$\mathcal{PT}$-symmetric Hamiltonians and their application in quantum information

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We discuss the prospect of $\mathcal{PT}$-symmetric Hamiltonians finding applications in quantum information science, and conclude that such evolution is unlikely to provide any benefit over existing techniques. Although it has been known for some time that $\mathcal{PT}$-symmetric quantum theory, when viewed as a unitary theory, is exactly equivalent to standard quantum mechanics, proposals continue to be put forward for schemes in which $\mathcal{PT}$-symmetric quantum theory can outperform standard quantum theory. The most recent of these is the suggestion to use $\mathcal{PT}$-symmetric Hamiltonians to perform an exponentially fast database search, a task known to be impossible with a quantum computer. Further, such a scheme has been shown to apparently produce effects in conflict with fundamental information-theoretic principles, such as the impossibility of superluminal information transfer, and the invariance of entanglement under local operations. In this paper we propose three inequivalent experimental implementations of $\mathcal{PT}$-symmetric Hamiltonians, with careful attention to the resources required to realize each such evolution. Such an operational approach allows us to resolve these apparent conflicts, and evaluate fully schemes proposed in the literature for faster time evolution and state discrimination.

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I. INTRODUCTION

In standard quantum theory, observables are associated with Hermitian operators, and time evolution is generated by a Hermitian Hamiltonian. The Hermiticity (or more precisely self-adjointness [1–4]) of the Hamiltonian ensures both the reality of the spectrum of allowed energy eigenvalues, and arguably more importantly, that the resulting time evolution is unitary. Non-Hermitian Hamiltonians are nevertheless ubiquitous in quantum physics as *effective* Hamiltonians, describing the effective dynamics on a restricted subspace of a quantum system, or the coherent part of the evolution in Markovian master equations in the study of open quantum systems (see, e.g., [5–8]).

Surprisingly, some non-Hermitian Hamiltonians can also describe unitary evolution, if we are prepared to redefine the inner product on the linear space of quantum states [9–16]. Such unitary theories are possible for so-called quasi-Hermitian Hamiltonians[1]—those with an entirely real spectrum and a complete set of linearly independent eigenvectors. Further, these turn out to be equivalent to standard, Hermitian quantum theory, in that there exists a one-to-one unitary mapping from states and observables in a unitary quasi-Hermitian theory to states and observables in a regular, Hermitian quantum theory [15].

Of these quasi-Hermitian theories, those which are also $\mathcal{PT}$ symmetric in particular have received a lot of attention (see, e.g., [17] for a review). $\mathcal{PT}$-symmetric Hamiltonians are those which are invariant under the combined symmetry operations of parity $\mathcal{P}$ (spatial reflection) and time reversal $\mathcal{T}$. Bender and Boettcher studied such a Hamiltonian in 1998 [18], showing through numerical and asymptotic studies that the non-Hermitian but $\mathcal{PT}$-symmetric Hamiltonian

$$H = p^2 + m^2x^2 - (ix)^N \tag{1}$$

has a real, positive spectrum for $N \geqslant 2$. It was later shown that so-called unbroken $\mathcal{PT}$ symmetry, when the eigenstates of a $\mathcal{PT}$-symmetric Hamiltonian are also eigenstates of $\mathcal{PT}$,[2] guarantees the reality of the spectrum [19]. In the region of unbroken symmetry therefore a $\mathcal{PT}$-symmetric Hamiltonian is also quasi-Hermitian, and can be considered to generate unitary evolutions in an appropriately defined Hilbert space. In the early years of $\mathcal{PT}$ symmetry it was further suggested that the physically motivated symmetry requirement of invariance under $\mathcal{PT}$ is perhaps more appealing than the seemingly purely mathematical condition of Hermiticity [17].

The study of $\mathcal{PT}$-symmetric quantum mechanics has since flourished into a thriving field of research. Nonetheless, although there are sometimes advantages in performing calculations in one theory over the other [20], $\mathcal{PT}$-symmetric quantum theory, when considered as a unitary theory, and when defined in a dynamically consistent way [16,21–23], is a special case of a quasi-Hermitian theory, and is known to be exactly equivalent to standard quantum theory [15].

In light of this equivalence, two proposed applications of $\mathcal{PT}$-symmetric quantum mechanics in quantum information theory seem somewhat surprising; namely faster time evolution in the so-called quantum brachistochrone [24], and single-shot discrimination of nonorthogonal states [25]. On

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[1]For a yet more general class of Hamiltonians - pseudo-Hermitian [10] - an inner product can also be defined which is invariant under the evolution generated by H. The inner product so defined however is indefinite - that is, assigns negative norm to some states. For the purposes of the present work we restrict attention to quasi-Hermitian Hamiltonians, for which the re-defined inner product retains a clear physical interpretation.

[2]Note that although H commutes with $\mathcal{PT}$ this is not automatically the case since $\mathcal{PT}$ is antilinear.

first sight, each of these seems to conflict with fundamental physical principles: the known bound on the speed of evolution between some specified initial and final states under an energy constraint is closely related to the energy-time uncertainty principle [26,27], while the ability to distinguish nonorthogonal states better than the known quantum bound leads to a violation of the no-signaling principle [28]. Although in [25] the authors state that each of the brachistochrone and state discrimination schemes can only be successful with some probability less than 1, an analysis of the expected performance (i.e., probability of success) of either scheme is lacking. Further, the authors go on to suggest considerable benefits of the state discrimination scheme in quantum information theory, including searching a database exponentially fast. As it is well known that Grover's quantum search algorithm [29], which gives a square-root speedup over the classical case—searching a database of size 2^n in time $O(2^{n/2})$—is optimal on a quantum computer [30–32], such a suggestion indicates that the schemes may be expected to be able to perform better than is allowed by standard quantum theory. It is this claim that we seek to refute in this paper.

The quantum brachistochrone sparked a lively debate in the literature [33–44], in which it was shown that non-Hermitian Hamiltonians obey the same bounds as Hermitian ones as long as in each case the respective theory is globally valid. In the gedanken experiment of [24], however, a quantum system passes from a region governed by a Hermitian Hamiltonian to one governed by a non-Hermitian Hamiltonian, and it is at the boundary between these regions that the apparent speedup happens. More recently it has been pointed out that failing to take proper care at this boundary leads to a violation of the no-signaling principle [45], at the heart of the "peaceful coexistence" of quantum mechanics and special relativity [46].

Despite this already quite extensive discussion, it seems that there is still some confusion in the literature surrounding how to treat the boundary between regions of space in which evolution is governed by a Hermitian Hamiltonian, and those in which it is governed by a non-Hermitian Hamiltonian. This confusion appears to stem from the fact that it is not known how to simulate $\mathcal{PT}$-symmetric Hamiltonians in quantum systems, even as effective Hamiltonians. Although there are various experimental implementations of $\mathcal{PT}$-symmetry in the literature [47–51], with the noteable exception of [52], these all use classical systems governed by an effective $\mathcal{PT}$-symmetric Hamiltonian. Without an understanding of how to physically implement a $\mathcal{PT}$-symmetric Hamiltonian in a quantum system, it has not been possible to evaluate the efficacy of schemes involving such evolutions. Thus, even several years after the quantum brachistochrone debate was settled, similar arguments led to the erroneous suggestion discussed above, that $\mathcal{PT}$-symmetric Hamiltonians could be used to search a database exponentially fast. The purpose of this paper therefore is to fill this gap in the literature. We propose three inequivalent implementations in a two-level system, each corresponding to a different physical situation. We also discuss the physics at the boundary in each case, and the relationship between nonunitarity at the boundary and no-signaling.

In Sec. II we provide a self-contained review of $\mathcal{PT}$ symmetry and the relationship of $\mathcal{PT}$-symmetric quantum theory (and more generally quasi-Hermiticity) to standard quantum theory accessible to quantum information theorists. Although such material is available in the reviews [16,24], it will not be familiar to quantum information theorists, who may be wondering if there is anything to the suggestions made of the potential benefits of $\mathcal{PT}$-symmetric Hamiltonians in quantum information. Readers already familiar with the field of $\mathcal{PT}$ symmetry may wish to skip this section. The new material appears in Sec. III, in which we provide a comprehensive discussion of the prospects for experimental implementation of $\mathcal{PT}$-symmetric Hamiltonians in two-level systems. Although for simplicity we discuss two-level systems, the arguments presented apply equally to higher-dimensional systems, and in the limiting case to continuous variable systems. A full discussion of infinite-dimensional systems however is beyond the scope of this work. Finally we conclude in Sec. IV.

II. REVIEW OF $\mathcal{PT}$-SYMMETRY AND QUASI-HERMITICITY

A. $\mathcal{PT}$ symmetry

A $\mathcal{PT}$-symmetric Hamiltonian is one which is invariant under the combined symmetry operations of parity ($\mathcal{P}$), and time reversal ($\mathcal{T}$). Due to the presence of the antilinear $\mathcal{PT}$ symmetry [12], such Hamiltonians have a spectrum which is either entirely real, or is composed of real eigenvalues and complex conjugate pairs. The condition that the eigenvectors of H are also eigenvectors of $\mathcal{PT}$ is sufficient to ensure the reality of the spectrum—if this condition is satisfied the Hamiltonian is said to have *unbroken* $\mathcal{PT}$ symmetry. Typically, $\mathcal{PT}$-symmetric Hamiltonians encountered in the literature are characterized by a set of parameters, and the $\mathcal{PT}$ symmetry may be broken for some regions of parameter space and unbroken in others. For example, the Hamiltonian in Eq. (1) has unbroken symmetry for $N \geqslant 2$, but the symmetry is broken for $N < 2$. A $\mathcal{PT}$ phase transition occurs at symmetry-breaking points—parameter values at which the symmetry changes from unbroken to broken. Such phase transitions have been demonstrated experimentally in a variety of physical systems [47–51], in which classical systems evolve under a $\mathcal{PT}$-symmetric effective Hamiltonian.

Evolution under a $\mathcal{PT}$-symmetric *effective* Hamiltonian is nonunitary evolution, involving a balance of loss and gain. When the symmetry is unbroken, and the spectrum entirely real, the resulting evolution has stable states, despite the non-Hermiticity of H (the eigenstates however are nonorthogonal with regard to the standard Hilbert space inner product). This case has been described as intermediate between open and closed quantum system evolution [53]. In the region of broken symmetry, the spectrum contains complex-conjugate pairs, resulting in exponential growth and exponential decay—the exponentially growing eigenstates then dominate.

Alternatively, in the region of unbroken $\mathcal{PT}$ symmetry, H is quasi-Hermitian, and can be considered to define unitary evolution in an appropriately defined Hilbert space. Since a full discussion of implementation of $\mathcal{PT}$-symmetric Hamiltonians must consider unitary and nonunitary theories, we review quasi-Hermiticity in the rest of this section.

B. Preliminaries: Self-adjointness as a physically motivated requirement

We begin with some preliminaries regarding the mapping of the physical system to mathematical theory, which although likely to be familiar to many readers are necessary for clarity of language in what follows. We also defend the requirement that Hamiltonians should be represented by Hermitian operators.

The mathematical description of physical systems in quantum theory is through the introduction of a Hilbert space—essentially a linear vector space endowed with an inner product (together with the mathematical requirement of completeness). Allowed states of the physical system are mapped one-to-one to rays in the Hilbert space, while observables are mapped to operators. Note that neither "an observable" nor "a physical state" correspond to *directly* measurable quantities, at least not independently of one another. An observable can only be measured on a physical system prepared in some physical state, and measurable quantities are then the frequencies of occurrence of different possible results in such an experiment. To calculate the expectation value of an observable $\mathcal{O}_A$ in a physical state λ_ψ, the corresponding mathematical objects A, ψ are combined in the familiar way,

$$\langle A\rangle = (\psi, A\psi),$$

where (,) denotes the inner product. Thus, to state the obvious, not only do we require the mapping from states and observables to vectors and operators, but also the definition of inner product in order to map a physical system to a theory that allows us to make predictions about physically measurable quantities.

To clarify the role of Hermiticity in the theory, note that the designation of an operator as Hermitian or otherwise is, of necessity, relative to an underlying inner product. Indeed, recall the definition of the adjoint of an operator A: it is the operator $A^\dagger$ such that

$$(u, Av) = (A^\dagger u, v)$$

for all v in the domain of A. Although the physics literature often uses the terms "Hermitian" and "self-adjoint" interchangeably, in the mathematical literature, an operator A is *Hermitian*, if

$$(u, Av) = (Au, v)$$

for all u,v in the domain of A. A more restrictive definition, which is however the relevant concept to quantum theory, is that of self-adjointness; an operator A is *self-adjoint* if it is Hermitian and the domain of A is the same as that of $A^\dagger$. Indeed, the theory of self-adjoint operators was essentially invented by von Neumann [1] (see also, e.g., [2–4]) to put the then new quantum theory on a rigorous mathematical footing. The difference is of physical importance, since it is self-adjoint operators which have a spectral theorem [1], and which, via Stone's theorem [54,55], which we discuss next, are the generators of continuous unitary evolution.

Once we have accepted that physical states are represented by vectors in Hilbert space, along with the probabilistic interpretation of the norm of the state, we can ask what sort of evolution is possible for a closed quantum system. Conservation of probability leads to the requirement that evolution during any time interval τ should be described by a unitary operator $U(\tau)$.[3] We further expect that evolution should be continuous, and for a closed conservative system, invariant under time translation. Mathematically, these requirements may be expressed as

$$\lim_{\tau\to 0} U(\tau) = I,$$
$$U(t+\tau) = U(t)U(\tau).$$

That every such evolution is generated by a self-adjoint operator H such that $U(\tau) = e^{-iH\tau}$ is the content of Stone's theorem [54,55]. Physically, this self-adjoint operator may be identified with the system Hamiltonian. Far from being a purely mathematical constraint, the requirement that the Hamiltonian operator be self-adjoint follows directly from physical considerations. Although the details and the proof are rather mathematical in nature, the motivations are quite firmly physical.

In the remainder of the paper we do not distinguish between Hermitian and self-adjoint operators, and use the rather looser terminology Hermitian to mean self-adjoint, as is common in the physics literature. For the most part we will be interested in finite-dimensional systems, for which the two definitions coincide.

C. Quasi-Hermiticity: Non-Hermitian Hamiltonians generating unitary evolution

What then is meant by the statement that some non-Hermitian Hamiltonians can describe unitary evolution on a Hilbert space with a suitably modified inner product? As we have discussed, the classification of an operator as non-Hermitian is relative to some assumed inner product. Consider two Hilbert spaces $\mathcal{H}$, $\mathcal{H}'$, which share the same linear space of vectors V, but differ in their inner product. We have thus far avoided using bra-ket notation, which assumes the inner product

$$(\phi, \psi) = \langle\phi|\psi\rangle, \tag{2}$$

where $\langle\phi|$ is the dual vector to $|\phi\rangle$, obtained by Dirac conjugation. The choice of inner product is implicit in the mapping from vector space (kets) to dual space (bras). Recall that the square overlap $|\langle\phi|\psi\rangle|^2$ may be interpreted physically as the probability that state $|\psi\rangle$ can pass as $|\phi\rangle$ in a measurement to verify $|\phi\rangle$.

We now wish to be able to talk about the two different Hilbert spaces $\mathcal{H}$ and $\mathcal{H}'$, representing the same physical system. For clarity we will use the following notation: the state of the physical system is denoted λ_ψ, the vector in $\mathcal{H}$ representing this physical state is denoted $|\psi\rangle$, while that in $\mathcal{H}'$ is denoted $|\psi'\rangle$). $\mathcal{H}$ and $\mathcal{H}'$ share the same linear vector space V, and the inner product on $\mathcal{H}$ is given in the usual way, as in Eq. (2).

By definition, any other inner product on V (and thus that of $\mathcal{H}'$) must be linear in one argument and antilinear in the other, and so may be expressed relative to $\mathcal{H}$ through the introduction

[3] An antiunitary operator would also preserve probabilities, but turns out to be ruled out by the other considerations listed.

of a linear metric operator η,

$$\langle\langle\phi'|\psi'\rangle\rangle = (\phi',\psi')_\eta = \langle\phi'|\eta|\psi'\rangle.$$

We restrict attention to theories with positive-definite norm, in order to retain the probabilistic interpretation of the resulting theory. This requirement thus gives

$$\langle\langle\psi'|\psi'\rangle\rangle = (\psi',\psi')_\eta = \langle\psi'|\eta|\psi'\rangle > 0,$$

for all nonzero vectors ψ'. In other words, the metric operator η should be positive-definite with respect to the usual Dirac inner product on $\mathcal{H}$. Equivalently, the eigenvalues of η are strictly positive, and since η has no zero eigenvalues it is therefore an invertible operator. We also assume, for simplicity, that η is bounded, although we note that unbounded metric operators have been considered in the literature [56].

As the adjoint depends on the definition of inner product, for any operator A on V we define $A^\dagger$, the adjoint in $\mathcal{H}$ and $A^\ddagger$, the adjoint in $\mathcal{H}'$ via

$$\begin{aligned}(u,Av) &= (A^\dagger u,v),\\ (u,Av)_\eta &= (A^\ddagger u,v)_\eta\\ &= (\eta A^\ddagger u,v),\end{aligned}$$

for all v in the domain of A. The two are related since

$$\begin{aligned}(u,Av)_\eta &= (\eta u,Av)\\ &= (A^\dagger \eta u,v),\end{aligned}$$

and thus $A^\dagger = \eta A^\ddagger \eta^{-1}$.

We are now in a position to ask what properties must an operator H have in order to be the generator of unitary evolution on $\mathcal{H}'$. The answer of course [10] is that H must be Hermitian on $\mathcal{H}'$: $H = H^\ddagger$, or equivalently

$$H^\dagger = \eta H \eta^{-1}. \tag{3}$$

For nontrivial η, H is manifestly non-Hermitian on $\mathcal{H}$, $H \neq H^\dagger$, but *is* Hermitian on $\mathcal{H}'$—a space with a suitably modified inner product. It follows from the above discussion that

(i) Every operator H on V which is Hermitian with respect to some inner product $(,)_\eta$ has the form Eq. (3).

(ii) For every operator H of the form Eq. (3), there exists a Hilbert space $\mathcal{H}'$ with an inner product $(,)_\eta$ with respect to which H is Hermitian.

Operators of this form are called quasi-Hermitian, and are the most general type of operators that may be associated physically with Hamiltonians (assuming a Hilbert space with positive-definite norm).

Finally we note that for quasi-Hermitian H satisfying Eq. (3), the combination

$$h = \rho H \rho^{-1}$$

is Hermitian for any invertible ρ satisfying $\rho^\dagger\rho = \eta$ [11]:

$$\begin{aligned}h^\dagger &= (\rho^\dagger)^{-1} H^\dagger \rho^\dagger\\ &= (\rho^\dagger)^{-1}\eta H \eta^{-1}\rho^\dagger\\ &= (\rho^\dagger)^{-1}\eta\rho^{-1} h \rho\eta^{-1}\rho^\dagger\\ &= h.\end{aligned}$$

The time evolution operator e^{-iHt} may similarly be expressed,

$$e^{-iHt} = \rho^{-1} e^{-iht}\rho, \tag{4}$$

as is easily verified by Taylor expansion of each side. Evolution is unitary in $\mathcal{H}'$:

$$\begin{aligned}\langle\langle\phi(t)'|\psi(t)'\rangle\rangle &= \langle\phi(t)'|\eta|\psi(t)'\rangle\\ &= \langle\phi(0)'|(e^{-iHt})^\dagger\eta e^{-iHt}|\psi(0)'\rangle\\ &= \langle\phi(0)'|\rho^\dagger e^{iht}(\rho^{-1})^\dagger\rho^\dagger\rho\rho^{-1}e^{-iht}\rho|\psi(0)'\rangle\\ &= \langle\phi(0)'|\rho^\dagger\rho|\psi(0)'\rangle\\ &= \langle\langle\phi(0)'|\psi(0)'\rangle\rangle.\end{aligned}$$

Each ρ defines a similarity transform mapping Hermitian operators on $\mathcal{H}'$ to Hermitian operators on $\mathcal{H}$. Note that for bounded η the most general ρ satisfying $\rho^\dagger\rho = \eta$ may be written $\rho = U\eta^{1/2}$ for an arbitrary unitary operator U (recall that η is positive definite, and so $\eta^{1/2}$ is well-defined and may be chosen positive definite).

D. Observables in quasi-Hermitian theories

An observable A in the quasi-Hermitian theory may be represented by an operator which is Hermitian with respect to the appropriate inner product, $A = A^\ddagger$. As above, for any invertible ρ satisfying $\rho^\dagger\rho = \eta$, the combination

$$a = \rho A \rho^{-1} \tag{5}$$

is Hermitian with respect to the usual inner product, $a = a^\dagger$ [21]. The expectation value of the observable A, when measured on a system prepared in state $|\psi'\rangle$ is thus given by

$$\begin{aligned}\langle A\rangle = (\psi',A\psi')_\eta &= \langle\psi'|\eta A|\psi'\rangle\\ &= \langle\psi'|\rho^\dagger\rho(\rho^{-1}a\rho)|\psi'\rangle\\ &= \langle\psi'|\rho^\dagger a\rho|\psi'\rangle\\ &= \langle\psi|a|\psi\rangle,\end{aligned} \tag{6}$$

where in the last line we have defined

$$|\psi\rangle = \rho|\psi'\rangle. \tag{7}$$

Note that if $|\psi'\rangle$ is normalized in the quasi-Hermitian theory, $\langle\psi'|\eta|\psi'\rangle = 1$, then $|\psi\rangle$ is normalized according to the standard inner product $\langle\psi|\psi\rangle = 1$. Further, if $|a_i\rangle$ is an eigenket of a with eigenvalue a_i, then $|a_i'\rangle = \rho^{-1}|a_i\rangle$ is an eigenket of A with the same eigenvalue:

$$\begin{aligned}A|a_i'\rangle &= (\rho^{-1}a\rho)|a_i'\rangle\\ &= \rho^{-1}a|a_i\rangle\\ &= a_i\rho^{-1}|a_i\rangle = a_i|a_i'\rangle.\end{aligned}$$

The eigenstates of a Hermitian operator a form a complete orthonormal set. As ρ is invertible, it follows that the eigenstates of A form a complete, linearly independent set.

It also follows from the above that A and a can be considered to describe the same physical observable, and further that the physical state for which measurement of that observable yields value a_i with certainty is associated with $|a_i'\rangle$, $|a_i\rangle$ respectively. For each orthonormal basis $\{|a_i'\rangle\}$ in $\mathcal{H}'$, representing a complete set of physically distinguishable states, there is a corresponding basis $\{|a_i\rangle\}$ in $\mathcal{H}$ representing the same physical set of states. The two bases are related via $|a_i\rangle = \rho|a_i'\rangle$.

Equations (5) and (7) thus provide a one-to-one mapping between states and observables in a quasi-Hermitian theory to those in a standard, Hermitian theory [15]. Since the measurable quantities, Eq. (6), are the same in each case, the two theories are indistinguishable by any physically allowed measurement.

It is worth stressing that the Hermitian and quasi-Hermitian theories describe the *same* physical system with the *same* set of physical observables. There is a one-to-one mapping from physical states of that system to vectors in a linear vector space V in each case, and from physical observables to operators in $\mathcal{H}$ and $\mathcal{H}'$ respectively. The resulting vectors may be related via the (nonunique) invertible mapping Eq. (7), while the operators representing observables are related via the similarity transform Eq. (5). Further, the transformation ρ, when considered as a mapping from $\mathcal{H}'$ to $\mathcal{H}$, is a unitary transformation [15].

In the $\mathcal{PT}$-symmetric literature the inner product is said to be "dynamically determined," that is, the system Hamiltonian determines the inner product [13,14,17,24,25,41]. It is worth stressing, to avoid confusion, that this is purely a mathematical consequence with no physical meaning, and is not related to the physical dynamics of the system as may be construed from the term "dynamically determined." That this must be the case is demonstrated by the fact that the same dynamics may just as well be described in a different Hilbert space, with a different but physically equivalent Hamiltonian. We note further that it is equally valid of course to consider the converse to be true—that it is the inner product which determines those operators which may play the role of Hamiltonian in the theory. The freedom in choosing an inner product has been described as analogous to a gauge freedom [16]—in certain cases the choice of one inner product over another simplifies calculations [20], but there is no physical significance to the choice.

III. EXPERIMENTAL SIMULATIONS OF PT SYMMETRIC SYSTEMS

The equivalence of quasi-Hermitian theories and Hermitian quantum mechanics is thus well understood. More recently attention has turned to the interaction between systems governed by Hermitian and non-Hermitian Hamiltonians, with studies of scattering from $\mathcal{PT}$-symmetric potentials [57,58], coupling between Hermitian and non-Hermitian Hamiltonians [59], and the gedanken experiment of [24,25], which is the focus of this paper, in which a Hermitian quantum system is subjected to a $\mathcal{PT}$-symmetric (non-Hermitian) Hamiltonian for a period of time.

Our aim in this section is to give a comprehensive treatment of the prospects for physical implementation of this gedanken experiment, providing three physically inequivalent implementations. We begin by briefly reviewing the proposed applications to the quantum brachistochrone [24,41] and to quantum state discrimination [25].

In the quantum brachistochrone, the problem is to find the shortest time for evolution from some specified initial state $|\psi_I\rangle$ to some specified final state $|\psi_F\rangle$. For a two-level system with time-independent Hamiltonian the time for unitary evolution from $|\psi_I\rangle$ to $|\psi_F\rangle$ is lower bounded by

$$\Delta t \geqslant \frac{2\hbar}{\Delta E} \arccos |\langle\psi_F|\psi_I\rangle|, \tag{8}$$

where $\Delta E = E_2 - E_1$ is the difference in energies between the two eigenstates of the Hamiltonian. This bound is a special case of the so-called Anandan-Aharonov bound [26]. As well as being of theoretical interest, the speed of unitary evolution between states is relevant in quantum computation, as it determines the time needed for elementary gate operations.

In [24] the authors considered evolution between orthogonal states $|0\rangle$ and $|1\rangle$, and showed that apparently faster evolution can be achieved given the ability to apply a $\mathcal{PT}$-symmetric Hamiltonian. The gedanken experiment presented therein is as follows: a Stern-Gerlach device is used to prepare a beam of spin-1/2 particles in a spin-up state, along some axis z. The beam then passes through a black box in which the evolution of the spin state is governed by a $\mathcal{PT}$-symmetric Hamiltonian. Finally the outgoing beam enters a second Stern-Gerlach device which performs a σ_z measurement on the spin state. The second Stern-Gerlach device acts as a verifier that the desired evolution from spin-up to spin-down has been achieved. The authors showed that the time needed in the black box could be chosen to be arbitrarily small for fixed ΔE (now the energy gap for the non-Hermitian Hamiltonian H). Note that in the limit of vanishingly small passage times however, the matrix elements of the non-Hermitian Hamiltonian become arbitrarily large (see, e.g., [44,60]).

Nevertheless, the Anandan-Aharanov bound turns out to hold also for $\mathcal{PT}$-symmetric (and more general quasi-Hermitian) theories, as long as the appropriate inner product is used in the evaluation of the overlap between initial and final states [33,34,37,38]. The apparent speedup happens entirely at the boundary between Hermitian and non-Hermitian regions—by simply choosing a non-Hermitian Hamiltonian whose inner product interprets the initial and final states to be closer than in the Hermitian region, we can achieve faster time evolution while still respecting the Anandan-Aharanov bound. Note that this proposal explicitly assumes nonunitary evolution, since the inner product changes at the boundary. (This nonunitarity at the boundary seems to have been recognized already in [24], and is stated explicitly in [41,61].) Inspired by the quantum brachistochrone, nonunitary evolution is used to speed up energy transfer between two coupled *classical* oscillators in [62].

A similar effect is used in the more recently proposed application of $\mathcal{PT}$-symmetric Hamiltonians to state discrimination [25]. The problem discussed therein is the following: given a system prepared in one of two possible nonorthogonal states $|\psi_1\rangle$, $|\psi_2\rangle$, make a measurement to determine which one was actually prepared. Perfect discrimination is possible only for orthogonal states. Surprisingly however, for two nonorthogonal states *error-free* discrimination is possible, but only at the cost of allowing for an inconclusive result (see, e.g., the reviews [63–65]). When this result occurs we learn nothing about the identity of the state, and tight bounds are known on the probability of occurrence of this inconclusive result [66–69]. In particular it can be shown that error-free discrimination with a higher probability of success than the known bounds leads to the possibility of using quantum correlations to instantaneously send information, a violation of the no-signaling principle [28]. The central idea in [25] is to choose a non-Hermitian Hamiltonian with an associated inner product under which the states $|\psi_1\rangle$, $|\psi_2\rangle$ are orthogonal, and simply measure in the region governed by this Hamiltonian. Alternatively, let the system evolve under a non-Hermitian Hamiltonian for a time such that on re-entering the Hermitian region, they are orthogonal under the standard inner product. We note again that in either case, the proposal explicitly involves nonunitary evolution (nonorthogonal states evolve to orthogonal ones).

In a recent paper Lee *et al.* showed [45] that the nonunitary evolution necessary for either of the above schemes, if assumed to occur with probability 1, can allow two spacelike separated parties to communicate faster than light through local measurements on preshared entangled states. In related work Pati [70] also showed that this evolution leads to a violation of invariance of measures of entanglement under local unitaries (see also the earlier work [71] on the apparent dependence of the entanglement entropy on the choice of metric). In the $\mathcal{PT}$-symmetric literature, it is however accepted that the change in Hilbert space necessary at the boundary can only happen with some probability less than 1 [25]. Thus an open question remains of how to properly treat the boundary between Hermitian and non-Hermitian regions, and with what probability of success such an evolution can be achieved.

To move from a region in space in which the system is described in the standard way to one in which the evolution is governed by a non-Hermitian Hamiltonian H there are only four options:

1. The Hilbert space in the two regions is the same. There is no change in the inner product. H is a non-Hermitian effective Hamiltonian, and evolution under H is nonunitary.

2. There is a change of the inner product at the boundary, and the system is described by two different Hilbert spaces, $\mathcal{H}$ in the Hermitian region and $\mathcal{H}'$ in the non-Hermitian region. The two Hilbert spaces describe the same physical system, with the same physical observables. The transformation is passive.

3. There is a change in Hilbert space at the boundary, and the two Hilbert spaces describe the same physical system, with the same physical observables. The transformation is active.

4. There is a change in Hilbert space at the boundary, and the two Hilbert spaces describe the same physical system, but with a *different* set of physical observables.

We may immediately discount the last option, since as we have shown above, there is always a one-to-one mapping from observables in the non-Hermitian theory to observables in a physically equivalent Hermitian theory. We note that each of the other options correspond to distinct physical situations, and discuss each of these in turn. Moreover, we claim that these four possibilities are exhaustive: either there is no change in Hilbert space at the boundary, or there is a change in Hilbert space. If there is a change in Hilbert space either the two Hilbert spaces describe the same physical system, or they describe different ones. Finally, if the two spaces describe the same physical system we must transform between the Hilbert space descriptions—this transformation can either be passive or active. These are *only* options that do not introduce new physics.[4]

Evolution under H is thus either nonunitary, in which case there is no troublesome change in Hilbert space, or unitary, in which case H describes evolution in a transformed frame. Transformation to this frame can be passive—requiring an update in the mathematical description of the state at the boundary, or active—evolution in a transformed frame is simulated entirely within the original frame through a physical transformation of the system.

The physically distinct scenarios of *nonunitary* evolution under a non-Hermitian $\mathcal{PT}$-symmetric *effective* Hamiltonian and *unitary* evolution under the same Hamiltonian on a Hilbert space with a suitably modified inner product are sometimes conflated in the literature. In [25] the authors refer in the same paragraph to the fact that the time evolution is unitary under an appropriately chosen inner product, and to experimental implementations requiring a delicate balance of loss and gain. A system evolves unitarily if and only if there is no flow of information to the environment [72], and true open system evolution with loss and gain *cannot* simulate unitary evolution.

In each case the physical setup we are considering is the following: we consider a two-level quantum system, and assume that at time $t < 0$ our physical system is described by a state $|\psi\rangle$ in Hilbert space $\mathcal{H}$, endowed with the usual inner product. At time $t = 0$ the system enters a region in which the evolution is governed by a non-Hermitian Hamiltonian H, in which it remains for some finite time, exiting at time $t = t_0$. The system may undergo measurement at some time $t > t_0$, at which point it is again described by a state in $\mathcal{H}$, and probabilities are calculated according to the usual rules of quantum theory. The question then is how to describe the evolution of the state throughout this sequence, in order to predict the statistics of the final measurement. For concreteness we will consider the Hamiltonian H used in [24,25,38,45] (written in $\mathcal{H}$ and in the eigenbasis of the σ_z operator $\{|0\rangle,|1\rangle\}$):

$$H = s\begin{pmatrix} i\sin\alpha & 1 \\ 1 & -i\sin\alpha \end{pmatrix}, \quad s,\alpha \in \mathbb{R}, \tag{9}$$

where s is a scaling constant, and α is a measure of the non-Hermiticity. For $|\alpha| < \frac{\pi}{2}$, H has real eigenvalues $E_\pm = \pm s\cos\alpha$, with corresponding (right) eigenstates

$$|E_+(\alpha)\rangle = \frac{e^{i\alpha/2}}{\sqrt{2\cos\alpha}}\begin{pmatrix} 1 \\ e^{-i\alpha} \end{pmatrix},$$
$$|E_-(\alpha)\rangle = \frac{ie^{-i\alpha/2}}{\sqrt{2\cos\alpha}}\begin{pmatrix} 1 \\ -e^{i\alpha} \end{pmatrix}.$$

These states are nonorthogonal in $\mathcal{H}$, but are orthonormal under a suitably modified inner product, with metric operator given by

$$\eta = \frac{1}{\cos\alpha}\begin{pmatrix} 1 & -i\sin\alpha \\ i\sin\alpha & 1 \end{pmatrix}. \tag{10}$$

For $\alpha = \frac{\pi}{2}$ the states become the same, and the metric becomes singular—this is the so-called $\mathcal{PT}$ symmetry breaking point.

[4]At least the only independent ones—it is always possible to consider combinations of these three extremes.

For $\rho = \eta^{1/2}$, we can calculate the corresponding Hermitian h, which is given by

$$h = \rho H \rho^{-1} = s \cos\alpha \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{11}$$

A. Evolution under a local $\mathcal{PT}$-symmetric *effective* Hamiltonian

In this case the system is described at all times in the same Hilbert space, and nothing special happens at the boundary. The physical state of the system is described as the vector $|\psi\rangle$ in $\mathcal{H}$ at time $t = 0$. H is an effective Hamiltonian. One of the reasons it has not been possible to evaluate the probability of success of the schemes discussed above is because there appear to be as yet no examples in the literature of physical processes under which a quantum system undergoes such effective evolution. Physically, if we consider the action of H on the orthonormal basis $\{|0\rangle, |1\rangle\}$ it is tempting to interpret the diagonal terms as gain or loss respectively to and from states $|0\rangle$, $|1\rangle$, at rate $s \sin\alpha$, while the off-diagonal terms represent coupling between the states. In classical simulations of $\mathcal{PT}$-symmetric evolution, this is precisely the interpretation given, for a variety of physical systems [47–51]. In quantum systems however, such an interpretation is problematic, as gain leads to an increase in the norm of a state, and is unphysical.

Consider the evolution of a normalized state $|\psi\rangle$ in the infinitesimal time interval δt:

$$|\psi\rangle \to (I - i\delta t H)|\psi\rangle.$$

Since the evolution is not unitary, the norm is not preserved, and we obtain

$$\begin{aligned}\langle\psi(\delta t)|\psi(\delta t)\rangle &= \langle\psi|(I + iH^\dagger\delta t)(I - iH\delta t)|\psi\rangle \\ &= 1 + i\delta t\langle\psi|(H^\dagger - H)|\psi\rangle + O(\delta t^2).\end{aligned}$$

The operator $i(H^\dagger - H)$ is a Hermitian operator, with in general both positive and negative eigenvalues. For H given in Eq. (9) we find

$$i(H^\dagger - H) = 2s \begin{pmatrix} \sin\alpha & 0 \\ 0 & -\sin\alpha \end{pmatrix},$$

and there exist states [e.g., $|0\rangle = (1 \;\; 0)^T$] which, to first order in δt, have a norm greater than 1 after evolution. For such states we can no longer retain the probabilistic interpretation of the norm of the state, and the evolution is thus unphysical. Note that a *decrease* in the norm on the other hand is perfectly acceptable and can be interpreted as a process which occurs with some probability less than 1.

Thus H can represent a physically allowed effective Hamiltonian only for initial states which evolve to physically allowed states, with a norm less than 1. We solve this problem by considering instead the Hamiltonian $\widetilde{H}$:

$$\widetilde{H} = H - is\sin\alpha I = s \begin{pmatrix} 0 & 1 \\ 1 & -2i\sin\alpha \end{pmatrix}.$$

The evolution generated by $\widetilde{H}$ does have a clear physical interpretation, as unitary coupling between states $|0\rangle$ and $|1\rangle$, together with loss from state $|1\rangle$. As a result of the loss, the evolution generated by this Hamiltonian is a probabilistic process: after time t there is some state-dependent probability of having lost the system entirely. Physically, quite analogously to classical demonstrations of $\mathcal{PT}$-symmetric Hamiltonians, this could describe a single photon in one of two coupled waveguides, one of which is lossy. With some probability the photon is absorbed in the lossy waveguide, but if it is not absorbed, it undergoes nonunitary (but coherent) evolution generated by $\widetilde{H}$.

As an alternative to a coupled waveguide system, the Hamiltonian $\widetilde{H}$ may be realized in an optical system with polarization encoding. The loss may be achieved using fiber with polarization-dependent loss. Indeed the first demonstration of unambiguous state discrimination used polarization encoding and polarization-dependent lossy fibers [73]. We also require coupling between orthogonal polarizations, to realize the off-diagonal terms in $\widetilde{H}$, which can be achieved using birefringent material. Although it may be possible to manufacture a fiber with both properties, this would require a birefringent material with different optical axes for the real and imaginary parts of the refractive index. An alternative, perhaps, would be to alternate regions of polarization-dependent loss with regions of lossless birefringence.

In a transformed frame, $\widetilde{H}$ can be interpreted as generating evolution under the desired $\mathcal{PT}$-symmetric Hamiltonian H: if state $|\widetilde{\psi}\rangle$ evolves under the Schrödinger equation with Hamiltonian $\widetilde{H}$,

$$i\frac{\partial}{\partial t}|\widetilde{\psi}\rangle = \widetilde{H}|\widetilde{\psi}\rangle,$$

then the transformed state defined via $|\psi\rangle = e^{s(\sin\alpha)t}|\widetilde{\psi}\rangle$ evolves under

$$\begin{aligned}i\frac{\partial}{\partial t}|\psi\rangle &= i(s\sin\alpha)e^{s(\sin\alpha)t}|\widetilde{\psi}\rangle + ie^{s(\sin\alpha)t}\frac{\partial}{\partial t}|\widetilde{\psi}\rangle \\ &= [i(s\sin\alpha)I + \widetilde{H}]|\psi\rangle \\ &= H|\psi\rangle.\end{aligned}$$

Performing calculations in a transformed frame is a common technique in quantum optics and related fields, and usually involves a unitary, time-dependent transformation from the laboratory frame to some rotating frame. This corresponds to a mathematical transformation to an interaction picture intermediately between the Schrödinger and Heisenberg pictures (see, e.g., [74]). Here we have used a nonunitary transformation, corresponding to uniform decay. We do not claim any particular physical significance of this transformation, we simply use it here to give one possible physical situation in which evolution is generated by the $\mathcal{PT}$-symmetric non-Hermitian H. The problematic increase in norm under H for some states is balanced by the exponential decay in transforming back from the transformed frame to the physical frame, so that $e^{-iHt}|\psi\rangle$ has a physical interpretation at all times. Evolution under $\widetilde{H}$ is referred to as passive $\mathcal{PT}$ symmetry in the analogous classical case in the experimental literature [47]. That this is also readily applicable to quantum systems does not appear to have been recognized to date in the literature.

We finally note that, as the entire procedure above is described by standard quantum theory, by definition it does not provide any additional capabilities compared to standard quantum theory, when the fact that the processes are probabilistic is properly taken into account. The probability that a system prepared in some initial state $|\widetilde{\psi}(0)\rangle = |\psi(0)\rangle$ has not been lost at time t is simply given by the norm of the state at time t, $|\langle\widetilde{\psi}(t)|\widetilde{\psi}(t)\rangle|$. Note that in the region of unbroken $\mathcal{PT}$ symmetry, the (nonorthogonal) eigenstates of H are stable under evolution generated by H. However, the transformation to the physical frame means that even for eigenstates of H, the probability that the evolution is successful is exponentially small in $(s \sin\alpha)t$. This seems to be unavoidable.

B. Unitary evolution under a local $\mathcal{PT}$-symmetric Hamiltonian

In this case the non-Hermitian Hamiltonian H is considered to generate unitary evolution in the region in which it acts. We thus require a change of inner product at the boundary between Hermitian and non-Hermitian regions. This corresponds to a change in reference frame from one in which states are described by vectors $|\psi\rangle$ normalized according to the standard inner product

$$\langle\psi|\psi\rangle = 1$$

and Hamiltonians by Hermitian operators $H = H^\dagger$ to one in which states are described by vectors $|\psi'\rangle\rangle$ normalized according to a modified inner product

$$\langle\langle\psi'|\psi'\rangle\rangle = \langle\psi'|\eta|\psi'\rangle$$

and Hamiltonians are described by operators satisfying $H = H^\ddagger$. The change from one frame to another can be either passive—we simply relabel the states and operators representing physical quantities, or active—we perform a physical operation from one frame to the other.

1. *Passive transformation*

We begin with the passive case. For concreteness let us introduce an orthonormal basis $\{|a_i\rangle\}$ for $\mathcal{H}$, where by orthonormal basis implicitly we mean that there exists some physical measurement that can perfectly distinguish the states of this basis. The state $|\psi\rangle$ in the Hermitian region may be written in this basis as

$$|\psi\rangle = \sum_i c_i|a_i\rangle \tag{12}$$

for some $c_i \in \mathbb{C}$ satisfying $|c_i|^2 = 1$ and with the interpretation that $|c_i|^2$ is the probability of obtaining result a_i in a measurement in the basis $\{|a_i\rangle\}$. It is tempting to consider the state vector $|\psi\rangle$ to be continuous across the boundary, and thus retain the representation Eq. (12) in the non-Hermitian region. Indeed, this has generally been the approach taken in the literature [24,25,45,70]. In $\mathcal{H}'$ however, the basis $\{|a_i\rangle\}$ is nonorthogonal. Thus although the components c_i in this basis are continuous across the boundary with this choice, the physical interpretation of these has been lost. There is no measurement in $\mathcal{H}'$ which distinguishes perfectly the nonorthogonal basis $\{|a_i\rangle\}$, and thus $|c_i|^2$ can no longer be interpreted as a probability distribution associated with this measurement. Since we are considering here a passive transformation, we instead impose the physically reasonable condition that the *physical* state be continuous across the boundary.

To retain the physical interpretation of the state $|\psi\rangle$, we need to identify the orthogonal basis $\{|a_i'\rangle\rangle\}$ in $\mathcal{H}'$ corresponding to $\{|a_i\rangle\}$ in $\mathcal{H}$. The state $|\psi'\rangle\rangle$ in $\mathcal{H}'$ representing the same physical state λ_ψ may then be written

$$|\psi'\rangle\rangle = \sum_i c_i|a_i'\rangle\rangle,$$

which is normalized in $\mathcal{H}'$ since by assumption $\langle\langle a_i'|\eta|a_j'\rangle\rangle = \langle a_i'|\eta|a_j'\rangle = \delta_{ij}$. Every such basis is related to a basis $\{|a_i\rangle\}$ in $\mathcal{H}$ by an invertible mapping ρ such that $\rho^\dagger\rho = \eta$. Thus, using notation now in $\mathcal{H}$ alone,

$$\begin{aligned}|\psi'\rangle &= \sum_i c_i\rho^{-1}|a_i\rangle\\ &= \rho^{-1}|\psi\rangle.\end{aligned}$$

Note that the form of this transformation follows from assuming only that the physical state is continuous across the boundary. To do otherwise is to introduce new physics at the boundary, which has nothing to do with $\mathcal{PT}$ symmetry, and rather is due to assigning physical meaning to a particular representation of the state.

The transformation at the boundary is passive, as it involves simply a relabelling of the state vector. To now return to the gedanken experiment, we start with an initial state $|\psi\rangle$, relabel the state vector at the boundary, evolve under H, and relabel again at the boundary. The net effect is as follows, where for convenience, we express the state in $\mathcal{H}$ throughout:

$$\begin{aligned}|\psi\rangle &\to |\psi'\rangle = \rho^{-1}|\psi\rangle\\ &\to e^{-iHt}|\psi'\rangle = (\rho^{-1}e^{-iht}\rho)\rho^{-1}|\psi\rangle\\ &\to \rho e^{-iHt}|\psi'\rangle = e^{-iht}|\psi\rangle.\end{aligned}$$

Thus the whole experiment may be simulated by simply evolving under the Hermitian Hamiltonian h. This evolution is clearly unitary, may be entirely described within standard, Hermitian quantum theory, and thus leads neither to applications in quantum information nor to a violation of no signaling.

We note that time-dependent metrics have been considered in the literature; in particular Gong and Wang [75] present a Schrödinger-like equation for a theory in which the metric is allowed to be time dependent. There seems to be an assumption however that the metric is continuous, and they do not explicitly address the discontinuous case. The discontinuous change in the metric at the boundary *has* been addressed for the quantum brachistochrone; we note that the argument presented here is similar to that of both Mostafazadeh [33] and Martin [34]. Both were subsequently criticized [37,38,59] for assuming that the whole system could be described as $\mathcal{PT}$ symmetric, while the original proposal assumed the co-existence of a Hermitian region and a non-Hermitian, $\mathcal{PT}$-symmetric region. It seems that Refs. [37,38,59] were advocating the co-existence of Hermitian and non-Hermitian evolution in the *same* frame. In the passive transformation, discussed so far, the physical state is continuous across the boundary. The alternative is to keep the *representation* continuous across the boundary but to perform an active transformation to the physical state so that evolution in a transformed frame may be simulated by evolution in the original frame.

2. Active transformation

The alternative to simply relabelling the state is thus to introduce an active transformation at the boundary. As before the system at time $t < 0$ is described by a state $|\psi\rangle$ in $\mathcal{H}$. At $t = 0$ we retain $|\psi\rangle$ as the description of the state in $\mathcal{H}$, but we wish to *simulate* evolution in $\mathcal{H}'$, through operations in $\mathcal{H}$ alone.

For an initial state $|\psi\rangle$, we apply the physical transformation ρ, and then evolve under the Hermitian Hamiltonian h. Note that since the transformation between frames involves a change in inner product, the physical operation ρ when considered as an active transformation is nonunitary, and in general can only be applied with some probability (discussed below). The state conditional on the success of this first step is updated via

$$|\psi\rangle \to \frac{\rho|\psi\rangle}{\sqrt{\langle\psi|\rho^\dagger\rho|\psi\rangle}} = \rho|\psi'\rangle,$$

where we have defined $|\psi'\rangle = |\psi\rangle/\sqrt{\langle\psi|\eta|\psi\rangle}$, and interpret this as the initial state normalized in $\mathcal{H}'$. (Note that we have chosen here to use the notation $|\psi'\rangle$ rather than $|\psi'\rangle\rangle$ as we are working throughout in $\mathcal{H}$, and simply simulating evolution in $\mathcal{H}'$.)

In the next step we evolve unitarily under h. To prove that the resulting description is equivalent to evolving $|\psi'\rangle$ as defined above in $\mathcal{H}'$, we consider our ability to predict physical quantities in $\mathcal{H}'$. Suppose at time t we perform a measurement in basis $|a_i\rangle$ of $\mathcal{H}$. The probability of obtaining outcome i is given by

$$\begin{aligned}
\Pr(i) &= |\langle a_i|\psi(t)\rangle|^2 \\
&= \frac{|\langle a_i|e^{-iht}\rho|\psi\rangle|^2}{\langle\psi|\eta|\psi\rangle} \\
&= |\langle a_i|e^{-iht}\rho|\psi'\rangle|^2 \\
&= |\langle a_i|(\rho^{-1})^\dagger\rho^\dagger\rho\rho^{-1}e^{-iht}\rho|\psi'\rangle|^2 \\
&= |\langle a_i'|\eta e^{-iHt}|\psi'\rangle|^2 \\
&= |\langle\langle a_i'|\psi'(t)\rangle\rangle|^2,
\end{aligned}$$

where as previously, $|a_i'\rangle = \rho^{-1}|a_i\rangle$, $\eta = \rho^\dagger\rho$ and we have used Eq. (4). Note that $\{|a_i'\rangle\}$ defines an orthonormal basis in $\mathcal{H}'$, and indeed for each such basis there exists a measurement in $\mathcal{H}$ that reproduces the statistics of measurement in that basis.

We can thus consider the physical operation ρ to be a transformation from $\mathcal{H}'$ to $\mathcal{H}$. Although the mapping is unitary when considered as a transformation in this way, as an operator acting on $\mathcal{H}$ alone ρ is nonunitary. How can we apply this physically?

Every physically allowed map in quantum theory is described by a trace-preserving completely positive (TPCP) map. Every such map has a Kraus representation (see, e.g., [76–78]):

$$|\psi\rangle\langle\psi| \to \sum_k E_k|\psi\rangle\langle\psi|E_k^\dagger,$$

where $\sum_k E_k^\dagger E_k = I$. We can interpret this as a statistical mixture of evolutions

$$|\psi\rangle \to \frac{E_k|\psi\rangle}{\sqrt{\langle\psi|E_k^\dagger E_k|\psi\rangle}},$$

each occurring with probability $\Pr(k) = \langle\psi|E_k^\dagger E_k|\psi\rangle$. It is further always possible to implement such a transformation in a heralded way—that is, so that we know which one of the operators E_k has been applied in a given run of an experiment. To implement the transformation ρ we simply choose a physical transformation with a Kraus operator $E_0 = c\rho$ for some constant c, which may be chosen to be real. When this transformation occurs we thus obtain

$$|\psi\rangle \to \frac{\rho|\psi\rangle}{\sqrt{\langle\psi|\rho^\dagger\rho|\psi\rangle}},$$

as desired. In order that this describes a physically realizable operation we require that there exists some E_1 such that $E_0^\dagger E_0 + E_1^\dagger E_1 = I$. Since $E_1^\dagger E_1$ is a positive operator, we therefore require $I - E_0^\dagger E_0 \geqslant 0$, i.e.,

$$I - c^2\rho^\dagger\rho \geqslant 0.$$

The probability of success in implementing this transformation is given by $c^2\langle\psi|\rho^\dagger\rho|\psi\rangle$; this is maximized while still satisfying the constraint above if we choose $c = (\lambda_{\max})^{-1/2}$ where $\lambda_{\max}$ is the largest eigenvalue of $\rho^\dagger\rho = \eta$. Thus the transformation from $\mathcal{H}'$ to $\mathcal{H}$ is successful with probability

$$\Pr(\text{succ}) \leqslant \frac{\langle\psi|\rho^\dagger\rho|\psi\rangle}{\lambda_{\max}}.$$

This gives a tight upper bound on the probability of success of such a transformation. A probability of success greater than this is introducing new physics, and will lead to effects such as faster than Hermitian evolution, single shot state discrimination with a higher probability of success than standard quantum theory, and violation of no signalling. A probability of success less than this bound is entirely implementable within standard quantum theory and thus offers no new capabilities but similarly suffers no new pitfalls.

We return now to the gedanken experiment with Hamiltonian H given in Eq. (9). The corresponding metric operator η is given in Eq. (10). A short calculation shows that this has eigenvalues $\lambda_\pm = (1 \pm \sin\alpha)/\cos\alpha$, corresponding to eigenvectors $|y\pm\rangle$, the ± 1 eigenstates of σ_y. Thus choosing $\rho = \eta^{1/2}$, the desired transformation from $\mathcal{H}'$ to $\mathcal{H}$ is given by

$$\begin{aligned}
E_0 &= \frac{1}{\sqrt{\lambda_{\max}}}\eta^{1/2} \\
&= |y+\rangle\langle y+| + \sqrt{\frac{1-\sin\alpha}{1+\sin\alpha}}|y-\rangle\langle y-|.
\end{aligned}$$

A physical implementation of the whole procedure in a spin-1/2 system is thus as follows: the initial state passes into a Stern-Gerlach device with an inhomogeneous magnetic field in the y direction. The $|y-\rangle$ component passes through an absorbing region, in which any given system is absorbed with probability $(1 - \sin\alpha)/(1 + \sin\alpha)$. The $|y\pm\rangle$ beams are recombined through the use of an inhomogeneous magnetic field equal and opposite to the first. Finally the Hamiltonian $h = \rho H \rho^{-1}$ may be implemented by applying a homogeneous magnetic field in the x direction.

Alternatively, the transformation E_0 is exactly that used in unambiguous state discrimination, and an alternative realization using polarization as our two-level system could be achieved using fiber with polarization-dependent loss [73], or indeed an interferometer with polarizing beamsplitters [79]. On exiting the fiber or interferometer, we only need implement the Hamiltonian $h = \rho H \rho^{-1}$ using a birefringent material.

3. $\mathcal{PT}$-symmetric evolution of a subsystem

Günther and Samsonov [39] suggested an embedding of the two-dimensional $\mathcal{PT}$-symmetric brachistochrone into a four-dimensional space, in an approach inspired by the Naimark extension of a POVM, and later implemented experimentally by Zheng *et al.* [52]. For a specified initial state of the $\mathcal{PT}$-symmetric system, the scheme describes how to prepare an appropriate initial state of the four-dimensional conventional quantum system, evolve, and finally measure the extended system in order to simulate $\mathcal{PT}$-symmetric evolution on a two-dimensional subsystem. However the authors of [39] do not address how to simulate $\mathcal{PT}$-symmetric evolution for an arbitrary and *unknown* initial state $|\psi\rangle$, and thus do not address the issue of the boundary between conventional and $\mathcal{PT}$-symmetric regions. Here we discuss where the subsystem scheme fits into the alternatives described above.

The embedding of a two-dimensional $\mathcal{PT}$-symmetric system into a four-dimensional unitary system proceeds as follows: the initial state of the four-dimensional system is given by

$$|\Psi\rangle_{AB} = \frac{|0\rangle_A \otimes |\psi\rangle_B + |1\rangle_A \otimes (\rho^2|\psi\rangle)_B}{\sqrt{1+\langle\psi|(\rho^\dagger)^2\rho^2|\psi\rangle}}, \tag{13}$$

where $\rho = \eta^{1/2}$, and $|\psi\rangle$ is the state in a $\mathcal{PT}$-symmetric region, and thus is normalized according to the $\mathcal{PT}$-symmetric inner product $\langle\psi|\eta|\psi\rangle = 1$. $|\Psi\rangle_{AB}$ then evolves unitarily under a Hermitian Hamiltonian. Finally, system A is measured, and conditional on being found in state $|0\rangle_A$, system B has undergone $\mathcal{PT}$-symmetric, nonunitary evolution. Thus it is the subspace spanned by $|0\rangle_A \otimes |0\rangle_B$, $|0\rangle_A \otimes |1\rangle_B$ which evolves under the $\mathcal{PT}$-symmetric Hamiltonian H.

Now suppose we start with an arbitrary but unknown state $|\psi\rangle$ (in a conventional quantum system) and wish to simulate $\mathcal{PT}$-symmetric evolution. How do we achieve the embedding of this initial state into a four-dimensional conventional quantum-mechanical system? We first note that, as used in [39] and may easily be verified using Eq. (10),

$$\eta^{-1} + \eta = aI,$$

where $a = 2/\cos\alpha$. Thus the operation

$$|0\rangle_A \otimes |\psi\rangle_B \rightarrow$$
$$|\Psi\rangle_{AB} = \frac{1}{\sqrt{a}}(|0\rangle_A \otimes (\rho^{-1}|\psi\rangle_B) + \otimes|1\rangle_A(\rho|\psi\rangle_B)),$$

which may be achieved by introducing an ancilla in state $|0\rangle_A$, and evolving under a suitably chosen joint operation V_{AB}, preserves inner products:

$${}_{AB}\langle\Phi|\Psi\rangle_{AB} = \frac{1}{a}{}_B\langle\phi|(\rho^{-2}+\rho^2)|\psi\rangle_B = {}_B\langle\phi|\psi\rangle_B.$$

V_{AB} thus may be chosen to be unitary. $|\Psi\rangle_{AB}$ is however not yet in the form given in Eq. (13). We now have a choice in order to prepare the initial state of the extended system—we either associate the initial state $|\psi\rangle$ in the conventional quantum system with a state $\rho^{-1}|\psi\rangle$ in the $\mathcal{PT}$-symmetric region (passive transformation), or we apply a transformation $I \otimes \rho$ to the joint system (active transformation), to recover the desired initial state $|\Psi\rangle_{AB}$.

In the remainder of the scheme the Hamiltonian applied to the extended system is unitarily equivalent to evolution under h (specifically, it is given by $V_{AB}(I_A \otimes h_B)V_{AB}^\dagger$). Finally, on exiting the $\mathcal{PT}$-symmetric region, we measure the ancilla qubit, and if found in state $|0\rangle_A$, the $\mathcal{PT}$ symmetric evolution is successful. This operation is always probabilistic, and corresponds to an active transformation from the simulated $\mathcal{PT}$-symmetric region to the conventional quantum region.

Closer inspection of the subsystem scheme therefore reveals that it is equivalent to either our passive or our active transformation. The construction in [39] appears to be a purely formal mathematical procedure inspired by the Naimark extension of a positive operator-valued measure (or more accurately, the Stinespring dilation of a CP map). This dilation and postselection is just one possible implementation of the Kraus operator transforming between frames. Although the physical picture of a subspace evolving under a $\mathcal{PT}$-symmetric Hamiltonian is not without appeal, the explicit introduction of the ancilla system obscures the connection between the transformed and untransformed systems. More importantly, the problem of how to prepare the initial state in the extended system seems to not have been addressed in the literature up to now, seriously limiting the applicability and interpretation of the subsystem scheme.

IV. DISCUSSION

In this paper our aim has been to clarify the requirements for physical implementation of $\mathcal{PT}$-symmetric Hamiltonians in quantum systems, and thereby evaluate the prospects for applications of $\mathcal{PT}$-symmetric Hamiltonians in quantum information science. We have presented three physically inequivalent proposed experimental implementations of $\mathcal{PT}$-symmetric Hamiltonians, and have discussed how to treat the boundary between Hermitian and non-Hermitian regions in each case. Note that the only option not requiring external intervention is the passive transformation case. In the absence of intervention the *only* physically reasonable boundary theory is to impose continuity of the physical state across the boundary. Changing mathematical description requires us to update the representation of the physical state accordingly. Failure to do so amounts to introducing new physics, which has nothing to do with $\mathcal{PT}$ symmetry, but rather is due to erroneously assigning physical meaning to a particular representation of the state. It seems there has been considerable confusion in the literature caused by the assumption that it is the *representation* of the state rather than the physical state which is continuous across the boundary.

The other implementations suggested both involve *simulation* of a $\mathcal{PT}$-symmetric Hamiltonian, and are presented in order to clarify some remaining points of disagreement in the literature regarding the co-existence of Hermitian and non-Hermitian regions, as well as the conflation of unitary evolution under a non-Hermitian H with nonunitary evolution under an effective Hamiltonian. We have outlined how to calculate the probability of success of various simulation schemes. By providing experimental implementations we pinpoint exactly where assumptions can enter which represent a departure from standard quantum theory. In light of this, the mounting list of strange effects suggested in the literature ranging from vanishingly small evolution times, to searching a database exponentially fast, to violation of no signaling and of invariance of measures of entanglement are, of course, excluded.

Although $\mathcal{PT}$-symmetric quantum theory as a unitary theory has long been known to be exactly equivalent to conventional quantum theory, Lee *et al.* [45] have recently questioned the validity of $\mathcal{PT}$ symmetry as a local theory, suggesting three alternative possibilities regarding its viability. These are as follows: $\mathcal{PT}$ symmetry is not a valid local theory; $\mathcal{PT}$-symmetric quantum theory may be applied consistently locally, but the boundary must be treated in a way to avoid superluminal signaling; or $\mathcal{PT}$ symmetry is a valid local theory which allows violation of no signaling. We find that the violation of no signaling is unrelated to $\mathcal{PT}$ symmetry, and have shown that the second option is the only physically reasonable one.

Finally we return to the question of an exponentially fast database search—or more precisely, a polynomial time search of an exponentially large database. Since any simulation of $\mathcal{PT}$-symmetric schemes may be performed entirely within quantum theory, by definition any scheme proposed thus far cannot out-perform existing techniques. The scheme suggested in [25] (referring to [80]) is based on the ability to distinguish unambiguously between exponentially close states. Even assuming perfect noiseless operations, unambiguous discrimination between exponentially close states may be achieved in quantum theory, but only with an exponentially small probability of success. Thus a polynomial time database search is achieved only with an exponentially small probability of success. To achieve any given constant probability of success we must repeat the attempted search exponentially many times, and thus the promise of an "exponentially fast" search is something of a red herring. Indeed, there exists a simple classical algorithm that searches a database in polynomial time with exponentially small probability of success—pick an entry at random from the database and check whether it is the marked item. Repeat a polynomial number of times.

More generally, the simulation of $\mathcal{PT}$-symmetric Hamiltonians is either trivial (the passive transformation case) or involves postselection, a probabilistic element. Although generically quantum algorithms are probabilistic, this usually enters at the readout stage. Probabilistic quantum gates are to be avoided wherever possible, as the probability of success of a circuit composed of such gates falls exponentially with the number of gates. Moreover postselection is known to be suboptimal for estimation tasks [81], and phase estimation is an important subroutine for several quantum algorithms, including Shor's famous factoring algorithm [82,83]. Finally, any $\mathcal{PT}$-symmetric implementation can, by definition, perform at best only as well as existing techniques, in terms of the probability of success of a given evolution. Thus it seems unlikely that $\mathcal{PT}$-symmetric Hamiltonians will find a use in quantum information science.

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