

**Max-Planck-Institut
für Mathematik
in den Naturwissenschaften
Leipzig**

**Simulating broken PT -symmetric
Hamiltonian systems by weak
measurement**

by

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Preprint no.: 75

2019



Simulating broken \mathcal{PT} -symmetric Hamiltonian systems by weak measurement

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By embedding a \mathcal{PT} -symmetric (pseudo-Hermitian) system into a large Hermitian one, we disclose the relations between \mathcal{PT} -symmetric quantum theory and weak measurement theory. We show that the weak measurement can give rise to the inner product structure of \mathcal{PT} -symmetric systems, with the pre-selected state and its post-selected state resident in the dilated conventional system. Typically in quantum information theory, by projecting out the irrelevant degrees and projecting onto the subspace, even local broken \mathcal{PT} -symmetric Hamiltonian systems can be effectively simulated by this weak measurement paradigm.

Introduction Generalizing the conventional Hermitian quantum mechanics, Bender and his colleagues established the Parity (\mathcal{P})-time (\mathcal{T})-symmetric quantum mechanics in 1998 [1]. With the additional degree of freedom from a non-conservative Hamiltonian, as well as the existence of exceptional points between unbroken and broken \mathcal{PT} -symmetries, optical \mathcal{PT} -symmetric devices have been demonstrated with many useful applications [2–7]. Although calling for more caution on physical interpretations, especially on the consistency problem of local \mathcal{PT} -symmetric operation and the no-signaling principle [8], \mathcal{PT} -symmetric quantum mechanics has been stimulating our understanding on many interesting problems such as spectral equivalence [9], quantum brachistochrone [10] and Riemann hypothesis [11].

Compared with the Dirac inner product in conventional quantum mechanics, \mathcal{PT} -symmetric quantum theory can be well manifested by the η -inner product [12, 13]. In the broken \mathcal{PT} -symmetry case, the η -inner product of a state with itself can be negative, which makes the broken \mathcal{PT} -symmetric quantum systems a complete departure from conventional quantum mechanics. While in the unbroken \mathcal{PT} -symmetry case, the η -inner product presents a completely analogous physical interpretation to the Dirac inner product, giving rise to many similar properties between \mathcal{PT} -symmetric and conventional quantum mechanics. Recent works also show that the η -inner product is tightly related to the properties of superposition and coherence in conventional quantum mechanics [14].

Despite the original motivation to build a new framework of quantum theory, researchers are aware of the importance of simulating \mathcal{PT} -symmetric systems with conventional quantum mechanics. It will help explore the properties and physical meaning of \mathcal{PT} -symmetric quantum systems. On this issue, one should answer the question in what sense a quantum system can be

viewed as \mathcal{PT} -symmetric. One approach, initialized by Günther and Samsonov, is to embed unbroken \mathcal{PT} -symmetric Hamiltonians into higher dimensional Hermitian Hamiltonians [15–17]. By dilating the system to a large Hermitian one and projecting out the ancillary system, this paradigm successfully simulates the evolution of unbroken \mathcal{PT} -symmetric Hamiltonians. Such a way, inspired by Naimark dilation and typical ideas in quantum simulation, endows direct physical meaning of \mathcal{PT} -symmetric quantum systems in the sense of open systems. However, the simulation of broken \mathcal{PT} -symmetric systems is still in suspense, due to its essential distinctions with conventional quantum systems.

In this Letter, we illustrate the simulation for broken \mathcal{PT} -symmetric systems based on weak measurement [18]. For a system weakly coupled to the apparatus, the pointer state will be shifted by the weak value when a weak measurement is performed. The weak value, tightly related to the non-classical features of quantum mechanics, such as the Hardy’s paradox [19], three box paradox [20] and Leggett-Garg inequalities [21], can take values beyond the expected values of an observable, and even be a complex number. The weak measurement theory has provided new ways to measure geometric phases [22–25] and non-Hermitian systems [26, 27], as well as to amplify signals as a sensitive estimation of small evolution parameters [28–30]. Our aim is to propose a concrete scenario in which the quantum system can be viewed as \mathcal{PT} -symmetric by utilizing the weak measurement. Our result reveals the connections between \mathcal{PT} -symmetry and the weak measurement theory, providing the important missing point for the simulation problem of broken \mathcal{PT} -symmetric quantum systems.

Generalized embedding of \mathcal{PT} -symmetric systems Consider n -dimensional discrete quantum systems. A linear operator P is said to be a parity operator if $P^2 = I$, where I denotes the $n \times n$ identity matrix. An anti-

linear operator T is said to be a time reversal operator if $TT = I$ and $PT = T\bar{P}$, where \bar{T} (\bar{P}) stands for the complex conjugation of T (P). A Hamiltonian H is said to be PT -symmetric if $HPT = PT\bar{H}$ [31]. H is called unbroken \mathcal{PT} -symmetric if it is diagonalizable and all of its eigenvalues are real. Otherwise, H is called broken \mathcal{PT} -symmetric.

In quantum mechanics, a Hamiltonian H gives rise to a unitary evolution of the system. Let ϕ_1 and ϕ_2 be two states. One can introduce a Hermitian operator η to define the η -inner product by $\langle \phi_1 | \phi_2 \rangle_\eta = \langle \phi_1 | \eta | \phi_2 \rangle$. With respect to the η -inner product, H presents a unitary evolution if and only if $H^\dagger \eta = \eta H$ [12, 13, 32–34], where H^\dagger denotes the conjugation and transpose of H . Here, η is said to be the metric operator of H . Moreover, for a generic \mathcal{PT} -symmetric operator H and its metric operator η , there always exist some matrix Ψ' such that $\Psi'^{-1} H \Psi' = J$ and $\Psi'^\dagger \eta \Psi' = S$, where

$$J = \text{diag}(J_{n_1}(\lambda_1, \bar{\lambda}_1), \dots, J_{n_p}(\lambda_p, \bar{\lambda}_p), J_{n_{p+1}}(\lambda_{p+1}), \dots, J_r(\lambda_r)), \quad (1)$$

$J_{n_k}(\lambda_k, \bar{\lambda}_k) = \begin{pmatrix} J_{n_k}(\lambda_k) & 0 \\ 0 & J_{n_k}(\bar{\lambda}_k) \end{pmatrix}$, $J_{n_j}(\lambda_j)$ are the Jordan blocks, $\lambda_1, \dots, \lambda_p$ are complex numbers and $\lambda_{p+1}, \dots, \lambda_r$ are real numbers,

$$S = \text{diag}(S_{2n_1}, \dots, S_{2n_p}, \epsilon_{n_q} S_{n_q}, \dots, \epsilon_{n_r} S_{n_r}), \quad (2)$$

n_i denote the orders of Jordan blocks in Eq. (1), i.e., $S_k = \begin{pmatrix} 1 & & \\ & \ddots & \\ 1 & & \end{pmatrix}_{k \times k}$ and $\epsilon_i = \pm 1$ is uniquely determined by η [16, 35]. For convenience, we only consider the situations in which $\epsilon_i = 1$. In this case, S is a permutation matrix and $S^2 = I$. Note that S can be equal to I if and only if H is unbroken \mathcal{PT} -symmetric [16]. Henceforth we always assume $S = I$ in the unbroken case. The following theorem gives an important property of \mathcal{PT} -symmetric Hamiltonians.

Theorem 1. Let H be an $n \times n$ \mathcal{PT} -symmetric matrix and η be the metric matrix of H . Let J and S be matrices in Eqs (1) and (2). Then, there exist $n \times n$ invertible matrices Ψ , Ξ , Σ and a $2n \times 2n$ Hermitian matrix \tilde{H} such that for $\tilde{\Psi} = \begin{pmatrix} \Psi \\ \Xi \end{pmatrix}$ and $\tilde{\Phi} = \begin{pmatrix} \Psi \\ \Sigma \end{pmatrix}$, the following equations hold,

$$\tilde{\Phi}^\dagger \tilde{\Psi} = S, \quad \tilde{\Phi}^\dagger \tilde{H} \tilde{\Psi} = SJ. \quad (3)$$

Proof. As was discussed, there exist a matrix Ψ' such that $\Psi'^{-1} H \Psi' = J$ and $\Psi'^\dagger \eta \Psi' = S$ [16, 35]. Since $\Psi'^\dagger \Psi' > 0$, there always exists a positive number c such that $c^2 \Psi'^\dagger \Psi' > I$. Set $\Psi = c \Psi'$. Since $\Psi^\dagger \Psi > I \geq S$, $\Psi^\dagger \Psi - S$ is invertible.

Let Ξ be an $n \times n$ invertible matrix. Taking $\Sigma = (\Xi^{-1})^\dagger (S - \Psi^\dagger \Psi)$, $\eta = (\Psi^{-1})^\dagger S \Psi^{-1}$, $H_1 = \eta H$, $H_2 = (\Psi^\dagger)^{-1} (\Xi)^\dagger$ and $H_4 = -H_2^\dagger \Psi \Xi^{-1} - (\Sigma^\dagger)^{-1} \Psi^\dagger H_2$, one

can directly verify that $\tilde{H} = \begin{pmatrix} H_1 & H_2 \\ H_2^\dagger & H_4 \end{pmatrix}$ is Hermitian and Eq. (3) holds. \square

Theorem 1 actually gives out the inner product structure of H in a subspace. Note that the matrix Ψ in Theorem 1 can be written as $\Psi = (|\psi_1\rangle, \dots, |\psi_n\rangle)$, where the column vectors $\{|\psi_i\rangle\}$ form a linear basis of \mathbb{C}^n . Similarly, $\Xi = (|\xi_1\rangle, \dots, |\xi_n\rangle)$ and $\Sigma = (|\sigma_1\rangle, \dots, |\sigma_n\rangle)$. Correspondingly we have $\tilde{\Psi} = (|\tilde{\psi}_1\rangle, \dots, |\tilde{\psi}_n\rangle)$ and $\tilde{\Phi} = (|\tilde{\phi}_1\rangle, \dots, |\tilde{\phi}_n\rangle)$, where $|\tilde{\psi}_i\rangle = \begin{pmatrix} |\psi_i\rangle \\ |\xi_i\rangle \end{pmatrix}$ and $|\tilde{\phi}_i\rangle = \begin{pmatrix} |\psi_i\rangle \\ |\sigma_i\rangle \end{pmatrix}$. Moreover, $\tilde{\Phi} S = (|\tilde{\mu}_1\rangle, \dots, |\tilde{\mu}_n\rangle) = (|\tilde{\phi}_{s(1)}\rangle, \dots, |\tilde{\phi}_{s(n)}\rangle)$, where S is the permutation matrix in Theorem 1, and s is the permutation induced by S . Similarly, we can write $\tilde{\Psi} S = (|\mu_1\rangle, \dots, |\mu_n\rangle)$, where $|\mu_i\rangle = |\psi_{s(i)}\rangle$. From the definition of $|\tilde{\mu}_i\rangle$, we have $\langle \tilde{\mu}_i | \tilde{\psi}_j \rangle = (S \tilde{\Phi}^\dagger \tilde{\Psi})_{ij}$ and $\langle \tilde{\mu}_i | \tilde{H} | \tilde{\psi}_j \rangle = (S \tilde{\Phi}^\dagger \tilde{H} \tilde{\Psi})_{ij}$. According to Eq. (3), we have

$$\langle \tilde{\mu}_i | \tilde{\psi}_j \rangle = \delta_{ij}, \quad \langle \tilde{\mu}_i | \tilde{H} | \tilde{\psi}_j \rangle = J_{ij}, \quad (4)$$

where J_{ij} is the (i, j) -th entry of J .

On the other hand, note that the metric matrix η of H is $(\Psi^\dagger)^{-1} S \Psi^{-1}$. Thus we have the following relations between the Dirac and η -inner products

$$\langle \tilde{\mu}_i | \tilde{\psi}_j \rangle = \langle \mu_i | \psi_j \rangle_\eta, \quad (5)$$

$$\langle \tilde{\mu}_i | \tilde{H} | \tilde{\psi}_j \rangle = \langle \mu_i | H | \psi_j \rangle_\eta, \quad (6)$$

where $\langle \mu_i | H | \psi_j \rangle_\eta = \langle \mu_i | \eta H | \psi_j \rangle$. The results show that there exist two different basis with the same projections onto the subspace of the \mathcal{PT} -symmetric system, with respect to the η -inner product. When confined to the subspace, the Hermitian Hamiltonian \tilde{H} in large space has the same effect as a \mathcal{PT} -symmetric Hamiltonian H , in the sense of this η -inner product.

Simulation of \mathcal{PT} -symmetric Hamiltonian systems To infer a quantum system is \mathcal{PT} -symmetric, it is sufficient to identify the Hamiltonian and its inner product structure. In the weak measurement formalism, one starts by pre-selecting an initial state $|\varphi_i\rangle$. The target system is coupled to the measurement apparatus, which is in a pointer state $|P\rangle$. Usually, $|P\rangle = (2\pi\Delta^2)^{-\frac{1}{4}} \exp(-\frac{Q^2}{4\Delta^2})$, a Gaussian state with Δ its standard deviation. Let A be an observable of the system and M be that of the apparatus, conjugate to Q [18]. The interaction Hamiltonian between the system and apparatus is $H_{int} = f(t)A \otimes M$, with interaction strength $g = \int f(t)dt$. The state evolves as $|\varphi_i\rangle \otimes |P\rangle \rightarrow e^{-igA \otimes M} |\varphi_i\rangle \otimes |P\rangle$. Now if the system satisfies the weak condition that g/Δ is sufficiently small, then for a post-selected state $|\varphi_f\rangle$ that $\langle \varphi_f | \varphi_i \rangle \neq 0$, one has $\langle \varphi_f | e^{-igA \otimes M} | \varphi_i \rangle | P \rangle \approx \langle \varphi_f | \varphi_i \rangle e^{-ig\langle A \rangle_w M} | P \rangle = \langle \varphi_f | \varphi_i \rangle (2\pi\Delta^2)^{-\frac{1}{4}} \exp(-\frac{(Q-g\langle A \rangle_w)^2}{4\Delta^2})$, where $\langle A \rangle_w =$

$\frac{\langle \varphi_f | A | \varphi_i \rangle}{\langle \varphi_f | \varphi_i \rangle}$ is called the weak value. That is, the state is shifted by $g\langle A \rangle_w$. Thus the weak value $\langle A \rangle_w$ can be read out experimentally, as a generalization of the eigenvalues in Von Neumann measurement [36].

From Eq. (4), we have $\lambda_i = J_{i,i} = \langle \tilde{\mu}_i | \tilde{H} | \tilde{\psi}_i \rangle = \frac{\langle \tilde{\mu}_i | \tilde{H} | \tilde{\psi}_i \rangle}{\langle \tilde{\mu}_i | \tilde{\psi}_i \rangle}$. Therefore, the eigenvalues of H can be obtained via a weak measurement, by pre-selecting the vector $|\tilde{\psi}_i\rangle$ and post-selecting the vector $|\tilde{\mu}_i\rangle$. This observation implies that one can use weak measurement to simulate the measurements on a \mathcal{PT} -symmetric system.

In conventional quantum mechanics, the expectation value of a Hermitian Hamiltonian $H_0 = \sum_i \lambda_i |u_i\rangle\langle u_i|$ with respect to a state $|\psi_0\rangle = \sum_i d_i |u_i\rangle$ is given by the inner product $\langle \psi_0 | H_0 | \psi_0 \rangle$. For a \mathcal{PT} -symmetric Hamiltonian system with the metric matrix η , the expectation value of a Hamiltonian H with respect to a state $|u\rangle = \sum_i a_i |\psi_i\rangle$ is instead given by $\langle u | H | u \rangle_\eta$. Given two vectors $|v\rangle = \sum_i b_i |\mu_i\rangle$ and $|w\rangle = \sum_i c_i |\psi_i\rangle$ of the \mathcal{PT} -symmetric system. Let $|\tilde{v}\rangle = \sum_i b_i |\tilde{\mu}_i\rangle$ (unnormalized for convenience) and $|\tilde{w}\rangle = \sum_i c_i |\tilde{\psi}_i\rangle$ be two vectors in the extended system. It follows from Eq. (6) that $\langle v | H | w \rangle_\eta = \langle \tilde{v} | \tilde{H} | \tilde{w} \rangle$. Assume that $|u\rangle$ satisfies the condition $\langle u | u \rangle_\eta = \pm 1$. Now take two states $|\tilde{u}_1\rangle = \sum_i a_{s(i)} |\tilde{\mu}_i\rangle$ and $|\tilde{u}_2\rangle = \sum_i a_i |\tilde{\psi}_i\rangle$, whose projections to the \mathcal{PT} -symmetric subspace are both $|u\rangle$. Then we have

$$\frac{\langle u | H | u \rangle_\eta}{\langle u | u \rangle_\eta} = \frac{\langle \tilde{u}_1 | \tilde{H} | \tilde{u}_2 \rangle}{\langle \tilde{u}_1 | \tilde{u}_2 \rangle}. \quad (7)$$

Therefore, confined to the \mathcal{PT} -symmetric subspace, a weak measurement can completely describe the expectations of H .

In conventional quantum mechanics, when an eigenvalue is detected, the measured state collapses to the corresponding eigenstate. However, the problem in \mathcal{PT} -symmetric system is subtle. According to Eq. (5), $\langle \psi_i | \psi_i \rangle_\eta \neq 0$ only if $i = s(i)$. This observation makes it reasonable to assume that for any vector $|u\rangle = \sum_i a_i |\psi_i\rangle$ satisfying $\langle u | u \rangle_\eta \neq 0$, if $a_i \neq 0$, then $a_{s(i)} \neq 0$. That is, if $\langle u | u \rangle_\eta \neq 0$, its vector components of $|\psi_i\rangle$ and $|\psi_{s(i)}\rangle$ take zero or nonzero values simultaneously, while the eigenvalues associated with ψ_i and $\psi_{s(i)}$ are either equal or complex conjugations. In this case, one can generalize the detection of an eigenvalue of λ_i in conventional quantum mechanics to the following. For $|u\rangle = \sum_i a_i |\psi_i\rangle$, if the value of

$$\frac{a_i \bar{a}_{s(i)} \lambda_i + \bar{a}_i a_{s(i)} \bar{\lambda}_i}{a_i \bar{a}_{s(i)} + \bar{a}_i a_{s(i)}}$$

is detected [37], the state $|u\rangle$ will collapse to

$$\frac{a_i |\psi_i\rangle + a_{s(i)} |\psi_{s(i)}\rangle}{|a_i \bar{a}_{s(i)} + a_{s(i)} \bar{a}_i|^{\frac{1}{2}}}.$$

Apparently, when $i = s(i)$, the state $|u\rangle$ will collapse to $|\psi_i\rangle$, similar to the case of conventional quantum mechanics. Note that $i = s(i)$ only if the system is unbroken \mathcal{PT} -symmetric, for which it is analogous to conventional quantum mechanics and such an analogy in state collapse is not unexpected.

By pre- and post-selecting the states, we see that the weak measurements can successfully simulate an arbitrary η -inner product. Furthermore, when confined to the subspace, the measurement results actually abstract the same information as a \mathcal{PT} -symmetric Hamiltonian system. Such information help us eventually infer that the subsystem is \mathcal{PT} -symmetric.

Discussions and conclusion We further discuss the mechanism and physical implications related to the weak measurement paradigm, by comparing it with the embedding paradigm [15, 16]. The essence of the embedding paradigm is to realize the evolution of a \mathcal{PT} -symmetric Hamiltonian, by evolving the state under the Hermitian Hamiltonian in the large space and then project it to the subspace. The key to this paradigm can be mathematically described as follows [16]: For a given $n \times n$ unbroken \mathcal{PT} -symmetric Hamiltonian H , find a $2n \times 2n$ Hermitian matrix \tilde{H} , $n \times n$ invertible matrices Ψ, Ξ so that $\tilde{\Psi}^\dagger \tilde{\Psi} = I$ and the following equations

$$e^{-it\tilde{H}} \tilde{\Psi} = \tilde{\Psi} e^{-itJ}, \quad e^{-itH} \Psi = \Psi e^{-itJ} \quad (8)$$

hold, where $\tilde{\Psi} = \begin{pmatrix} \Psi \\ \Xi \end{pmatrix}$. The equations are actually equivalent to the following conditions [38]:

$$\tilde{\Psi}^\dagger \tilde{\Psi} = I, \quad \tilde{H} \tilde{\Psi} = \tilde{\Psi} J, \quad H \Psi = \Psi J. \quad (9)$$

Equation (8) ensures that the unitary evolution $\tilde{U}(t)$ gives the evolution $U(t)$ of a \mathcal{PT} -symmetric Hamiltonian H in a subspace. In this sense, the embedding paradigm gives a natural way of simulation. Nevertheless, in the broken \mathcal{PT} -symmetric case, the solutions do not exist [16]. In fact, Eq. (3) is mathematically a generalization of Eq. (9) [39]. Like the case of the embedding paradigm, it is natural to further require that $\tilde{\Phi}^\dagger e^{-it\tilde{H}} \tilde{\Psi} = S e^{-itJ}$, so that $e^{-it\tilde{H}}$ gives the same effect as e^{-itH} in the subspace. However, such a requirement cannot be satisfied for broken \mathcal{PT} -symmetry, which is obvious from the unboundedness of $S e^{-itJ}$.

However, consider sufficiently small time $t \in [0, \epsilon]$. We have $|\tilde{u}(t)\rangle = e^{-it\tilde{H}} |\tilde{u}\rangle \approx (I - it\tilde{H}) |\tilde{u}\rangle$. On the other hand, $|u(t)\rangle = e^{-itH} |u\rangle \approx (I - itH) |u\rangle$. Now equations Eqs. (5) and (6) insure that when confined to the subspace, $|\tilde{u}(t)\rangle$ is equivalent to $|u(t)\rangle$ in the sense of η -inner product (see Supplemental Material for an example). This observation implies that \mathcal{PT} -symmetric quantum systems can be well approximated in a sufficiently small time evolution, by choosing two different sets of basis $\{|\tilde{\phi}_i\rangle\}$ and $\{|\tilde{\psi}_i\rangle\}$ with the same components in the subspace, which can be realized by weak

measurement. Here instead of the small time interval, the weak condition that g/Δ is sufficiently small ensures the approximation. The weak measurement paradigm can be viewed as a generalization of the embedding paradigm, due to the fact that Eq. (9) is a special case of Eq. (3) in the \mathcal{PT} -symmetric unbroken case. Hence, the Hamiltonian \tilde{H} in the embedding paradigm can also be utilized in the weak measurement approach, although the embedding paradigm itself does not work. Comparing our approach with that in [26], where one obtains the expected value of a Hamiltonian in the Dirac inner product by using the polar decomposition, our method lays emphasis on the properties of a \mathcal{PT} -symmetric Hamiltonian with respect to the η -inner product.

In summary, we have proposed a weak measurement paradigm to investigate the behaviors of broken \mathcal{PT} -symmetric Hamiltonian systems. By embedding the \mathcal{PT} -symmetric system into a large Hermitian system and utilizing weak measurements, we have shown how a \mathcal{PT} -symmetric Hamiltonian can be simulated. Our paradigm may shine new light on the study of \mathcal{PT} -symmetric quantum mechanics and its physical implications and applications.

This work is supported by National Natural Science Foundation of China (11171301, 11571307, 11690032, 61490711, 61877054 and 11675113), National Key R&D Program of China under Grant No. 2018 YFA0306202 and the NSF of Beijing under Grant No. KZ201810028042.

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- [38] Equation (8) is actually the matrix version of the embedding in [16]. Denote $\Xi = \tau\Psi$. Then (9) reduces to $H_1 + H_2\tau = H$ and $H_2^\dagger + H_4\tau = \tau H$, which gives the equivalent description of the embedding property. A concrete solution to (8) can also be found in [17].
- [39] When unbroken \mathcal{PT} -symmetric, it is always possible to

take $\Xi = \Sigma$ and $S = I$, Eq. (9) is a special case of Eq. (3).

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Supplemental Material

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(Dated: May 31, 2019)

An example

To illustrate the validity of our theoretic results, an example is given based on the two dimensional model proposed by Bender et al. [1]:

$$H = \begin{bmatrix} re^{i\theta} & s \\ s & re^{-i\theta} \end{bmatrix}, \quad P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad T = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Here, as $HPT = P\overline{T}H$, the Hamiltonian H is \mathcal{PT} -symmetric. In particular, when $\Delta = s^2 - r^2 \sin^2 \theta < 0$, H is broken \mathcal{PT} -symmetric. The corresponding eigenvalues and eigenvectors (without normalization) are:

$$\lambda_1 = r \cos \theta + i\sqrt{-\Delta}, \quad \lambda_2 = r \cos \theta - i\sqrt{-\Delta}.$$

$$\psi_1 = \begin{bmatrix} i(\sqrt{-\Delta} + r \sin \theta) \\ s \end{bmatrix}, \quad \psi_2 = \begin{bmatrix} -s \\ i(\sqrt{-\Delta} + r \sin \theta) \end{bmatrix}.$$

Then, by denoting the eigenvectors in the matrix form, we have:

$$\Psi = [\psi_1, \psi_2] = \begin{bmatrix} i(\sqrt{-\Delta} + r \sin \theta) & -s \\ s & i(\sqrt{-\Delta} + r \sin \theta) \end{bmatrix}, \quad (S1)$$

It can be verified that $\Psi^{-1}H\Psi = J$ and $\Psi^\dagger \eta \Psi = S$, where

$$J = \begin{bmatrix} r \cos \theta + i\sqrt{-\Delta} & 0 \\ 0 & r \cos \theta - i\sqrt{-\Delta} \end{bmatrix}, \quad S = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \quad (S2)$$

Now, with the short-handed notations,

$$u = \sqrt{-\Delta} + r \sin \theta, \quad a = 2r \sin \theta.$$

we have

$$\Psi = \begin{bmatrix} iu & -s \\ s & iu \end{bmatrix}, \quad \Psi^{-1} = \frac{1}{s^2 - u^2} \begin{bmatrix} iu & s \\ -s & iu \end{bmatrix}, \quad (S3)$$

$$S - \Psi^\dagger \Psi = \begin{bmatrix} -au & 1 - 2sui \\ 1 + 2sui & -au \end{bmatrix}, \quad (S4)$$

$$\det(S - \Psi^\dagger \Psi) = -4\Delta u^2 - 1. \quad (S5)$$

For simplicity, we also assume $-4\Delta u^2 - 1 \neq 0$. Otherwise, as showed in the proof of Theorem 1, we can take a constant value c such that $S - c^2\Psi^\dagger\Psi$ is invertible, i.e., with $c\Psi$ instead of Ψ . Now

$$(S - \Psi^\dagger\Psi)^{-1} = \frac{1}{-4\Delta u^2 - 1} \begin{bmatrix} -au & -1 + 2sui \\ -1 - 2sui & -au \end{bmatrix}.$$

To introduce our simulating scenario, we take $\Psi = \Xi$ for convenience, as Ξ is arbitrary. By using the construction in Theorem 1, one can have $\Sigma = (\Xi^{-1})^\dagger(S - \Psi^\dagger\Psi)$, $\eta = (\Psi^{-1})^\dagger S \Psi^{-1}$, $H_1 = \eta H$, $H_2 = (\Psi^\dagger)^{-1}(\Xi)^\dagger$ and $H_4 = -H_2^\dagger \Psi \Xi^{-1} - (\Sigma^\dagger)^{-1} \Psi^\dagger H_2 = -I - \Xi(S - \Psi^\dagger\Psi)^{-1} \Xi^\dagger$.

Then, direct calculations give us

$$\tilde{H} = \begin{bmatrix} A_1 & A_2 & 1 & 0 \\ A_3 & A_4 & 0 & 1 \\ 1 & 0 & -1 - KB_1 & -KB_2 \\ 0 & 1 & -KB_3 & -1 - KB_4 \end{bmatrix}, \quad (S6)$$

$$\tilde{\Psi} = \begin{bmatrix} iu & -s \\ s & iu \\ iu & -s \\ s & iu \end{bmatrix}, \quad (S7)$$

$$\tilde{\Phi}^\dagger = \begin{bmatrix} -iu & s & iu - K_2s & iK_2u - s \\ -s & -iu & iK_2u + s & iu + K_2s \end{bmatrix}, \quad (S8)$$

with the notations

$$\begin{aligned} K &= \frac{1}{-4\Delta u^2 - 1}, \quad K_2 = \frac{1}{s^2 - u^2}, \\ A_1 &= \frac{s}{u^2 - s^2}, \quad A_2 = \frac{re^{-i\theta}}{u^2 - s^2}, \\ A_3 &= \frac{re^{i\theta}}{u^2 - s^2}, \quad A_4 = \frac{s}{u^2 - s^2}, \\ B_1 &= B_4 = -(u^2 - s^2)^2, \\ B_2 &= B_3 = s^2 - u^2. \end{aligned}$$

Based on these solutions, it can be easily verified that $\tilde{\Phi}^\dagger \tilde{\Psi} = S$, $\tilde{\Phi}^\dagger \tilde{H} \tilde{\Psi} = SJ$, such that

$$\langle \tilde{\phi}_i, e^{-it\tilde{H}} \tilde{\psi}_j \rangle \approx \tilde{\phi}_i^\dagger (I - it\tilde{H}) \tilde{\psi}_j = \psi_i^\dagger \eta (I - itH) \psi_j \approx \langle \psi_i, e^{-itH} \psi_j \rangle_\eta. \quad (S9)$$

Thus, under the η -inner product, the reduced system resembles a broken \mathcal{PT} -symmetric one. In order to illustrate the validity of our simulating paradigm, we introduce four parameters defined below:

$$Z_{11} = |\langle \tilde{\phi}_1, e^{-it\tilde{H}} \tilde{\psi}_1 \rangle|, \quad (\text{S10})$$

$$Z_{22} = |\langle \tilde{\phi}_2, e^{-it\tilde{H}} \tilde{\psi}_2 \rangle|, \quad (\text{S11})$$

$$Z_{12} = |\langle \tilde{\phi}_1, e^{-it\tilde{H}} \tilde{\psi}_2 \rangle - \langle \psi_1, e^{-itH} \psi_2 \rangle_\eta| |\langle \psi_1, e^{-itH} \psi_2 \rangle_\eta|^{-1}, \quad (\text{S12})$$

$$Z_{21} = |\langle \tilde{\phi}_2, e^{-it\tilde{H}} \tilde{\psi}_1 \rangle - \langle \psi_2, e^{-itH} \psi_1 \rangle_\eta| |\langle \psi_2, e^{-itH} \psi_1 \rangle_\eta|^{-1}. \quad (\text{S13})$$

The reason Z_{11} and Z_{22} have different forms from Z_{12} and Z_{21} is that $\langle \psi_1, e^{-itH} \psi_1 \rangle_\eta = \langle \psi_2, e^{-itH} \psi_2 \rangle_\eta = 0$, but $\langle \psi_1, e^{-itH} \psi_2 \rangle_\eta \neq 0$, $\langle \psi_2, e^{-itH} \psi_1 \rangle_\eta \neq 0$. With the definitions above, apparently, Z_{ij} reflects the difference between $\langle \tilde{\phi}_i, e^{-it\tilde{H}} \tilde{\psi}_j \rangle$ and $\langle \psi_i, e^{-itH} \psi_j \rangle_\eta$, as shown in FIG. S1.

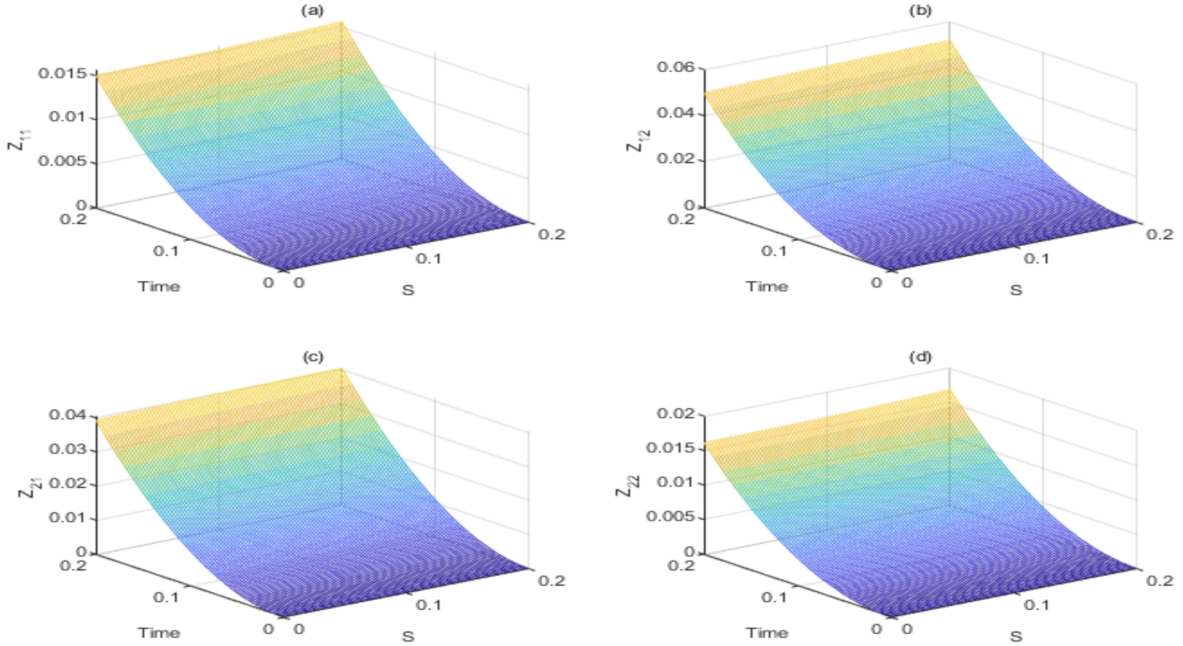


FIG. S1. Direct calculation on the parameters Z_{ij} . The corresponding values of Z_{ij} given in Eqs. (S10-S13) are shown in (a-d), respectively, for the range of $r = \sqrt{2}, \theta = \frac{\pi}{4}, t \in [0, 0.2], s \in [0, 0.2]$.

In the range of $r = \sqrt{2}, \theta = \frac{\pi}{4}, t \in [0, 0.2], s \in [0, 0.2]$, the differences between $\langle \tilde{\phi}_i, e^{-it\tilde{H}} \tilde{\psi}_i \rangle$ and $\langle \psi_i, e^{-itH} \psi_i \rangle_\eta$ are less than 2×10^{-2} ; while the relative differences between $\langle \tilde{\phi}_i, e^{-it\tilde{H}} \tilde{\psi}_j \rangle$ and $\langle \psi_i, e^{-itH} \psi_j \rangle_\eta$ are less than 6×10^{-2} .

In addition, when $t \rightarrow 0$, Z_{ij} and thus $\langle \tilde{\phi}_i, e^{-it\tilde{H}} \tilde{\psi}_j \rangle - \langle \psi_i, e^{-itH} \psi_j \rangle_\eta$, tend to zero. This means that Eq. (S9) is valid for a sufficiently small time interval t , which supports our theoretical conclusion. We want to emphasize that $e^{-it\tilde{H}}$ behaves like a broken \mathcal{PT} -symmetric evolution under the η -inner product, but not under the standard Dirac inner product. Hence in this case, the projection of $e^{-it\tilde{H}} \tilde{\psi}_i$ is not expected to be the same as that of $e^{-itH} \psi_i$.

Moreover, our theorem gives the same results for unbroken \mathcal{PT} -symmetry. When \mathcal{PT} -symmetry is unbroken, then $S = I$, $\eta = (\Psi^{-1})^\dagger \Psi^{-1} > 0$, J is diagonal, resulting in Eq. (9) being just a special case of our Theorem 1. Apparently, Eq. (9) implies that the projection of $e^{-it\tilde{H}} \tilde{\psi}_i$ is numerically equal to $e^{-itH} \psi_i$. Hence the embedding paradigms illustrated in Refs. [2–4] are also included in our method, although in those papers the η -inner product and measurements are not considered on purpose.

With the help of the analogy between Dirac inner product and η -inner product of unbroken \mathcal{PT} -symmetry, the example illustrated in Ref. [2] can be viewed as a proof for our paradigm in the unbroken \mathcal{PT} -symmetry. Explicitly, one can verify that Eq. (3) holds for the construction given below:

$$\begin{aligned}
H &= \begin{bmatrix} E_0 + is \sin \theta & s \\ s & E_0 - is \sin \theta \end{bmatrix}, \quad S = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad J = \begin{bmatrix} E_0 + s \cos \theta & 0 \\ 0 & E_0 - s \cos \theta \end{bmatrix}, \\
\tilde{H} &= \begin{bmatrix} E_0 & s \cos^2 \theta & is \cos \theta \sin \theta & 0 \\ s \cos^2 \theta & E_0 & 0 & -is \cos \theta \sin \theta \\ -is \cos \theta \sin \theta & 0 & E_0 & s \cos^2 \theta \\ 0 & is \cos \theta \sin \theta & s \cos^2 \theta & E_0 \end{bmatrix}, \\
\tilde{\Psi} = \tilde{\Phi} &= \begin{bmatrix} \frac{e^{\frac{i\theta}{2}}}{2} & \frac{ie^{-\frac{i\theta}{2}}}{2} \\ \frac{e^{-\frac{i\theta}{2}}}{2} & -\frac{ie^{\frac{i\theta}{2}}}{2} \\ \frac{e^{-\frac{i\theta}{2}}}{2} & \frac{ie^{\frac{i\theta}{2}}}{2} \\ \frac{e^{\frac{i\theta}{2}}}{2} & -\frac{ie^{-\frac{i\theta}{2}}}{2} \end{bmatrix}.
\end{aligned}$$

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