Particle in a box in $\mathcal{PT}$-symmetric quantum mechanics and an electromagnetic analog

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In $\mathcal{PT}$-symmetric quantum mechanics a fundamental principle of quantum mechanics, that the Hamiltonian must be Hermitian, is replaced by another set of requirements, including notably symmetry under $\mathcal{PT}$, where $\mathcal{P}$ denotes parity and $\mathcal{T}$ denotes time reversal. Here we study the role of boundary conditions in $\mathcal{PT}$-symmetric quantum mechanics by constructing a simple model that is the $\mathcal{PT}$-symmetric analog of a particle in a box. The model has the usual particle-in-a-box Hamiltonian but boundary conditions that respect $\mathcal{PT}$ symmetry rather than Hermiticity. We find that for a broad class of $\mathcal{PT}$-symmetric boundary conditions the model respects the condition of unbroken $\mathcal{PT}$ symmetry, namely, that the Hamiltonian and the symmetry operator $\mathcal{PT}$ have simultaneous eigenfunctions, implying that the energy eigenvalues are real. We also find that the Hamiltonian is self-adjoint under the $\mathcal{PT}$-symmetric inner product. Thus we obtain a simple soluble model that fulfills all the requirements of $\mathcal{PT}$-symmetric quantum mechanics. In the second part of this paper we formulate a variational principle for $\mathcal{PT}$-symmetric quantum mechanics that is the analog of the textbook Rayleigh-Ritz principle. Finally we consider electromagnetic analogs of the $\mathcal{PT}$-symmetric particle in a box. We show that the isolated particle in a box may be realized as a Fabry-Perot cavity between an absorbing medium and its conjugate gain medium. Coupling the cavity to an external continuum of incoming and outgoing states turns the energy levels of the box into sharp resonances. Remarkably we find that the resonances have a Breit-Wigner line shape in transmission and a Fano line shape in reflection; by contrast, in the corresponding Hermitian case the line shapes always have a Breit-Wigner form in both transmission and reflection.

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I. INTRODUCTION

In $\mathcal{PT}$-symmetric quantum mechanics the canonical principle that the Hamiltonian must be Hermitian is relaxed. Nonetheless it remains possible to consistently formulate quantum mechanics if the Hamiltonian operator respects certain conditions, notably $\mathcal{PT}$ symmetry. In principle, $\mathcal{PT}$ quantum mechanics expands the set of Hamiltonians that can be used to describe natural phenomena. The purpose of this paper is to add to known examples of $\mathcal{PT}$ quantum mechanics by formulating an especially simple model: the particle in a box.

Prior work on $\mathcal{PT}$ quantum mechanics has considered Hamiltonians in which the potential is imaginary [1–3] and hence the Hamiltonian is manifestly non-Hermitian. Here we keep the usual particle-in-a-box Hamiltonian. Non-Hermiticity enters the problem through the boundary conditions. There is a well-developed theory of self-adjoint extensions that determines the boundary conditions that are permissible in quantum mechanics if one imposes Hermiticity on the Hamiltonian [4,5]. Here we develop the $\mathcal{PT}$ counterpart of this body of knowledge by consideration of a simple example. In complementary prior work Nelson and Hatano [6] have studied a model with non-Hermitian periodic boundary conditions.

Another result in this paper is the formulation of a variational principle that is the $\mathcal{PT}$ quantum mechanics analog of the textbook Rayleigh-Ritz variational principle.

In a development parallel to, but separate from, $\mathcal{PT}$ quantum mechanics it has been found that photonic structures with $\mathcal{PT}$ symmetry have many remarkable properties [7–9], notably the coexistence of lasing and perfect coherent absorption [10–13]. In this paper we also construct a classical electromagnetic analog of the $\mathcal{PT}$-symmetric particle in a box. By allowing the modes of the box to couple to an external continuum of incoming and outgoing modes we obtain an electromagnetic structure that has sharp resonances in place of the bound states of an isolated box. Remarkably we find that these resonances have a Breit-Wigner line shape in transmission and a Fano line shape in reflection.

II. PARTICLE IN A BOX

A. Boundary conditions

We consider a nonrelativistic spinless particle in one dimension with position x confined to lie in a box of size L so that $0 \leqslant x \leqslant L$. The particle is governed by the Hamiltonian

$$h = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}; \tag{1}$$

hereafter we shall work in units wherein $\hbar = 1$ and $m = 1$. Parity applied to the wave function has the effect

$$\mathcal{P}\psi(x) = \psi(L - x), \tag{2}$$

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while time reversal is the antilinear operator

$$\mathcal{T}\psi(x) = \psi^*(x). \tag{3}$$

Note that $\mathcal{P}^2 = 1$ and $\mathcal{T}^2 = 1$ while $[\mathcal{P},\mathcal{T}] = 0$. By the linearity of quantum mechanics the wave function must obey the boundary conditions [14]

$$\psi(0) = \lambda_1\psi'(0), \quad \psi(L) = \lambda_2\psi'(L), \tag{4}$$

where (λ_1,λ_2) are complex numbers. Thus any boundary condition is fully characterized by the pair (λ_1,λ_2).

Thus far we have described features common to both the canonical particle in a box and its $\mathcal{PT}$-symmetric counterpart being introduced here. We now turn to the differences. In canonical quantum mechanics one supposes that the inner product of two states is defined as

$$(\phi,\psi) = \int_0^L dx\, \phi^*(x)\psi(x) \tag{5}$$

and moreover, the Hamiltonian is Hermitian or self-adjoint with respect to this inner product. In order to ensure that the Hamiltonian is self-adjoint we must pay attention to the boundary conditions that are imposed on the wave functions. Integration by parts reveals that the self-adjointness condition $(\phi,h\psi) = (h\phi,\psi)$ is fulfilled provided the surface term

$$[\phi^*\psi' - \psi^*\phi']_0^L = 0 \tag{6}$$

vanishes.

If we impose the boundary conditions (4) on ψ, then it is easy to verify that one must impose the boundary conditions

$$\phi(0) = \lambda_1^*\phi'(0), \quad \phi(L) = \lambda_2^*\phi'(L) \tag{7}$$

on $\phi(x)$ in order to fulfill the surface condition (6). Note that in general the boundary conditions we must impose on ϕ are different from those we must impose on ψ; the boundary conditions on ϕ are said to be the adjoint of the boundary conditions on ψ.

In the special case that λ_1 and λ_2 are real, the same boundary condition is imposed on ψ and ϕ, and the boundary condition is said to be self-adjoint. To ensure that the Hamiltonian equation (1) is Hermitian we must impose self-adjoint boundary conditions on the wave functions. Textbook treatments of the particle in a box tend to focus exclusively on the hard wall case $\lambda_1 = \lambda_2 = 0$ but in fact any member of the two-parameter family of self-adjoint boundary conditions may be used. Which one should be used in practice depends on the physics of the problem that is being modeled as a particle in a box. So long as we use self-adjoint boundary conditions we may be sure that the eigenvalues of the Hamiltonian h are real and the eigenfunctions are complete.

Now let us put aside considerations of Hermiticity and ask what kinds of boundary conditions are permissible in $\mathcal{PT}$ quantum mechanics. The criterion we impose is that the boundary conditions must be $\mathcal{PT}$ symmetric in the sense that if $\psi(x)$ obeys the boundary conditions, then so does

$$\xi(x) = \mathcal{PT}\psi(x) = \psi^*(L - x). \tag{8}$$

It is only with $\mathcal{PT}$-symmetric boundary conditions that the Hamiltonian may properly be said to commute with the operator $\mathcal{PT}$, one of three necessary conditions for $\mathcal{PT}$ quantum mechanics, according to the criteria enumerated by Jones-Smith and Mathur [15].

To obtain the form of the $\mathcal{PT}$-symmetric boundary conditions more explicitly, note that Eq. (8) implies $\xi(0) = \psi^*(L)$ and $\xi(L) = \psi^*(0)$. Also $\xi'(0) = -\psi'^*(L)$ and $\xi'(L) = -\psi'^*(0)$. If we now impose that ψ obeys Eq. (4) we find that ξ automatically follows suit if and only if $\lambda_2 = -\lambda_1^*$. Thus $\mathcal{PT}$-symmetric boundary conditions form the two-parameter family $(\ell_1 + i\ell_2, -\ell_1 + i\ell_2)$ where ℓ_1 and ℓ_2 are real, whereas Hermitian boundary conditions correspond to (λ_1,λ_2) where λ_1 and λ_2 are real. Note that the two families intersect along the lines $\ell_2 = 0$ and $\lambda_1 = -\lambda_2$, respectively. On the other hand, the case that $\ell_1 = 0$ is maximally non-Hermitian [16].

We now briefly consider the $\mathcal{PT}$-symmetric generalization of periodic boundary conditions. We will show that these boundary conditions lead to a model studied many years ago by Nelson and Hatano [6] in connection with the pinning of superconducting vortex lines. To this end we consider a particle on a ring. In canonical quantum mechanics the wave function of the particle must obey periodic boundary conditions, or, for a ring threaded by flux, twisted boundary conditions, given by

$$\psi(\theta + 2\pi) = \lambda\psi(\theta). \tag{9}$$

Here $\lambda = \exp(i\phi)$, where ϕ is the flux threading the ring in units of the Aharonov-Bohm flux quantum and θ is the angular coordinate around the ring. If we relax the condition of Hermiticity it is permissible to consider λ to be an arbitrary complex number, not necessarily of unit modulus. The criterion we now impose is that the boundary condition (9) must be $\mathcal{PT}$ symmetric in the sense that if $\psi(\theta)$ obeys the boundary condition, then so does

$$\xi(\theta) = \mathcal{PT}\psi(\theta) = \psi^*(\theta + \pi). \tag{10}$$

Imposition of this constraint forces the boundary parameter λ to be real. Whereas in the Hermitian case the parameter λ must lie on the unit circle in the complex plane, in the $\mathcal{PT}$-symmetric case it must lie on the real axis. These are precisely the boundary conditions studied by Nelson and Hatano. For a free particle Nelson and Hatano's boundary conditions do not lead to real eigenvalues, except for the Hermitian cases $\lambda = \pm 1$, but if there is a potential well, or a disordered potential, real eigenvalues are obtained for some range of λ, followed by a $\mathcal{PT}$ transition to complex eigenvalues (dubbed a delocalization transition by Nelson and Hatano). It is worth noting that one can further generalize the Nelson and Hatano model to the case that the wave function and its derivative at θ and $\theta + 2\pi$ are related by a 2×2 transfer matrix which may be constrained by either Hermiticity or by $\mathcal{PT}$ symmetry. However, in this paper we will not investigate periodic boundary conditions further. Instead we focus on the complementary problem of a particle in a box with $\mathcal{PT}$-symmetric boundary conditions.

B. Eigenvalues and eigenfunctions

Now let us compute the eigenvalues and eigenfunctions of the particle in a box subject to $\mathcal{PT}$-symmetric boundary conditions (hereafter called the $\mathcal{PT}$-symmetric particle in a box). Since we are now analyzing a non-Hermitian eigenvalue problem there is no guarantee that we will obtain real eigenvalues or that the eigenfunctions we obtain will be complete. Nonetheless we find that under a broad set of circumstances the spectrum of the $\mathcal{PT}$-symmetric particle in a box is entirely real. Furthermore the corresponding eigenfunctions can therefore be chosen to be simultaneous eigenfunctions of the Hamiltonian and $\mathcal{PT}$, a condition called "unbroken $\mathcal{PT}$" in the literature [2]. Unbroken $\mathcal{PT}$ is the second condition a Hamiltonian must fulfill according to the criteria of Ref. [15]. Thus we arrive at the important conclusion that the $\mathcal{PT}$-symmetric particle in a box meets the condition of unbroken $\mathcal{PT}$ for a broad range of circumstances.

We attempt solutions of the form

$$\psi = A\exp(ikx) + B\exp(-ikx), \tag{11}$$

where k may be complex. These solutions are eigenfunctions of the Hamiltonian equation (1) with energy

$$E = \tfrac{1}{2}k^2. \tag{12}$$

Note that the energy is real only if k is real or pure imaginary.

Imposing $\mathcal{PT}$-symmetric boundary conditions leads to the quantization condition

$$\exp(i2kL) = \frac{1 - i2k\ell_1 - k^2(\ell_1^2 + \ell_2^2)}{1 + i2k\ell_1 - k^2(\ell_1^2 + \ell_2^2)} \tag{13}$$

and the amplitude ratio

$$\frac{A}{B} = -\frac{1 - k\ell_2 + ik\ell_1}{1 + k\ell_2 - ik\ell_1}. \tag{14}$$

The quantization condition (13) determines the allowed values of k and hence the energy levels; Eqs. (11) and (14) then determine the corresponding eigenfunctions.

Note that in the Hermitian case $\ell_2 = 0$ the right-hand side of the quantization condition has magnitude unity leading to the expected result that the allowed k values and hence the energy levels are both real. Remarkably for the maximally non-Hermitian case $\ell_1 = 0$, the right-hand side of the quantization condition is exactly unity, once again leading to real k values and energy levels. It is also clear that the only solutions to Eq. (13) lie on the real axis in the complex k plane so long as $\ell_1 > 0$. For $\ell_1 < 0$ it is possible to obtain complex solutions corresponding to broken $\mathcal{PT}$ symmetry.

Here for simplicity let us focus on the maximally non-Hermitian case $\ell_1 = 0$ where it is easy to see that the allowed wave vectors are

$$k_n = \frac{\pi n}{L} \quad \text{with} \quad n = 1,2,3,\ldots \tag{15}$$

with corresponding energy levels

$$E_n = \frac{\pi^2 n^2}{2L^2}. \tag{16}$$

The corresponding eigenfunctions are

$$\psi_n(x) = N_n\left[\sin(k_n x) + ik_n\ell_2\cos(k_n x)\right], \tag{17}$$

where N_n is a normalization factor to be determined. Thus we see that the energy levels of the maximally non-Hermitian box are identical to the energy levels of the textbook particle in a box with hard wall boundary conditions. The eigenfunctions, however, are quite different. The relationship between the maximally non-Hermitian model and the textbook particle in a box is discussed further in the Appendix. It is easy to verify that the eigenfunctions (17) are also eigenfunctions of the symmetry operator $\mathcal{PT}$ with eigenvalue $(-1)^{n+1}$. Thus $\mathcal{PT}$ is unbroken.

We turn now to the normalization of the eigenfunctions (17). Note that eigenfunctions corresponding to distinct eigenvalues are not orthogonal with respect to the canonical inner product (5), reflecting the non-Hermiticity of the problem. Thus we cannot use this inner product for normalization. Although the eigenfunctions of a non-Hermitian operator are not orthogonal, a weaker result called biorthogonality remains applicable [17]. One can show that the eigenvalues of h and its adjoint $h^\dagger$ are complex conjugates of each other. Moreover if ψ is an eigenfunction of h and φ is an eigenfunction of $h^\dagger$ with eigenvalues that are not complex conjugates of each other, then φ and ψ will be orthogonal. Translated to the present context, the adjoint of a particle in a box with boundary conditions $(i\ell_2, i\ell_2)$ is a particle in a box with the adjoint boundary conditions $(-i\ell_2, -i\ell_2)$. The eigenfunctions of the former problem are given by Eq. (17); the eigenfunctions of the latter by

$$\varphi_n(x) = \tilde{N}_n\left[\sin(k_n x) - ik_n\ell_2\cos(k_n x)\right]. \tag{18}$$

These eigenfunctions will respect the biorthonormality

$$(\varphi_n, \psi_m) = \int_0^L dx\, \varphi_n^*(x)\psi_m(x) = \delta_{n,m} \tag{19}$$

if we choose the normalization factors

$$\tilde{N}_n N_n = \frac{2}{L}\frac{1}{1 - k_n^2\ell_2^2}. \tag{20}$$

A symmetric way to partition Eq. (20) is to choose

$$N_n = \sqrt{\frac{2}{L}}\frac{1}{\left|1 - k_n^2\ell_2^2\right|^{1/2}} \tag{21}$$

and $\tilde{N}_n = -\mathrm{sgn}(n)N_n$, where the $\mathrm{sgn}(n)$ is the sign of $k_n^2\ell_2^2 - 1$.

For some non-hermitian operators the eigenfunctions also satisfy a bi-completeness relation which in the present context would state

$$\sum_{n=1}^{\infty}\varphi_n^*(x)\psi_n(x') = \delta(x - x') \tag{22}$$

However, bicompleteness is not guaranteed and must be proved on a case by case basis. We do not at present have a proof that it holds in the case under consideration here.

In summary, in this section we have shown that the $\mathcal{PT}$-symmetric particle in a box has unbroken $\mathcal{PT}$ symmetry for all boundary conditions wherein $\ell_1 > 0$. We have explicitly computed the eigenvalues and eigenfunctions for the maximally non-Hermitian case $\ell_1 = 0$ and found that the eigenvalues are real for all ℓ_2 and that the eigenfunctions of the Hamiltonian may also be chosen to be eigenfunctions of the operator $\mathcal{PT}$. Finally, we have used biorthogonality to normalize the eigenfunctions.

C. Inner products

In this section we introduce the $\mathcal{PT}$-symmetric inner product and demonstrate that the Hamiltonian equation (1) subject to $\mathcal{PT}$-symmetric boundary conditions is self-adjoint with respect to the $\mathcal{PT}$ inner product. Self-adjointness under the $\mathcal{PT}$ inner product is the third key condition that a $\mathcal{PT}$

quantum Hamiltonian must meet according to Ref. [15]. It follows from $\mathcal{PT}$ self-adjointness that the eigenfunctions of the $\mathcal{PT}$-symmetric particle in a box are orthogonal under the $\mathcal{PT}$ inner product. At least conceptually, this eigenfunction orthogonality is different from the biorthogonality discussed above and it provides another way to normalize the eigenfunctions. These results then allow us to define the $\mathcal{C}$ operator and the associated $\mathcal{CPT}$ inner product and thereby complete the formulation of the particle in a box in $\mathcal{PT}$ quantum mechanics.

For a finite-dimensional system the wave function may be represented as a column of complex numbers denoted ψ and the canonical inner product (5) of two states ψ and ϕ may be written as $(\phi,\psi) = \phi^\dagger\psi$. On the other hand, the $\mathcal{PT}$ inner product is given by $(\phi,\psi)_{\mathcal{PT}} = (\mathcal{PT}\phi)^T\psi$ [2,15]. Generalizing to a particle in a box we may write the $\mathcal{PT}$ inner product as

$$(\phi,\psi)_{\mathcal{PT}} = \int_0^L dx\, \phi^*(L-x)\psi(x). \tag{23}$$

Equation (23) should be contrasted with the standard inner product (5). The $\mathcal{PT}$ inner product suffers from the defect that it is not positive definite; nonetheless, it plays an important role in the formulation of $\mathcal{PT}$ quantum mechanics.

Having defined the $\mathcal{PT}$ inner product let us now show that the Hamiltonian equation (1) is self-adjoint under this inner product. To this end we equate $(\phi,h\psi)_{\mathcal{PT}} = (h\phi,\psi)_{\mathcal{PT}}$. Simple integration by parts then reveals this equality will hold provided the surface term

$$[\phi^*(L-x)\psi'(x) + \phi'^*(L-x)\psi(x)]_0^L \tag{24}$$

vanishes. If we now impose that ψ obeys the $\mathcal{PT}$-symmetric boundary condition $(\ell_1 + i\ell_2, -\ell_1 + i\ell_2)$ we find that in order for the surface term to vanish, ϕ must obey the same boundary condition. Thus we have shown that the Hamiltonian equation (1) subject to $\mathcal{PT}$-symmetric boundary conditions is self-adjoint under the $\mathcal{PT}$ inner product as claimed.

An immediate consequence of $\mathcal{PT}$ self-adjointness is that the eigenfunctions of the $\mathcal{PT}$-symmetric particle in a box with distinct eigenvalues should be orthogonal under the $\mathcal{PT}$ inner product. For the maximally non-Hermitian case $\ell_1 = 0$, a short calculation reveals

$$(\psi_n,\psi_m)_{\mathcal{PT}} = (-1)^{n+1}\frac{L}{2}\left(1 - k_n^2\ell_2^2\right)N_n^2\delta_{n,m}. \tag{25}$$

Here we have made use of Eqs. (17) and (23) but not yet committed ourselves to the choice equation (21) for the normalization factor. Note that there is a sequence of ℓ_2 values $\ell_2 = L/\pi n$, where $n = 1,2,3,\ldots$ for which we obtain an orthogonality catastrophe: The nth eigenfunction is self-orthogonal under the $\mathcal{PT}$ inner product. Except at these isolated points we may adopt the normalization equation (21) in which case the expression for the $\mathcal{PT}$ inner product simplifies to

$$(\psi_n,\psi_m)_{\mathcal{PT}} = (-1)^n \mathrm{sgn}(n)\delta_{n.m}, \tag{26}$$

where $\mathrm{sgn}(n)$ is the sign of $k_n^2\ell_2^2 - 1$.

Armed with these results we may now define the linear $\mathcal{C}$ operator via

$$\mathcal{C}\psi_n = (-1)^n \mathrm{sgn}(n)\psi_n. \tag{27}$$

Equation (27) fixes the action of the operator $\mathcal{C}$ in the Hilbert space of states spanned by the Hamiltonian eigenfunctions ψ_n. We shall call this space the physical space of the $\mathcal{PT}$-symmetric particle in a box. Within this space the $\mathcal{C}$ operator may be written as an integral kernel with the spectral representation

$$\mathcal{C}(x,x') = \sum_{n=1}^{\infty}(-1)^n \mathrm{sgn}(n)\psi_n(x)\varphi_n^*(x') \tag{28}$$

based on the biorthogonality equation (19). Noting that $\varphi_n^*(x')$ and $\psi_n(x')$ differ only by a factor of $-\mathrm{sgn}(n)$ we may simplify the expression for $\mathcal{C}$ to

$$\mathcal{C}(x,x') = \sum_{n=1}^{\infty}(-1)^{n+1}\psi_n(x)\psi_n(x'), \tag{29}$$

where $\psi_n(x)$ is given by Eqs. (17) and (21).

Finally, following [2,15], we define the $\mathcal{CPT}$ inner product of two states as

$$\begin{aligned}(\phi,\psi)_{\mathcal{CPT}} &= \int_0^L dx (\mathcal{CPT}\phi)(x)\psi(x)\\ &= \int_0^L dx \int_0^L dx' \psi(x)\mathcal{C}(x,x')\phi^*(L-x').\end{aligned} \tag{30}$$

Evidently for the eigenstates of h, by construction, $(\psi_n,\psi_m)_{\mathcal{CPT}} = \delta_{n,m}$. Thus the $\mathcal{CPT}$ inner product is positive definite.

In $\mathcal{PT}$ quantum mechanics the $\mathcal{CPT}$ inner product, also known as the dynamically determined inner product, is deemed the physically correct inner product [2,15]. It is positive definite and time evolution is unitary with respect to it. With the construction of the $\mathcal{CPT}$ inner product we have therefore completed our formulation of the $\mathcal{PT}$-symmetric particle in a box.

III. VARIATIONAL PRINCIPLE FOR $\mathcal{PT}$ QUANTUM MECHANICS

The variational principle is a powerful reformulation of Schrödinger's equation. It facilitates the proof of theorems, such as the existence of bound states for arbitrarily weak binding potentials in one and two dimensions, and it is the basis of fruitful approximation schemes, especially in quantum many-body physics. It is therefore worthwhile to ask whether there is a similar variational formulation in $\mathcal{PT}$ quantum mechanics. Remarkably we find that it is possible to reformulate $\mathcal{PT}$ quantum mechanics as a variational principle, but only for Hamiltonians that meet the threefold criteria of $\mathcal{PT}$ symmetry, unbroken $\mathcal{PT}$, and $\mathcal{PT}$ self-adjointness.

For comparative purposes it is useful to briefly recall the variational principle in the Hermitian case. For simplicity, consider a finite-dimensional Hilbert space in which the state ψ can be represented as an N component column vector with components ψ_i. The Hamiltonian is then an $N \times N$

matrix with elements h_{ij}. The Rayleigh functional R is defined as

$$R = \psi^\dagger h\psi. \tag{31}$$

It is easy to verify that R is real for Hermitian h. According to the variational principle the eigenstates of the Hamiltonian are the states that extremize the Rayleigh functional subject to the normalization constraint $\psi^\dagger\psi = 1$. According to the method of Lagrange multipliers we must therefore extremize

$$F = \psi^\dagger h\psi - \lambda(\psi^\dagger\psi - 1). \tag{32}$$

By setting $\partial F/\partial\psi_i^* = 0$ we recover the Schrödinger equation

$$h\psi = \lambda\psi. \tag{33}$$

On the other hand, the condition $\partial F/\partial\psi_i = 0$ implies

$$\psi^\dagger h = \lambda\psi^\dagger \Rightarrow h^\dagger\psi = \lambda^*\psi. \tag{34}$$

Note that for h Hermitian equations (33) and (34) are equivalent since $h^\dagger = h$ and λ is real. But for h non-Hermitian the two equations are not equivalent and indeed, in general, are incompatible. Thus Hermiticity plays an essential role in the variational principle. Minimization of R subject to normalization is equivalent to the Schrödinger eigenvalue problem only for Hermitian h.

We turn now to the $\mathcal{PT}$-symmetric case. Again for simplicity we consider a finite-dimensional Hilbert space. Without loss of generality [15] we may assume that we are in a basis such that $\mathcal{T}\psi = \psi^*$ and $P\psi = S\psi$, where S is a diagonal matrix with all its diagonal entries equal to ± 1. To be definite we assume that our Hilbert space is $2n$ dimensional and

$$S = \begin{pmatrix} \mathcal{I} & 0 \\ 0 & -\mathcal{I} \end{pmatrix}, \tag{35}$$

where $\mathcal{I}$ denotes the $n\times n$ identity matrix and 0 denotes the $n\times n$ matrix with all entries equal to zero. The $\mathcal{PT}$ inner product is then given by

$$(\phi,\psi)_{\mathcal{PT}} = (\mathcal{PT}\phi)^T\psi = \phi^\dagger S\psi. \tag{36}$$

The condition of $\mathcal{PT}$ symmetry, that the Hamiltonian should commute with $\mathcal{PT}$, implies $hS = Sh^*$. This enforces the form

$$h = \begin{pmatrix} a & ib \\ ic & d \end{pmatrix}, \tag{37}$$

where a, b, c, and d are real $n\times n$ matrices. The condition that the Hamiltonian is self-adjoint with respect to the $\mathcal{PT}$ inner product, $(\phi,h\psi)_{\mathcal{PT}} = (h\phi,\psi)_{\mathcal{PT}}$, implies $Sh = h^\dagger S$, or equivalently $c = b^T$ in Eq. (37).

Armed with this notation we now introduce the $\mathcal{PT}$ counterpart of the Rayleigh functional

$$B = (\psi,h\psi)_{\mathcal{PT}} = \psi^\dagger Sh\psi. \tag{38}$$

To show that the functional B is real it is convenient to write

$$\psi = \begin{pmatrix} \xi \\ \eta \end{pmatrix}, \tag{39}$$

where ξ and η are n component columns. Then

$$B = \xi^\dagger a\xi - \eta^\dagger d\eta + i\xi^\dagger b\eta - i\eta^\dagger b^T\xi. \tag{40}$$

The first two terms are evidently real and the last two are the sum of a conjugate pair, revealing that B is indeed real.

According to the variational principle for $\mathcal{PT}$ quantum mechanics we must extremize B subject to each of three constraints: (a) $(\psi,\psi)_{\mathcal{PT}} = 1$, (b) $(\psi,\psi)_{\mathcal{PT}} = 0$, and (c) $(\psi,\psi)_{\mathcal{PT}} = -1$. To show that the variational principle is equivalent to the eigenvalue equation for h let us examine case (a). The other cases can be handled similarly. By the method of Lagrange multipliers we must look for states ψ that extremize

$$F_B = \psi^\dagger Sh\psi - \lambda(\psi^\dagger S\psi - 1). \tag{41}$$

Imposing $\partial F_B/\partial\psi_i^* = 0$ yields the eigenvalue problem

$$Sh\psi = \lambda S\psi \Rightarrow h\psi = \lambda\psi, \tag{42}$$

the desired result, but imposing $\partial F_B/\partial\psi_i = 0$ leads to

$$\psi^\dagger Sh = \lambda\psi^\dagger S \Rightarrow h^\dagger S\psi = \lambda^* S\psi. \tag{43}$$

To show that Eq. (43) is equivalent to Eq. (42), we use $h^\dagger S = Sh$ ($\mathcal{PT}$ self-adjointness) and the reality of the eigenvalues $\lambda = \lambda^*$ (unbroken $\mathcal{PT}$). Thus we see that the three fundamental conditions of $\mathcal{PT}$ quantum mechanics play an essential role in the formulation of the variational principle just as Hermiticity does in the Hermitian case.

We conclude with a brief consideration of the variational principle for the particle in a box. Here we must extremize

$$B = -\frac{1}{2}\int_0^L dx\, \psi^*(L-x)\frac{\partial^2}{\partial x^2}\psi(x) \tag{44}$$

subject to the constraints $\int_0^L dx\, \psi^*(L-x)\psi(x) = -1$, 0, or 1. Making variations with respect to ψ^* leads immediately to the Schrödinger equation

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi = \lambda\psi. \tag{45}$$

Making variations with respect to ψ leads to the equation

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi^* = \lambda\psi^* \tag{46}$$

provided the surface term

$$[\psi^*(L-x)\delta\psi'(x) + \psi'^*(L-x)\delta\psi(x)]_0^L \tag{47}$$

vanishes. The vanishing of the surface term is ensured by requiring the variation $\delta\psi$ to obey the same $\mathcal{PT}$-symmetric boundary conditions as ψ. Thus we see the essential role for the variational principle of $\mathcal{PT}$-symmetric boundary conditions (which ensure both $\mathcal{PT}$ symmetry and $\mathcal{PT}$ self-adjointness). Finally we must invoke unbroken $\mathcal{PT}$ since Eqs. (45) and (46) are equivalent only if the eigenvalues λ are real.

IV. ELECTROMAGNETIC ANALOG

A. Isolated cavity

In order to construct the electromagnetic analog of the $\mathcal{PT}$-symmetric particle in a box let us examine more closely what happens at the boundary points. Close to the left boundary the wave function is

$$\psi = A_1\exp(ikx) + A_2\exp(-ikx). \tag{48}$$

By imposing $\psi(0) = (\ell_1 + i\ell_2)\psi'(0)$ we conclude that the reflection coefficient

$$r_L = \frac{A_1}{A_2} = -\frac{1 + k\ell_2 + ik\ell_1}{1 - k\ell_2 - ik\ell_1}. \tag{49}$$

On the other hand, if we write Eq. (48) as

$$\psi = A_1 \exp(ikL)e^{ik(x-L)} + A_2 \exp(-ikL)e^{-ik(x-L)} \tag{50}$$

and impose the boundary condition $\psi(L) = (-\ell_1 + i\ell_2)\psi'(L)$ we find that the right reflection coefficient is

$$r_R = \frac{A_2 \exp(-ikL)}{A_1 \exp(ikL)} = -\frac{1 - k\ell_2 + ik\ell_1}{1 + k\ell_2 - ik\ell_1}. \tag{51}$$

Thus we conclude

$$r_R = \frac{1}{r_L^*}. \tag{52}$$

The reflection coefficients have the same phase but reciprocal magnitudes. The quantized energy levels of the box may be determined by solving

$$r_L r_R \exp(i2kL) = 1. \tag{53}$$

This is identical to the quantization condition deduced earlier, Eq. (13). Equation (52) is the key feature of the $\mathcal{PT}$-symmetric particle in a box that we will seek to emulate in the electromagnetic analog.

To construct the electromagnetic analog first imagine that the half space $x < 0$ is occupied by an absorbing medium, while $x > 0$ is void. The electromagnetic field to the right of the interface may be written as a sum of an incident and reflected wave as

$$E_y = \mathcal{E}_1 e^{ikx} + \mathcal{E}_2 e^{-ikx}, \quad H_z = \frac{\mathcal{E}_1}{c\mu_0} e^{ikx} - \frac{\mathcal{E}_2}{c\mu_0} e^{-ikx}. \tag{54}$$

We consider only the case of normal incidence and linear polarization here. The field to the left of the interface may be written as

$$E_y = \beta \exp^{-inkx}, \quad H_z = -\frac{\beta n}{c} \frac{1}{\mu_0 \mu_r} e^{-iknx}. \tag{55}$$

Here $n = n' + in'' = \sqrt{\epsilon_r \mu_r}$ is the reflective index of the medium. We assume $n'' > 0$ corresponding to an absorbing medium. Note that the wave equation (55) is evanescent and decays inside the absorbing medium. The amplitude of the wave β is determined by the continuity of E_x and H_y across the interface [18]. Performing the match we find that the reflection coefficient is

$$r_{L\ \mathrm{em}} = \frac{\mathcal{E}_1}{\mathcal{E}_2} = \frac{1 - n/\mu_r}{1 + n/\mu_r}. \tag{56}$$

Next imagine that the half space $x > 0$ is occupied by an active medium, while $x < 0$ is empty. The active medium is assumed to have refractive index n^* and permeability μ_r^* conjugate to the absorbing medium considered in the preceding paragraph. Since $n'' < 0$, this medium is active. The electromagnetic field to the left of the interface may be written as a sum of an incident and reflected wave exactly as in Eq. (54). The field to the right, inside the medium, is given by

$$E_y = \alpha \exp(-ikn^* x), \quad H_z = -\alpha \frac{n^*}{c} \frac{1}{\mu_0 \mu_r^*} \exp(-ikn^* x). \tag{57}$$

Note that the field in the medium is evanescent and decays away from the interface. By continuity of E_x and H_y across the interface we may calculate the amplitude α and the reflection coefficient

$$r_{R\ \mathrm{em}} = \frac{\mathcal{E}_2}{\mathcal{E}_1} = \frac{1 + n^*/\mu_r^*}{1 - n^*/\mu_r^*}. \tag{58}$$

Note that $r_{L\ \mathrm{em}}$ and $r_{R\ \mathrm{em}}$ have the desired inverse conjugate relationship, Eq. (52).

It follows that if we build a structure wherein the space $x < 0$ is occupied by the absorbing medium, the space $x > L$ is occupied by its conjugate active medium, and the slot $0 < x < L$ is left empty, we will obtain an electromagnetic analog of the $\mathcal{PT}$-symmetric particle in a box. The electromagnetic cavity will support undamped oscillations at wave vectors that meet the quantization condition (53), where the reflection coefficients are given by Eqs. (56) and (58).

B. Scattering analysis

One way to realize a particle in a box in semiconductor physics is to create a double barrier structure, for example, a GaAs/AlGaAs sandwich [19]. In the limit that the barriers are infinitely high a particle localized in between is essentially a particle in a box. For finite barrier height, however, the eigenstates of the particle in a box broaden into long-lived resonances that can be mapped out by measuring the transmission through the double barrier structure as a function of energy. The resonances appear as Lorentzian peaks in the transmission plotted against energy. The natural $\mathcal{PT}$-symmetric analog of the double barrier model is a two-slab structure in which one slab is absorbing, and the other, its active conjugate.

In quantum mechanics scattering is powerfully constrained by current conservation which leads to unitarity for the scattering matrix and pseudounitarity [U(1,1) symmetry] for the transfer matrix. The structure we analyze is instead constrained by $\mathcal{PT}$ symmetry. Moreover, it is built of components that do not individually respect $\mathcal{PT}$ symmetry, though, for simplicity, we assume that they do respect parity. In the remainder of this section we discuss the form of S and T matrices in the absence of current conservation and with reduced symmetry. In the next section these results are used to analyze resonant scattering from the $\mathcal{PT}$-symmetric two-slab structure.

First let us consider a single slab. In general, the slab may be illuminated from both sides. Thus the field far from the slab is given by

$$\begin{aligned} E_y &= Ae^{ikx} + Be^{-ikx} \quad \text{as} \quad x \to -\infty \\ &= Ce^{ikx} + De^{-ikx} \quad \text{as} \quad x \to +\infty. \end{aligned} \tag{59}$$

As before, we consider only normal incidence and linearly polarized waves. By linearity it follows that the field amplitudes to the left of the slab are related to those on the right via the transfer matrix

$$\begin{pmatrix} C \\ D \end{pmatrix} = T \begin{pmatrix} A \\ B \end{pmatrix}. \tag{60}$$

We now make one simplifying assumption, namely, that the slab is parity symmetric. Parity applied to the field of Eq. (59) leads to a field in which the amplitudes to the left and right are exchanged, thus $A \leftrightarrow D$ and $B \leftrightarrow C$. Thus symmetry under parity has the consequence that

$$\sigma_x T \sigma_x = T^{-1}. \tag{61}$$

Equation (61) implies that $\det T = \pm 1$. The case $\det T = -1$ leads inexorably to the unphysical result $T = \pm\sigma_x$. Thus we focus on the physical case $\det T = 1$. Equation (61) then leads to the result

$$T = \begin{pmatrix} a & b \\ -b & d \end{pmatrix}. \tag{62}$$

Here the matrix elements a, b, and d are complex and satisfy $ad + b^2 = 1$. Thus a transfer matrix that is constrained only by parity has four real parameters.

The S matrix relates the outgoing amplitudes (C,B) to the incoming amplitudes (A,D) via

$$\begin{pmatrix} C \\ B \end{pmatrix} = S \begin{pmatrix} A \\ D \end{pmatrix}. \tag{63}$$

We write the elements of the S matrix as

$$S = \begin{pmatrix} t_L & r_R \\ r_L & t_R \end{pmatrix}. \tag{64}$$

t_L and r_L are the transmission and reflection amplitudes when there is an incoming wave from the left ($A = 1$, $D = 0$); t_R and r_R are for the case that the incoming wave is from the right ($A = 0$, $D = 1$). Straightforward algebra reveals that for the parity-symmetric transfer matrix equation (62) the corresponding S matrix is

$$S = \frac{1}{d}\begin{pmatrix} 1 & b \\ b & 1 \end{pmatrix}. \tag{65}$$

It is evident from this form that the eigenvalues of the S matrix are

$$z_1 = \frac{1+b}{d}, \quad z_2 = \frac{1-b}{d}. \tag{66}$$

The associated eigenvectors are, respectively, the symmetric vector $\binom{1}{1}$ and the antisymmetric vector $\binom{1}{-1}$.

Using Eq. (66) it is straightforward to write the elements of T in terms of z_1 and z_2, thus

$$a = \frac{2z_1z_2}{z_1+z_2}, \quad b = \frac{z_1-z_2}{z_1+z_2}, \quad d = \frac{2}{z_1+z_2}. \tag{67}$$

The expression for a results from rearranging the constraint $ad + b^2 = 1$ as $a = (1+b)(1-b)/d = z_1z_2d$. Thus we may treat z_1 and z_2 as two basic complex parameters in terms of which the transfer matrix may be written. The virtue of using z_1 and z_2 as the basic parameters is that they have a transparent physical interpretation. In quantum mechanics the S matrix is unitary and hence its eigenvalues are unimodular. Hence $|z_1| = |z_2| = 1$ corresponds to the unitary case. The case that $|z_1| < 1$ and $|z_2| < 1$ corresponds to a strictly absorbing slab; the case that $|z_1| > 1$ and $|z_2| > 1$ corresponds to a strictly gainful one.

In the following it will sometimes be convenient to decompose z_1 and z_2 into their magnitudes and phases as

$$z_1 = \rho e^{\mu} e^{i\phi_1}, \quad z_2 = \rho e^{-\mu} e^{i\phi_2}. \tag{68}$$

We will refer to ρ as the mean absorbance and to μ as the asymmetry parameter.

In the quantum or unitary case $\rho = 1$ and $\mu = 0$. In that case the expression for the T matrix simplifies to

$$T = \begin{bmatrix} \sec\left(\frac{\phi_1-\phi_2}{2}\right)e^{(1/2)(\phi_1+\phi_2)} & i\,\tan\left(\frac{\phi_1-\phi_2}{2}\right) \\ -i\,\tan\left(\frac{\phi_1-\phi_2}{2}\right) & \sec\left(\frac{\phi_1-\phi_2}{2}\right)e^{-(1/2)(\phi_1+\phi_2)} \end{bmatrix}. \tag{69}$$

We are at liberty to choose the phases ϕ_1 and ϕ_2 so that $-\pi < \phi_1 - \phi_2 \leqslant \pi$. Then it is permissible to write

$$\sec\left(\frac{\phi_1-\phi_2}{2}\right) = \cosh\theta, \quad \tan\left(\frac{\phi_1-\phi_2}{2}\right) = \sinh\theta, \quad e^{i(1/2)(\phi_1+\phi_2)} = e^{i\phi}, \tag{70}$$

and thereby replace the parameters (ϕ_1,ϕ_2) with new parameters (θ,ϕ). In terms of these parameters Eq. (69) becomes

$$T = \begin{pmatrix} \cosh\theta e^{i\phi} & i\sinh\theta \\ -i\sinh\theta & \cosh\theta e^{-i\phi} \end{pmatrix}. \tag{71}$$

The corresponding S matrix is

$$S = \begin{pmatrix} \operatorname{sech}\theta e^{i\phi} & i\tanh\theta e^{i\phi} \\ i\tanh\theta & \operatorname{sech}\theta e^{i\phi} \end{pmatrix}. \tag{72}$$

Comparing to Eq. (64) we see that the corresponding transmission probability is $1/\cosh^2\theta$. Thus θ is a measure of the penetrability of the barrier via quantum tunneling, with large θ corresponding to an impenetrable barrier.

Thus it will prove most transparent to write the parity symmetric transfer matrix equation (61) in terms of the parameters ρ, μ, θ, and ϕ. Making use of Eqs. (67), (68), and (70) we obtain

$$T = \frac{1}{\cosh\mu + i\sinh\mu\sinh\theta}\begin{bmatrix} \rho\cosh\theta e^{i\phi} & \sinh\mu + i\cosh\mu\,\sinh\theta \\ -\sinh\mu - i\cosh\mu\sinh\theta & \frac{1}{\rho}\cosh\theta e^{-i\phi} \end{bmatrix}. \tag{73}$$

Note that Eq. (73) reduces to Eq. (71) in the limit $\rho = 1$ and $\mu = 0$.

Equation (73) parametrizes the transfer matrix of any structure that respects parity. In the Appendix we compare the general expression to the transfer matrix of a simple rectangular slab of refractive index n and permeability μ_r.

Having parametrized the transfer matrix of a single slab we now determine T^R, the transfer matrix of its time reversed counterpart. Time reversing the field configuration equation (59) yields

$$\begin{aligned} E_y &= A^* e^{-ikx} + B^* e^{ikx} \quad \text{as} \quad x \to -\infty \\ &= C^* e^{-ikx} + D^* e^{ikx} \quad \text{as} \quad x \to +\infty. \end{aligned} \tag{74}$$

It follows that

$$\begin{pmatrix} D^* \\ C^* \end{pmatrix} = T^R \begin{pmatrix} B^* \\ A^* \end{pmatrix}, \tag{75}$$

where T^R is the transfer matrix of the time reversed slab. Comparing Eq. (75) to Eq. (60) we conclude that

$$T^R = \sigma_x T^* \sigma_x, \tag{76}$$

the result we sought.

Using Eqs. (62), (67), and (76) it is easy to verify that if T is characterized by the parameters (z_1,z_2), then the parameters of T^R are $(1/z_1^*,1/z_2^*)$. Physically this means that if T is absorbing ($|z_1| < 1$ and $|z_2| < 1$), then T^R has gain ($|z_1| > 1$ and $|z_2| > 1$) and vice versa, as one might expect intuitively. Note furthermore that if we impose time-reversal symmetry, $T = T^R$, we obtain a unitary S matrix since z_1 and z_2 are unimodular.

Explicitly if T is given by Eq. (73), then T^R is given by

$$T^R = \frac{1}{\cosh\mu - i\sinh\mu\,\sinh\theta} \begin{bmatrix} \frac{1}{\rho}\cosh\theta e^{i\phi} & -\sinh\mu + i\cosh\mu\,\sinh\theta \\ \sinh\mu - i\cosh\mu\,\sinh\theta & \rho\cosh\theta e^{-i\phi} \end{bmatrix}. \tag{77}$$

Finally we note that if the slab is shifted to the right by a distance δ, its transfer matrix changes according to

$$T \to U(\delta) T U^\dagger(\delta) \tag{78}$$

where the shift matrix

$$U(\delta) = \begin{pmatrix} e^{-ik\delta} & 0 \\ 0 & e^{ik\delta} \end{pmatrix}. \tag{79}$$

C. Transmission spectroscopy of a $\mathcal{PT}$-symmetric double barrier

We construct a structure with an absorbing slab at $x = -\delta/2$ and its time-reversed counterpart at $x = \delta/2$. The transfer matrix T^D of the composite structure is given by

$$T^D = U(-\delta/2) T U^\dagger(-\delta/2) U(\delta/2) T^R U^\dagger(\delta/2). \tag{80}$$

Here T is the transfer matrix of the absorber if it were located at $x = 0$; T^R, of its time reversed counterpart, at the same location. It is easy to verify that T^D satisfies the condition of $\mathcal{PT}$ symmetry $T^D T^{D*} = 1$ [12,13]. In addition, det $T^D = 1$ since it is a product of matrices with unit determinant. From the transfer matrix T^D we can easily construct the S matrix S^D which is more directly connected to the results of scattering experiments.

It is useful to first consider the unitary case $\rho = 1$, $\mu = 0$. In this case both T and T^R are given by Eq. (71). A short calculation reveals that $t_L = t_R = t$, given by

$$t = \frac{e^{i2\phi}}{\cosh^2\theta + \sinh^2\theta e^{i2k\delta} e^{i2\phi}}. \tag{81}$$

Equation (81) reveals the classic textbook resonance phenomenon. For

$$e^{i2k\delta} e^{i2\phi} = -1 \tag{82}$$

we obtain perfect transmission, $|t|^2 = 1$. To analyze this resonance write $k = k_c + q$, where k_c is the resonant wave vector that meets the condition (82) and q is the detuning. Close to resonance and in the limit of low penetrability (large θ), the expression for t simplifies to yield the classic Lorentzian line shape

$$|t|^2 = \frac{1}{1 + q^2/Q^2}, \tag{83}$$

where $1/Q = 2\delta\sinh^2\theta$. In deriving Eq. (83) we assume that (θ,ϕ) are independent of q, justified *a posteriori* if the resonance is sufficiently narrow [20]. Since $|t|^2 + |r|^2 = 1$, the reflection shows a corresponding feature as well.

Next up in complexity let us suppose the absorbing slab has $\rho < 1$ but the asymmetry $\mu = 0$. Making the same approximation, in this case the formula for the S matrix simplifies to

$$S = \frac{e^{i2\phi}}{1 - iq/Q} \begin{bmatrix} 1 & \pm i(q/Q)(1/\rho) \\ \pm i\rho(q/Q) & 1 \end{bmatrix}, \tag{84}$$

where the $-$ sign applies if the resonant numerator satisfies $\exp(ik_c\delta + i\phi) = +i$ (even resonance), and the $+$ sign if $\exp(ik_c\delta + i\phi) = -i$ (odd resonance). From the S matrix we see that there is again a Lorentzian peak in transmission given by Eq. (83). Furthermore the transmission is the same for incidence from the left or the right; $|t_L|^2 = |t_R|^2 = |t|^2$. The reflection, however, breaks left-right symmetry

$$|r_L|^2 = \rho^2 \frac{q^2}{Q^2 + q^2}, \quad |r_R|^2 = \frac{1}{\rho^2} \frac{q^2}{Q^2 + q^2}. \tag{85}$$

Since $\rho < 1$, the reflection for radiation incident from the right is enhanced relative to incidence from the left. Note that in the former situation the radiation is incident directly on the active slab; in the latter on the absorbing slab first. The absorption may be computed from the conservation law $|t|^2 + |r|^2 + |a|^2 = 1$. Thus we find

$$|a_L|^2 = (1 - \rho^2) \frac{q^2}{Q^2 + q^2}, \quad |a_R|^2 = \left(1 - \frac{1}{\rho^2}\right) \frac{q^2}{Q^2 + q^2}. \tag{86}$$

Note that $|a_R|^2$ is negative, corresponding to a net generation of radiation rather than absorption, in the case of incidence from the right.

It is instructive to calculate the eigenvalues and eigenvectors of the S matrix (84). Focusing on the case of even resonance we find that the eigenvalues of the S matrix are $e^{i2\phi}$ and $e^{i2\phi}e^{i2\xi}$, where $\tan\xi = q/Q$. The corresponding eigenvectors are

$$v_1 = \frac{1}{\sqrt{1+\rho^2}}\begin{pmatrix}1\\ \rho\end{pmatrix}, \quad v_2 = \frac{1}{\sqrt{1+\rho^2}}\begin{pmatrix}1\\ -\rho\end{pmatrix}, \tag{87}$$

respectively. Remarkably, although the S matrix is not unitary, its eigenvalues are unimodular, a circumstance dubbed unbroken $\mathcal{PT}$ by Ref. [13]. Note that the eigenvectors (87) are not orthogonal in the sense $v_1^\dagger v_2 = 0$ as they would be for a unitary S matrix.

Unbroken $\mathcal{PT}$ has the physical interpretation that absorption happens by interference. If the incident radiation is in either eigenmode, Eqs. (87), it will emerge unattenuated from the structure. If, however, the incident radiation is a superposition $\alpha v_1 + \beta v_2$, then the incident power is

$$|\alpha|^2 + |\beta|^2 + \frac{1-\rho^2}{1+\rho^2}(\alpha^*\beta + \beta^*\alpha), \tag{88}$$

while the transmitted power is

$$|\alpha|^2 + |\beta|^2 + \frac{1-\rho^2}{1+\rho^2}(\alpha^*\beta e^{i2\xi} + \beta^*\alpha e^{-i2\xi}). \tag{89}$$

Note that both expressions contain interference terms by virtue of the nonorthogonality of the S-matrix eigenmodes and this interference is modified by passage through the structure.

Finally we turn to the most general case $\rho < 1$ and permit nonzero asymmetry μ. Again we find $t_L = t_R = t$. Right on resonance we find the remarkable effect of superunitary transmission, $|t|^2 \geqslant 1$. More explicitly, we find $|t|^2 = 1/Z^2$, where

$$Z = \frac{1-\sinh^2\mu\,\cosh^2\theta}{1+\sinh^2\mu\,\cosh^2\theta}. \tag{90}$$

Near resonance we find

$$|t|^2 = \frac{1}{Z^2 + q^2/Q^2}, \tag{91}$$

a Lorentzian with reduced oscillator strength. Here Q is defined as

$$Q = \frac{1}{2\delta}\frac{1+\sinh^2\mu\,\cosh^2\theta}{\sinh^2\theta + \sinh^2\mu\,\cosh^2\theta}. \tag{92}$$

Although the transmission resonance remains Lorentzian, the reflection is found to be

$$|r_L|^2 = \rho^2\frac{(\Delta + q/Q_2)^2}{(1+q^2/Q^2)^2}, \quad |r_R|^2 = \frac{1}{\rho^2}\frac{(-\Delta + q/Q_2)^2}{1+q^2/Q^2}. \tag{93}$$

Here

$$Q_2 = \frac{1}{2\delta}\frac{1-\sinh^2\mu\,\cosh^2\theta}{\sinh\theta\,\cosh\theta\,\cosh\mu} \tag{94}$$

and

$$\Delta = \frac{\sinh\mu\,\cosh\theta}{1-\sinh^2\mu\,\cosh^2\theta}. \tag{95}$$

Thus the reflection coefficients have an asymmetric form associated with Fano rather than Lorentzian lines [21]. Note that r_L vanishes at $q = -\Delta Q_2$ and r_R at $q = \Delta Q_2$. Thus the reflection minima are displaced symmetrically away from the $q = 0$ peak in the transmission.

V. CONCLUSION

In this paper we study the role of boundary conditions in $\mathcal{PT}$ quantum mechanics by consideration of a simple example. There is a well developed theoretical understanding of the role of boundary conditions in determining whether an operator is self-adjoint [4,5], but the corresponding problem in $\mathcal{PT}$ quantum mechanics has not previously been investigated to our knowledge. We show that for a Hermitian particle in a box the allowed boundary conditions can be parametrized by the pair (λ_1,λ_2) where λ_1 and λ_2 are real numbers. On the other hand, for a $\mathcal{PT}$-symmetric particle in a box the allowed boundary conditions may be parametrized as $(\ell_1 + i\ell_2, -\ell_1 + i\ell_2)$ where ℓ_1 and ℓ_2 are real. Thus the two sets of boundary conditions overlap for the case that $\lambda_1 = -\lambda_2$ and $\ell_2 = 0$, respectively. This case corresponds to Hamiltonians that are Hermitian and separately respect both $\mathcal{P}$ and $\mathcal{T}$. Here, however, we are interested in Hamiltonians that are not Hermitian but respect the combined symmetry $\mathcal{PT}$. For such Hamiltonians we find that as long as $\ell_1 > 0$, not only does the Hamiltonian commute with $\mathcal{PT}$, one also obtains the stronger result that $\mathcal{PT}$ is unbroken. In other words one can find simultaneous eigenfunctions of the Hamiltonian and $\mathcal{PT}$ and the Hamiltonian eigenvalues are necessarily real. Furthermore we find that the Hamiltonian for a particle in a box with $\mathcal{PT}$-symmetric boundary conditions is self-adjoint under the $\mathcal{PT}$ inner product. Thus the $\mathcal{PT}$-symmetric particle in a box fulfills all three requirements of $\mathcal{PT}$ quantum mechanics of which it constitutes a simple soluble example.

A second development in this paper is the formulation of a variational principle for $\mathcal{PT}$ quantum mechanics that is the analog of the textbook Rayleigh-Ritz principle. The latter principle is the basis for many approximations and insights into quantum mechanics and its generalization to $\mathcal{PT}$ quantum mechanics may therefore prove of similar value.

Finally we study classical electromagnetic analogs of the $\mathcal{PT}$-symmetric particle in a box. We show that the natural photonic analog of the isolated particle in a box is a Fabry-Perot cavity bounded by an absorbing medium and its conjugate gain medium. One way to experimentally realize and probe a particle in a box is to consider a double barrier structure. In the limit of infinite barrier height this system is an ideal particle in a box but for finite height the bound states of the particle in a box are broadened into resonances that can be mapped out by measurements of the transmission, reflection, and absorption through the structure. In textbook quantum mechanics the transmission and reflection resonances have a classic Breit-Wigner shape; there is no absorption. In the $\mathcal{PT}$-symmetric case we find that the transmission has a

Breit-Wigner shape but the reflection and absorption have an asymmetric Fano line shape.

We conclude by identifying some problems that are left open. (a) The potential real x^M tends to the ordinary particle in a box in the limit $M \to \infty$. The authors of Ref. [3] have studied the eigenvalues of the $\mathcal{PT}$-symmetric potential $x^M x^{i\epsilon}$ and have derived asymptotic results in the limit $M \to \infty$ and $\epsilon \to \infty$. It would be desirable to study the relationship between their asymptotic results and the $\mathcal{PT}$-symmetric particle-in-a-box model studied here. (b) We do not at present have a proof of the completeness of the eigenfunctions for the non-Hermitian particle in a box. In the Hermitian case the completeness can be proved by regulation and direct evaluation of the completeness sum, Eq. (22), or by use of the variational principle [17]; it is guaranteed by general theorems moreover [5]. The non-Hermitian case is more subtle. In particular, the variational proof [17] does not generalize because the variational principle for $\mathcal{PT}$ quantum mechanics is based on the $\mathcal{PT}$-symmetric inner product which is indefinite. (c) Spontaneous $\mathcal{PT}$ symmetry breaking is a remarkable feature of $\mathcal{PT}$ quantum mechanics [2]. Our model may provide a simple tractable example of such a transition for $\ell_1 < 0$. (d) In the maximally non-Hermitian case $\ell_1 = 0$ our model has a sequence of critical points at which it has an orthogonality catastrophe. These critical points correspond to the circumstance that a particular eigenstate becomes weightless (zero norm) with respect to the $\mathcal{PT}$ inner product, a phenomenon worthy of further elucidation. (e) In this paper we limited attention to a nonrelativistic spinless particle for which time-reversal symmetry is even in the sense that $\mathcal{T}^2 = 1$. Two natural generalizations are to consider a particle with spin $\frac{1}{2}$ for which time-reversal symmetry is odd $\mathcal{T}^2 = -1$ and a particle that obeys the relativistic Dirac equation. (f) Finally we describe a possible experimental realization of the $\mathcal{PT}$-symmetric particle in a box using the Fe-doped $LiNbO_3$ system studied by Ref. [7]. We envisage forming a waveguide by forming a suitable refractive index profile $n_R(x)$ transverse to the direction of propagation as in Ref. [7]. Asymmetric optical gain can then be provided by two-wave mixing and a suitable amplitude mask that allows the pump beam to illuminate only one side of the waveguide. The temporal dynamics of the $\mathcal{PT}$-symmetric particle in a box can be mapped out by spatial propagation of light down the waveguide, much as the temporal dynamics of a two-level non-Hermitian system was mapped out in Ref. [7]. The experiment we envisage would be particularly well suited to study the $\mathcal{PT}$ phase transition and the orthogonality catastrophes that occur in our system. More detailed consideration of this and other experimental realizations are left for future investigation.

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APPENDIX: MAPPING TO TEXTBOOK PARTICLE IN A BOX

In this Appendix we examine more closely the relationship of the maximally non-Hermitian particle in a box with boundary conditions $(i\ell_2, i\ell_2)$ to the textbook particle in a box with boundary conditions (0,0). Since the two problems are isospectral it is easy to find a similarity transformation between them. Denoting the eigenfunctions of the textbook problem

$$\xi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}, \tag{A1}$$

with $n = 1,2,3,\ldots$, we see that the kernel

$$K(x,x') = \sum_{n=1}^{\infty} \psi_n(x)\xi_n(x') \tag{A2}$$

maps eigenfunctions of the textbook box to the eigenfunctions of the maximally non-Hermitian problem. Here $\psi_n(x)$ is given by Eq. (17). Conversely, the kernel

$$M(x,x') = \sum_{n=1}^{\infty} \xi_n(x)\varphi_n^*(x') \tag{A3}$$

maps eigenfunctions of the non-Hermitian box back to the textbook eigenfunctions by virtue of the biorthogonality equation (19). The kernel M is the inverse of K in the sense that

$$\int dx''\, M(x,x'')K(x'',x') = \delta(x - x') \tag{A4}$$

by virtue of the completeness of the eigenfunctions of the textbook particle in a box. At present we lack a proof that M is also the right inverse of K; that would be tantamount to a proof of bicompleteness.

The existence of a mapping between the two problems raises the question whether they in fact represent the same physics in a different representation. However, it can be shown that the kernels K and M are nonlocal. Thus the perturbation of the ideal box problem that is local in one representation will look nonlocal in the other. Thus the two problems may in fact be considered physically distinct. Note also that the existence of this mapping is a peculiarity of the maximally non-Hermitian box. More general $\mathcal{PT}$-symmetric boundary conditions should not be isospectral with any Hermitian boundary conditions.

To conclude we now prove that the kernel K is nonlocal. If K were local it would have a delta function spike at $x = x'$ and it would vanish for x and x' distinct. Thus our task is to show that $K(x,x') \neq 0$ for at least some distinct x and x'. To this end it is convenient to split the expression for K into a sum of two terms. The first of these terms is

$$K_1 = \frac{2}{\pi \ell_2} \sum_{n=1}^{\infty} \frac{1}{n} \sin \frac{\pi n x}{L} \sin \frac{\pi n x'}{L} + i \frac{2}{L} \sum_{n=1}^{\infty} \sin \frac{\pi n x'}{L} \cos \frac{\pi n x}{L}. \tag{A5}$$

The convergence of these sums is a bit delicate but they may be evaluated analytically with the result

$$K_1 = \frac{i}{L}\cot\frac{\pi(x'-x)}{L} + \frac{i}{L}\cot\frac{\pi(x'+x)}{L} + \frac{1}{\pi\ell_2}\ln\left|\frac{\sin[\pi(x+x')/L]}{\sin[\pi(x-x')/L]}\right|. \tag{A6}$$

Thus K_1 does not vanish for x and x' distinct. Indeed it diverges as $x \to x'$. We will now show that the second term, K_2, remains finite and therefore cannot cancel the divergent term. Hence $K_1 + K_2$ also does not vanish at least for x and x' sufficiently close, showing the K is indeed nonlocal.

The exact expression for the second term is

$$K_2 = \frac{2}{L}\sum_{n=1}^{\infty}\left[\left|\left(\frac{\pi\ell_2 n}{L}\right)^2 - 1\right|^{-1/2} - \left(\frac{\pi\ell_2 n}{L}\right)^{-1}\right] \times \sin\frac{\pi n x}{L}\sin\frac{\pi n x'}{L}$$

$$+ i\frac{2}{L}\sum_{n=1}^{\infty}\left[\frac{\pi\ell_2 n}{L}\left|\left(\frac{\pi\ell_2 n}{L}\right)^2 - 1\right|^{-1/2} - 1\right] \times \sin\frac{\pi n x'}{L}\cos\frac{\pi n x}{L}. \tag{A7}$$

Neither sum depends on the oscillatory terms for its convergence in contrast to the situation for K_1. It follows

$$|K_2| \leqslant \frac{2}{L}\sum_{n=1}^{\infty}\left|\left|\left(\frac{\pi\ell_2 n}{L}\right)^2 - 1\right|^{-1/2} - \left(\frac{\pi\ell_2 n}{L}\right)^{-1}\right| + \frac{2}{L}\sum_{n=1}^{\infty}\left|\frac{\pi\ell_2 n}{L}\left|\left(\frac{\pi\ell_2 n}{L}\right)^2 - 1\right|^{-1/2} - 1\right|. \tag{A8}$$

The right-hand side of Eq. (A8) is finite since the sum is highly convergent. It therefore provides a bound on K_2 that is constant (independent of x and x'). This completes the demonstration that K is nonlocal.

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