh, J. Math. Phys. **45**, 932 (2004).
[12] C. M. Bender, D. C. Brody, and H. F. Jones, Phys. Rev. Lett. **89**, 270401 (2002).
[13] A. Mostafazadeh, J. Phys. A **38**, 3213 (2005).
[14] F. G. Scholtz, H. B. Geyer, and F. J. W. Hahne, Ann. Phys. (N.Y.) **213**, 74 (1992).
[15] A. Mostafazadeh, preprint: quant-ph/0310164.
[16] A. Mostafazadeh, J. Phys. A **38**, 6557 (2005), quant-ph/0411137.
[17] H. F. Jones, preprint: quant-ph/0411171; A. Banerjee, preprint: quant-ph/0502163.
[18] A. Ruschhaupt, F. Delgado, and J. G. Muga, J. Phys. A **38**, L171 (2005).
[19] M. Znojil, Phys. Lett. A **285**, 7 (2001); B. Bagchi, S. Mallik, and C. Quesne, Mod. Phys. Lett. A **17**, 1651 (2002).

[20] R. N. Deb, A. Khare, and B. D. Roy, Phys. Lett. A **307**, 215 (2003); J. G. Muga, J. P. Palao, B. Navarro, and I. L. Egusquiza, Phys. Rep. **395**, 357 (2004).
[21] A. Mostafazadeh, Class. Quantum Grav. **20**, 155 (2003); Ann. Phys. (N.Y.) **309**, 1 (2004).
[22] A. Mostafazadeh, preprint: quant-ph/0307059.
[23] A. Bohm, *Quantum Mechanics: Foundations and Applications*, 3rd ed. (Springer, Berlin, 1993).