Efficient simulation of the dynamics of an *n*-dimensional $\mathcal{PT}$-symmetric system with a local-operations-and-classical-communication protocol based on an embedding scheme

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$\mathcal{PT}$-symmetric quantum theory has attracted extensive attention in recent years because of its novel properties, applications, and even controversial discussions. Many difficulties in applications stem from the unknown of how to simulate the dynamics of $\mathcal{PT}$-symmetric systems in conventional quantum systems. In this work, by clarifying some common confusion in the simulation of $\mathcal{PT}$-symmetric systems, we are able to naturally extend the application scope of the original embedding simulation scheme from pure states to arbitrary mixed states. Based on the above groundwork, we further propose a local-operations-and-classical-communication (LOCC) protocol scheme to simulate the dynamics of a $\mathcal{PT}$-symmetric system. Our LOCC protocol scheme, which needs one ancillary qubit only, can be applied to simulate any arbitrary finite-dimensional $\mathcal{PT}$-symmetric system in the $\mathcal{PT}$-unbroken phase and has several advantages over the original embedding scheme. The success probability is increased to $\lambda_{\min}$ ($\lambda_{\min} > 1$) times in general, even approaching 100% in some special cases, and has a concise bound that makes it easier to estimate the necessary experimental resources in advance. Furthermore, our LOCC protocol has less dependence on but more flexibility in the selection of the metric operator and more adaptability in practical applications, and it is more consistent with the physical intuition. Finally, the physical or philosophical meaning behind the embedding scheme and the LOCC protocol is discussed.

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I. INTRODUCTION

In conventional quantum mechanics (CQM), the requirement that physical observables, such as the Hamiltonians, should be Hermitian operators is considered one of the basic postulates. This postulate is consistent with our physical intuition that the eigenvalue spectrum and the measured value of observables are all real. However, this postulate has been questioned by more and more scholars in the past three decades [1–3]. In fact, there is no assumption that the eigenstates of an observable must form a set of complete orthogonal bases in quantum mechanics except that the spectrum of the observable is real [4–7], so the Hermitian system was extended to a quasi-Hermitian system by Scholtz *et al.*, who introduced a nontrivial metric operator in Hilbert space in 1992 [8] and in fact established quasi-Hermitian quantum mechanics (QQM). Then it was proved that QQM and CQM are equivalent and can be connected by the Dyson map [9,10]. Bender *et al.* found that some non-Hermitian Hamiltonians, which are parity-time-reversal ($\mathcal{PT}$)-symmetric, also have real eigenvalue spectrums, and then established $\mathcal{PT}$-symmetric quantum mechanics ($\mathcal{PT}$-QM) [11–14]. However, it was later recognized that $\mathcal{PT}$ symmetry is neither sufficient nor necessary for the real spectrum of the Hamiltonian [15–17], and in fact either the eigenvalues of the $\mathcal{PT}$-symmetric Hamiltonian are real ($\mathcal{PT}$-symmetry-unbroken case) or they appear as complex conjugate pairs ($\mathcal{PT}$-symmetry-broken case) [17–19]. The $\mathcal{PT}$-QM, QQM, and CQM can be proved to be equivalent in the $\mathcal{PT}$-symmetry-unbroken case [12,20–23]. Around 2002, Mostafazadeh pointed out that all the $\mathcal{PT}$-symmetric non-Hermitian Hamiltonians belong to the class of pseudo-Hermitian Hamiltonians and established pseudo-Hermitian quantum mechanics (PQM) [16,17,24–26], and then gave the necessary and sufficient condition for the reality of the spectrum of a non-Hermitian Hamiltonian with a complete set of biorthogonal eigenstates [17]. In addition, time-dependent pseudo-Hermitian theory was also developed [27]. In 2013, Brody established biorthogonal quantum mechanics (BQM) by replacing the notion of "complete orthogonal states" with "complete biorthogonal states" and gave a characterization of mixed states [7]. Biorthogonal quantum mechanics incorporates all the structures of $\mathcal{PT}$-symmetric quantum mechanics models and allows for generalizations, especially in situations where the $\mathcal{PT}$ construction of the dual space fails [6].

With the increasing interest in $\mathcal{PT}$-symmetric systems, many new properties and phenomena have been gradually discovered [23,28], such as the quantum brachistochrone

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problem [22,29–36] and the discrimination of nonorthogonal quantum states [37,38], and even some reports seem surprising because they seem to conflict with fundamental physical principles [39,40]. For example, Lee *et al.* found that local $\mathcal{PT}$ symmetry violates the no-signaling principle [40], which aroused widespread attention [35,41–43] and was then realized by Tang *et al.* in experiment [44]. However, some confusion and difficulties in applications appear to stem from not knowing how to simulate $\mathcal{PT}$-symmetric systems and their dynamic processes in conventional quantum systems. Huang *et al.* reinterpreted this phenomenon by simulating the $\mathcal{PT}$-symmetry-unbroken system with embedding technology based on the Naimark dilation theorem (Stinespring dilation theorem) [45–47], and proved that the phenomenon of violating the no-signaling principle stems from the fact that some probabilities are neglected in the process of simulation. In addition, some studies show that the $\mathcal{PT}$-symmetric Hamiltonian can also be regarded as part of an open system with dissipation [48,49], and the evolution of mixed states under an open system was also given [50,51]. Therefore, simulating PT-symmetric systems not only has very promising practical value, but also offers basic theoretical significance in understanding quantum mechanics [45,52–54].

The traditional method of linear combination of unitaries (LCU) can be used to simulate various non-Hermitian systems [55], such as $\mathcal{PT}$-symmetric systems in unbroken or broken phases [34,52,54,55], anti-$\mathcal{PT}$-symmetric systems [56], and others [57–59]. In general, at least one auxiliary qubit is necessary. Here we simulate the dynamic process of a $\mathcal{PT}$-symmetric system with the local-operations-and-classical-communication (LOCC) protocol based on an embedding scheme by using only one auxiliary qubit. The embedding scheme is a valuable approach to simulate the $\mathcal{PT}$-symmetry-unbroken system without manually adjusting the parameters related to the dynamic process [28,44,45,60,61], which is realized by dilating the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian to a higher-dimensional Hermitian one and then performing a fixed projection operation on the auxiliary qubit for postselection, and this method can also be realized by experiment [62]. However, the success probability of this scheme can still be improved because some resources in fact have been wasted, and the success probability is largely affected by the special selection of the metric operator. In this paper, we propose a LOCC protocol scheme based on an embedding scheme to efficiently simulate the $\mathcal{PT}$-symmetry-unbroken system, and we prove that our scheme increases the success probability of the embedding scheme to $\lambda_{\min}$ times that of the original scheme ($\lambda_{\min} > 1$, where $\lambda_{\min}$ is the minimum eigenvalue of the metric operator) and may even achieve a success probability supremum of up to 100%. Furthermore, our LOCC protocol depends less on the special selection of the metric operator and is more in line with the physical intuition. Finally, the physical or philosophical meaning behind the embedding scheme and the LOCC protocol is discussed.

The rest of this paper is organized as follows. In Sec. II, we review some basic concepts in $\mathcal{PT}$-symmetry theory. In Sec. III, we review the embedding theory and method, and extend it to an arbitrary mixed state in the QQM framework; then the success probability of the embedding scheme and its bound are also derived. Based on the groundwork we have done above, in Sec. IV we further propose our LOCC protocol scheme, and then give its success probability and a concise bound. We then further study the relation between the lower bound of the success probability and the degree of non-Hermiticity, and give a general lower bound that does not depend on the specific protocol, in Sec. V. After that, we demonstrate with an example of a two-dimensional $\mathcal{PT}$-symmetric system in Sec. VI. In Sec. VII, we give conclusions and discussions.

II. THEORETICAL PREPARATIONS

A. $\mathcal{PT}$-symmetry theory

Consider an n-dimensional discrete quantum system $\mathcal{H}$ and its Hamiltonian H, parity operator $\mathcal{P}$, and time-reversal operator $\mathcal{T}$ (their corresponding matrix representations can be recorded as P and T, respectively, and $P^2 = I$, $T\bar{T} = I$). If $\mathcal{PTH}=\mathcal{HPT}$ (equivalent to $PT\bar{H} = HPT$; in the following, the "operator" and "matrix" are common without causing confusion), then the system $H(\mathcal{H})$ is called $\mathcal{PT}$ symmetric. In particular, the Hamiltonian (system) H is called $\mathcal{PT}$-symmetry unbroken if and only if the H is similar to a real diagonal matrix. Otherwise, H is called $\mathcal{PT}$-symmetry broken if and only if it satisfies either of these two conditions [16,17,63]: (1) it cannot be diagonalized or (2) it has complex eigenvalues that come in complex conjugate pairs. We only consider the $\mathcal{PT}$-symmetry-unbroken situation in this paper.

First, we introduce the concept of an η inner product:

$$(|\psi_1\rangle, |\psi_2\rangle)_\eta \equiv \langle\psi_1 \mid \psi_2\rangle_\eta := \langle\psi_1|\eta|\psi_2\rangle,$$
$$\forall|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}, \tag{1}$$

where η is the metric operator; especially in the unbroken phase of $\mathcal{PT}$-QM, it can be a reversible positive Hermitian operator [17]. According to the above definition, the η-pseudo-Hermitian adjoint $O^\#$ of the operator O, which is different from the concept of a Hermitian adjoint, can be obtained through

$$(|\psi_1\rangle, O^\#|\psi_2\rangle)_\eta := \langle\psi_1|\eta \cdot O^\#|\psi_2\rangle = (O|\psi_1\rangle, \psi_2\rangle)_\eta$$
$$= \langle\psi_1|O^\dagger \cdot \eta|\psi_2\rangle. \tag{2}$$

Thus we can obtain the relation between $O^\#$ and $O^\dagger$:

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

In $\mathcal{PT}$-QM, the quantum observables are no longer Hermitian, but η-pseudo-Hermitian, i.e.,

$$O^\# = O \Rightarrow O^\dagger = \eta O \eta^{-1} \neq O. \tag{4}$$

The representation of the same quantum observable $\mathcal{O}$ under the two different theoretical frameworks of CQM and $\mathcal{PT}$-QM can be connected by the Dyson map [9,64]:

$$o = \eta^{\frac{1}{2}} O \eta^{-\frac{1}{2}}, \tag{5}$$

where O is the observable in the $\mathcal{PT}$-QM framework and o is the corresponding observable in CQM.

In the framework of $\mathcal{PT}$-QM (more generally, PQM), there are some operators satisfying

$$\eta H = H^\dagger \eta, \tag{6}$$

where η is called the metric operator of H and is the reversible Hermitian operator mentioned above. However, the metric operator is usually not unique; for instance, if η is a metric operator of H, so is $r\eta$ ($r \in \mathbb{R}$).

Then according to the Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{7}$$

for any two evolving states $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$, we have

$$i\frac{d}{dt}\langle\psi_1(t)|\psi_2(t)\rangle_\eta = \langle\psi_1(t)|(\eta H - H^\dagger\eta)|\psi_2(t)\rangle = 0, \tag{8}$$

which means that probability is conserved. Note that all the "$\hbar$'s" have been omitted in this paper.

B. Biorthogonal representation of arbitrary quantum states

The framework of CQM defined in a d-dimensional discrete Hilbert space is based on the orthogonal basis $\{|n,a\rangle\}$ that can usually be composed of the eigenstates of the Hamiltonian, while the framework of $\mathcal{PT}$-QM is based on the biorthogonal basis, and we record the complete biorthogonal basis of H as $\{|\chi_n,a\rangle, |\phi_n,a\rangle\}$. Then, according to the definition,

$$\langle\chi_m,a|\phi_n,b\rangle = \delta_{mn}\delta_{ab}, \tag{9a}$$

$$H|\phi_n,a\rangle = E_n|\phi_n,a\rangle, \quad H^\dagger|\chi_n,a\rangle = E_n|\chi_n,a\rangle, \tag{9b}$$

$$\sum_n\sum_{a=1}^{d_n}|\chi_n,a\rangle\langle\phi_n,a| = \sum_n\sum_{a=1}^{d_n}|\phi_n,a\rangle\langle\chi_n,a| = I, \tag{9c}$$

where d_n is the degree of degeneracy of the eigenvalue E_n, and a and b are degeneracy labels. Then according to Eq. (9) we have

$$H = \sum_n\sum_{a=1}^{d_n}E_n|\chi_n,a\rangle\langle\phi_n,a|. \tag{10}$$

We set the constraint

$$|\langle\phi_n,a|\phi_n,a\rangle|^2 = 1. \tag{11}$$

Then we can define a standard metric operator η_s and its inverse η_s^{-1}:

$$\eta_s = \sum_n\sum_{a=1}^{d_n}|\chi_n,a\rangle\langle\chi_n,a|, \tag{12}$$

$$\eta_s^{-1} = \sum_n\sum_{a=1}^{d_n}|\phi_n,a\rangle\langle\phi_n,a|. \tag{13}$$

Then we know $|\chi_n,a\rangle = \eta_s|\phi_n,a\rangle$. (For mathematics alone, Eq. (6) belongs to the Sylvester-type equation "$AX + XB = C$" [65], so the metric operator η can also be obtained directly according to the standard solution of the Sylvester equation.) For convenience, we assume the degeneracy $d_n = 1$ in the following paper.

In some of the literature, it is often recorded that $\Phi = [|\phi_1\rangle,\dots,|\phi_i\rangle,\dots,|\phi_n\rangle]$, $\Xi = [|\chi_1\rangle,\dots,|\chi_i\rangle,\dots,|\chi_n\rangle]$, and $E = \mathrm{diag}(E_1,\dots,E_i,\dots,E_n)$; then

$$\begin{aligned}\Phi^{-1}H\Phi = E, &\quad \Xi^{-1}H^\dagger\Xi = E,\\ \eta = \Xi\Xi^\dagger, &\quad \eta^{-1} = \Phi\Phi^\dagger,\\ \Xi = \eta\Phi, &\quad \Xi^\dagger\Phi = I_n.\end{aligned} \tag{14}$$

For an arbitrary pure state ψ, the associated state $\tilde{\psi}$ can be defined [7]:

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle \Leftrightarrow \langle\tilde{\psi}| = \sum_n c_n^*\langle\chi_n| \Rightarrow |\tilde{\psi}\rangle = \sum_n c_n|\chi_n\rangle. \tag{15}$$

The pure state ψ can be expressed separately in CQM (left) and $\mathcal{PT}$-QM (right) frameworks as follows, and they are equivalent in a physical sense in their respective theoretical systems:

$$\begin{aligned}|\psi\rangle = \sum_n c_n|n\rangle &\Leftrightarrow |\psi\rangle_{\mathcal{PT}} = \sum_n c_n|\phi_n\rangle,\\ \langle\psi| = \sum_n c_n^*\langle n| &\Leftrightarrow {}_{\mathcal{PT}}\langle\psi| = \sum_n c_n^*\langle\chi_n|,\end{aligned} \tag{16}$$

where $\sum_n |c_n|^2 = 1$.

The projection operator is

$$\pi_n = |n\rangle\langle n| \Leftrightarrow \pi_{\mathcal{PT}n} = |\phi_n\rangle\langle\chi_n|. \tag{17}$$

It is obvious that $\pi_m\pi_n = \delta_{mn}$ in both frameworks. Then we can obtain the biorthogonal representation of arbitrary quantum mixed states,

$$\rho_c = \sum_{mn}\rho_{cmn}|m\rangle\langle n| \Leftrightarrow \rho_{\mathcal{PT}} = \sum_{mn}\rho_{cmn}|\phi_m\rangle\langle\chi_n|, \tag{18}$$

where the left- and the right-hand sides of the symbol "$\Leftrightarrow$" are connected by a similarity transformation, i.e., the Dyson map mentioned above in Eq. (5), so the spectrum of the density operator remains unchanged, and they have the same physical meaning. It is worth nothing that in the framework of CQM, all the density operators are Hermitian (ρ_c), while in the framework of $\mathcal{PT}$-QM, in general, the density operators are all non-Hermitian ($\rho_{\mathcal{PT}}$), and the Hermitian property of the density operator is indeed an important distinctive external feature that distinguishes CQM from $\mathcal{PT}$-QM. Then according to Eq. (18) we know $\mathrm{Tr}(\rho_{\mathcal{PT}}) = \mathrm{Tr}(\rho_c) \equiv 1$.

Therefore, for the purpose of simulation with the embedding scheme [32,50], we can take

$$\begin{aligned}\rho_S &= \rho_{PT}\cdot\eta^{-1}\\ &= \sum_{mn}\rho_{cmn}|\phi_m\rangle\langle\phi_n|,\end{aligned} \tag{19}$$

which can be normalized by $\mathrm{Tr}(\eta\rho_S) = 1$, and it is worth noting that although $\mathrm{Tr}(\rho_S) < \mathrm{Tr}(\eta\rho_S) \equiv 1$, it is still reasonable, because it is actually an unnormalized density operator (see Appendix B). It is worth noting that, for the purpose of simulation, it is not necessary to pursue the complete equivalence in physical meaning between the simulated $\mathcal{PT}$-symmetric system and the system performing the simulation program in CQM, but only the suitability of its mathematical form and the physical realizability; however, we still need to remind that the two are actually different in the physical sense. Unfortunately, the existing literature rarely discusses this problem or is very vague about it [34,38,44–46,52,54,61], and only discusses the pure-states case. We have explained this problem clearly by combing the developmental history of quantum mechanics in our Introduction and the above analysis, which lays the foundation for us to naturally extend the embedding scheme to the mixed-states case in the following.

III. SIMULATION SCHEME OF THE DYNAMICS OF A $\mathcal{PT}$-SYMMETRIC SYSTEM WITH AN EMBEDDING SCHEME IN ARBITRARY MIXED STATES

A. The Hermitian dilation principle of a $\mathcal{PT}$-symmetric system

In 2008, Guenther *et al.* proposed the original simulation scheme of a $\mathcal{PT}$-symmetric system by using a Naimark dilation technique in a two-dimensional Hilbert space [28,32]. This scheme is valuable for understanding the relation between a $\mathcal{PT}$-symmetric system and a Hermitian system in conventional quantum mechanics; specifically, the former can be regarded as a subsystem of a higher-dimensional Hermitian system. At the same time, this scheme also gives an idea of simulating the dynamics of a $\mathcal{PT}$-symmetric system. However, this original scheme is based on the special property in a two-dimensional system where $\eta + \eta^{-1} = tI (t \in \mathbb{R})$, whereas this property does not hold in higher-dimensional systems. In 2018, Huang *et al.* extended this simulation scheme to an n-dimensional system and provided mathematical completeness [45]. However, the success probability of these schemes is usually not high enough because of a waste of resources in actual use. Besides, these schemes are only limited to pure states, while mixed states are not discussed; in fact, the simulation of mixed states in a $\mathcal{PT}$-symmetric system is not so obvious. Based on the above, we propose an efficient simulation scheme of the dynamics of a $\mathcal{PT}$-symmetric system with a LOCC protocol scheme based on the embedding scheme.

We assume H_S is a $\mathcal{PT}$-symmetric operator in an n-dimensional Hilbert space $L(\mathcal{H}^n)$, and $\hat{H}_{AS}$ is a Hermitian operator in $L(\mathcal{H}^m)$ $(m > n)$. $\rho_{AS} = \left(\begin{smallmatrix} \rho_S & \rho_2 \\ \rho_3 & \rho_4 \end{smallmatrix}\right)$ is the density operator of a quantum state, where $\rho_{AS} \in L(\mathcal{H}^m)$, $\rho_S \in L(\mathcal{H}^n)$, and $\rho_4 \in L(\mathcal{H}^{(m-n)})$. There is a map $\mathcal{M}$: $L(\mathcal{H}^m) \to L(\mathcal{H}^n)$ (the symbols S, A, and AS can be understood as the main system used to simulate the $\mathcal{PT}$-symmetric system, the auxiliary system, and the composite system, respectively). In addition, for the convenience of expression, we define the "$\circ$" operation like $B \circ \cdot \equiv B \cdot B^\dagger$, so we know $(B \cdot C) \circ \rho = (BC) \cdot \rho \cdot (C^\dagger B^\dagger) = B \circ C \circ \rho$, where ρ can represent any operator.

Next, for the convenience of narration and understanding, we first introduce the concept of embedding, and then elaborate on its constructions in the next section. In Appendix A, we also give more details about it.

Note that

$$\begin{aligned}\mathbb{K}_{\hat{H}_{AS}} = \{&\rho_{AS} | \rho_{AS} \in L(\mathcal{H}^m), \mathcal{M}[\hat{H}_{AS} \circ \rho_{AS}] \\ &= H_S \circ \mathcal{M}[\rho_{AS}], \mathcal{M}[U_{AS} \circ \rho_{AS}] = \mathcal{U}_S \circ \mathcal{M}[\rho_{AS}]\},\end{aligned} \tag{20}$$

where $U_{AS} = e^{-it\hat{H}_{AS}}$ and $\mathcal{U}_S = e^{-itH_S}$. If $\mathcal{M}[\mathbb{K}_{\hat{H}_{AS}}] = L(\mathcal{H}^n)$, then it is said that the operator H has the embedding property, or the operator H can be embedded into $\hat{H}$, or $\hat{H}$ is an expansion operator of H [45,46].

B. Simulating the dynamics of a $\mathcal{PT}$-symmetric system with an embedding scheme

1. The embedding scheme in arbitrary mixed states

The essence of the simulation of the dynamics of a $\mathcal{PT}$-symmetric system is to find a system in the CQM framework to simulate the evolution and properties of a known $\mathcal{PT}$-symmetric system. If the non-Hermitian $\mathcal{PT}$-symmetric H is known, according to Eq. (20), we can find the corresponding Hermitian Hamiltonian $\hat{H}_{AS}$. We assume that the composite system ρ_{AS} consists of the auxiliary system A and the main system S used to simulate the $\mathcal{PT}$-symmetric system. We define the measurement operator, $\Pi_k = |k\rangle_A\langle k| \otimes I_S$, $k \in \{0, 1\}$, and the map $\mathcal{M}_k$ is defined as $\mathcal{M}_k[\rho_{AS}] = \mathrm{Tr}_A[\Pi_k \circ \rho_{AS}]$; then after the measurement, the state of the composite system will be $\Pi_k \circ \rho_{AS}$ (unnormalized), and the state of the main system will be $M_k[\rho_{AS}]$ (unnormalized). At the same time, we assume the Hermitian Hamiltonian of the composite system is

$$\hat{H}_{AS} = \begin{pmatrix} H_1 & H_2 \\ H_2^\dagger & H_4 \end{pmatrix}, \tag{21}$$

where H_1 and H_4 are both Hermitian, and assume

$$\begin{aligned}\rho_{AS} &= (|0\rangle_A \otimes I_S + |1\rangle_A \otimes \xi)\rho_S({}_A\langle 0| \otimes I_S + {}_A\langle 1| \otimes \xi) \\ &= \begin{pmatrix} \rho_S & \rho_S\xi \\ \xi\rho_S & \xi\rho_S\xi \end{pmatrix},\end{aligned} \tag{22}$$

where ξ is a Hermitian operator corresponding to η, and we can check that $\rho_{AS}^\dagger = \rho_{AS}$. The ρ_S is an arbitrary state and can be expressed as $\rho_S = \sum_{mn} \rho_{cmn} |\phi_m\rangle\langle\phi_n|$, where $\sum_n \rho_{cnn} = 1$ and $\{|\phi_n\rangle\}$ are the eigenstates of $\mathcal{PT}$-symmetric H_S and are not usually orthogonal. The ρ_S is not normalized and can be normalized by $\mathrm{Tr}(\eta\rho_S) \equiv 1$ according to the $\mathcal{PT}$-symmetric inner product or $\mathrm{Tr}\rho_{AS} = 1$. It is worth stressing that the choices of metric operators are not unique; in fact, any metric operator that meets this condition $\eta > 1$ is legal. We have to mention that, in practical application, considering the balance of noise robustness between the main system S and auxiliary system A in practice, we usually do not choose η too large or too small; otherwise, for example, when we choose $\eta \to I_S$, then $\xi \to 0$, and the original entanglement state will become almost separable, $\rho_{AS} = |0\rangle_A\langle 0| \otimes \rho_S$, which means decoherence may easily occur.

According to Eq. (20), we obtain that

$$\mathcal{M}_0[\hat{H}_{AS} \circ \rho_{AS}] = H_S \circ \mathcal{M}_0[\rho_{AS}] = H_S \circ \rho_S, \tag{23a}$$

$$\mathcal{M}_0[e^{-it\hat{H}_{AS}} \circ \rho_{AS}] = e^{-itH_{AS}} \circ \mathcal{M}_0[\rho_{AS}] = e^{-itH_S} \circ \rho_S. \tag{23b}$$

Then, substituting each quantity into Eq. (23a), we get

$$\begin{aligned}\mathcal{M}_0\Bigg[&\begin{pmatrix} H_1 & H_2 \\ H_2^\dagger & H_4 \end{pmatrix} \circ [(|0\rangle_A \otimes I_S + |1\rangle_A \otimes \xi) \\ &\cdot \rho_S \cdot ({}_A\langle 0| \otimes I_S + {}_A\langle 1| \otimes \xi)]\Bigg] \\ = \mathcal{M}_0&\left[\begin{pmatrix} H_1 & H_2 \\ H_2^\dagger & H_4 \end{pmatrix} \cdot \begin{pmatrix} I_S \\ \xi \end{pmatrix} \circ \rho_S\right]\end{aligned}$$

$$= \mathcal{M}_0\left[\begin{pmatrix} H_1(t) + H_2(t)\xi \\ H_2^\dagger(t) + H_4(t)\xi \end{pmatrix} \circ \rho_S\right]$$
$$= H_S \circ \rho_S. \tag{24}$$

Then according to Eq. (23a), and according to Eqs. (18), (19), and (9), we can infer that

$$\mathrm{Tr}(\rho_{AS}) = \mathrm{Tr}[\rho_S(\xi^2 + I_S)] = \mathrm{Tr}[\rho_S\eta] = \mathrm{Tr}[\rho_{\mathcal{PT}}] = \mathrm{Tr}[\rho_c] \equiv 1, \tag{25a}$$
$$H_1 + H_2\xi = H_S, \tag{25b}$$
$$H_2^\dagger + H_4\xi = \xi H_S. \tag{25c}$$

Since the standard metric operator $\eta_s > 0$, we can always find a constant β that makes $\eta = \beta\eta_s > 1$. According to the above equations, and we know ξ is Hermitian, we can obtain

$$\xi^\dagger\xi + I_S = \eta \Rightarrow \xi = (\eta - I_S)^{\frac{1}{2}}, \tag{26a}$$
$$H_2 = (H_S - H_1)\xi^{-1}, \tag{26b}$$
$$H_4 = (\xi H_S - H_2^\dagger)\xi^{-1}. \tag{26c}$$

By observing the above equations, we know that H_1 is the only free Hermitian variable, and we may further determine it by adding more constraints.

Similar to the above, we can also assume that

$$\rho_{AS}^\perp = (-|0\rangle_A \otimes \xi + |1\rangle_A \otimes I_S) \cdot \rho_S \cdot (-{}_A\langle 0| \otimes \xi + {}_A\langle 1| \otimes I_S) = \begin{pmatrix} \xi\rho_S\xi & -\xi\rho_S \\ -\rho_S\xi & \rho_S \end{pmatrix}, \tag{27}$$

where $\rho_{AS}^\perp$ is defined in the orthogonal space with ρ_{AS}, and then we can infer that

$$\mathrm{Tr}(\rho_{\mathrm{AS}}^\perp) = (\mathrm{Tr})[(\xi^\dagger\xi + \mathrm{I_S})\rho_S] \equiv 1, \tag{28a}$$
$$-H_1\xi + H_2 = -\xi H_S, \tag{28b}$$
$$-H_2^\dagger\xi + H_4 = H_S. \tag{28c}$$

Then according to Eqs. (26) and (28) we can infer that

$$\xi = (\eta - I_S)^{\frac{1}{2}}, \tag{29a}$$
$$H_1 = H_S\eta^{-1} + \xi H_S\eta^{-1}\xi = \Phi E_S\Phi^\dagger + \xi \cdot \Phi E_S\Phi^\dagger \cdot \xi, \tag{29b}$$
$$H_2 = H_S\eta^{-1}\xi - \xi H_S\eta^{-1} = \Phi E_S\Phi^\dagger \cdot \xi - \xi \cdot \Phi E_S\Phi^\dagger = -H_2^\dagger, \tag{29c}$$
$$H_4 = H_S\eta^{-1} + \xi H_S\eta^{-1}\xi = \xi^{-1}(H_S\eta^{-1} + \eta H_S - H_S - H_S^\dagger)\xi^{-1} + H_S\eta^{-1} = H_1, \tag{29d}$$

where ξ, ηH_S, and $H_S\eta^{-1}$ are all Hermitian, so it is easy to verify that H_1 and H_4 are Hermitian, and H_2 is anti-Hermitian.

Therefore, we obtain the unique Hermitian dilation of H_S, i.e.,

$$\hat{H}_{AS} = I_A \otimes H_1 + i\sigma_y \otimes H_2 = I_A \otimes (H_S\eta^{-1} + \xi H_S\eta^{-1}\xi) + i\sigma_y \otimes (H_S\eta^{-1}\xi - \xi H_S\eta^{-1}) = V \circ [I_A \otimes E_S], \tag{30}$$

where

$$V = \frac{1}{\sqrt{2}}[(I_A + i\sigma_x) \otimes I_S - i(\sigma_y + \sigma_z) \otimes \xi] \cdot I_A \otimes \Phi = \frac{1}{\sqrt{2}}\begin{pmatrix} \Phi_+ & i\Phi_- \\ i\Phi_+ & \Phi_- \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} (I_S - i\xi)\Phi & i(I_S + i\xi)\Phi \\ i(I_S - i\xi)\Phi & (I_S + i\xi)\Phi \end{pmatrix}. \tag{31}$$

Noting that V is unitary but not unique, and we record $\Phi_+ = (I_S - i\xi)\Phi$ and $\Phi_- = (I_S + i\xi)\Phi$ here. Obviously, they are all unitary operators; then $H_1 + iH_2 = (I_S - i\xi)\Phi \circ E_S = \Phi_+ \circ E_S$, $H_1 - iH_2 = (I_S + i\xi)\Phi \circ E_S = \Phi_- \circ E_S$, and they are all Hermitian, $(I_S \pm i\xi) \cdot (I_S \pm i\xi)^\dagger = \eta$. By observing Eq. (30), we know this embedding scheme only needs one auxiliary qubit, and the dilated system $\hat{H}_{AS}$ actually doubles the degeneracy of the original system H_S. It is worth noting that the dilated method given in Ref. [32] is only the special case of two-dimensional and pure states, so it is not universal.

If we set $\rho_S = \rho_S(0)$, $\rho_{AS} = \rho_{AS}(0)$, then, according to the above analysis and Eq. (23b), we can get

$$\rho_{AS}(t) = U_{AS}(t) \circ \rho_{AS}(0) = e^{-it\hat{H}_{AS}} \cdot \rho_{AS}(0) \cdot e^{it\hat{H}_{AS}} \Rightarrow \rho_S(t) = \mathcal{U}_S(t) \circ \rho_S(0) = e^{-itH_S} \cdot \rho_S(0) \cdot e^{itH_S^\dagger}. \tag{32}$$

Therefore, the embedding scheme is completed (see Appendix A for details). It is worth emphasizing that $\rho_{AS}(t)$ is still the legal density operator, i.e., the positive-semidefinite (i.e., Hermitian) operator with unit trace (see Appendix B for the proof).

Reviewing the above whole embedding process, we know the low-dimensional non-Hermitian $\mathcal{PT}$-symmetry-unbroken system H_S dominated by the $\mathcal{PT}$-QM can be understood as being a result of the fixed postselection ($\prod_0$) of a higher-dimensional Hermitian system $\hat{H}_{AS}$ dominated by the CQM. After the fixed postselection, the system will evolve in the way required by $\mathcal{PT}$-QM in the remaining Hilbert subspace.

2. *The success probability of the embedding scheme*

The success probability is the key problem in the simulation of the dynamics of a $\mathcal{PT}$-symmetric system, which largely determines the applicability of the scheme; however, there are few discussions about it [23], so we discuss this particular problem in this section.

According to Eq. (32), the state $\rho_S(t)$ can be calculated as

$$\rho_S(t) = e^{-itH_S}\rho_S e^{itH_S^\dagger} = \eta^{-\frac{1}{2}}e^{-ith}\eta^{\frac{1}{2}} \cdot \rho_S \cdot \eta^{\frac{1}{2}}e^{ith}\eta^{-\frac{1}{2}} = \eta^{-\frac{1}{2}}e^{-ith} \cdot \Omega_S \cdot e^{ith}\eta^{-\frac{1}{2}} = \eta^{-\frac{1}{2}}\Omega_S(t)\eta^{-\frac{1}{2}}, \tag{33}$$

where

$$\begin{aligned}\Omega_S &= \eta^{\frac{1}{2}} \cdot \rho_S \cdot \eta^{\frac{1}{2}} \\ &= \sum_{mn} \rho_{S_{mn}} |\psi_m\rangle\langle\psi_n|.\end{aligned} \tag{34}$$

Here Ω_S is the density operator in the CQM framework, which is in fact the density operator $\rho_{\mathcal{PT}}$ in Eq. (18), and $\{|\psi_n\rangle = \eta^{1/2}|\phi_n\rangle\}$ constitutes a set of complete orthogonal eigenstates, while $\{|\phi_n\rangle, |\chi_n\rangle\}$ is the complete biorthogonal eigenstates of H_S. And then

$$\Omega_S(t) = e^{-iht} \cdot \Omega_S \cdot e^{iht}, \tag{35}$$

where

$$h = \eta^{\frac{1}{2}} \cdot H_S \cdot \eta^{-\frac{1}{2}} = W \cdot E_S \cdot W^\dagger \tag{36}$$

is the Hermitian Hamiltonian in the CQM framework corresponding to the non-Hermitian Hamiltonian H_S in $\mathcal{PT}$-QM, E_S is the diagonal matrix consisting of the eigenvalues of h, which has the same eigenvalues as H_S, and W is the unitary matrix in the spectral decomposition and not unique, and can be taken as $W = \eta^{\frac{1}{2}} \cdot \Phi$. The physical meanings of h and H_S are in fact similar with the corresponding operators in Eq. (5). We will see later that writing the density operator and the Hamiltonian with the CQM framework will provide us some mathematical intuition. After that, we know

$$\mathrm{Tr}(\eta\rho_S(t)) = \mathrm{Tr}(\Omega_S(t)) = \mathrm{Tr}(\Omega_S) = \mathrm{Tr}(\eta\rho_S) = 1. \tag{37}$$

At the same time, we can obtain the success probability of projection measurement Π_0 at time t:

$$\begin{aligned}P_0(t) &= \mathrm{Tr}(\rho_S(t)) \\ &= \mathrm{Tr}(\eta^{-1}\Omega_S(t)) \\ &= \mathrm{Tr}(\eta^{-1} \cdot We^{-iE_St} \cdot W^\dagger\Omega_S W \cdot e^{iE_St}W^\dagger).\end{aligned} \tag{38}$$

The physical meaning of P_0 is the success probability of simulating $\mathcal{PT}$-symmetric systems with the embedding method, so, in general, P_0 is not unitary except for some special cases (such as some special time for special states, which can be seen in the Fig. 3 in the examples given in Sec. VI).

However, according to Eq. (36), we can obtain that

$$\begin{aligned}[\eta^{-1}, h] &= \eta^{-1} \cdot \eta^{1/2}H_S\eta^{-1/2} - \eta^{1/2}H_S\eta^{-1/2} \cdot \eta^{-1} \\ &= \eta^{-1/2}(H_S - H_S^\dagger)\eta^{-1/2} \\ &\neq 0,\end{aligned} \tag{39}$$

i.e., η^{-1} does not commute with h, so they do not have a set of identical complete eigenstates, and thus the state $\Omega(t)$ will not always remain in the eigenstates of η^{-1}, which means the success probability $P_0(t)$ will not be constant. Besides, by observing Eq. (38), we know that $P_0(t)$ will oscillate periodically. Therefore, it will be very necessary and meaningful to estimate the upper and lower bounds of the success probability of the simulation scheme when considering practical applications in experiments, so the amount of resources needed can be estimated in advance when designing the experiment.

Assume that $\{\lambda_n\}$ is the spectrum of the metric operator η, according to our discussions above Eq. (26), and $\eta > 1$, so all $\lambda_n > 1$, and we record the maximum and minimum as $\lambda_{\max}$ and $\lambda_{\min}$, respectively. Then according to Eq. (38), the bound of the success probability can be obtained directly:

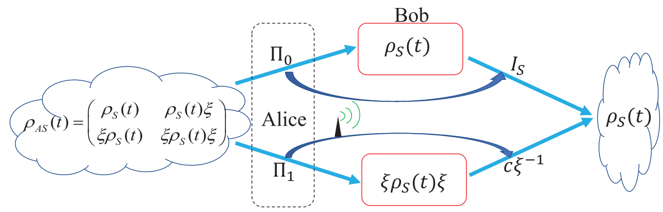

FIG. 1. The scheme of simulating the dynamics of a $\mathcal{PT}$-symmetric system with a LOCC protocol based on an embedding scheme.

$$\frac{1}{\lambda_{\max}} \leqslant P_0(t) = \mathrm{Tr}(\rho_S(t)) \leqslant \frac{1}{\lambda_{\min}}, \tag{40}$$

where the equal sign holds when the $\Omega_S(t)$ in Eq. (38) happens to be the eigenstate of η^{-1} corresponding to the minimum (maximum) eigenvalue at time t. It is particularly worth noting that $1/\lambda_{\max}$ and $1/\lambda_{\min}$ are the infimum and supremum of this embedding scheme, respectively, which do not depend on any state and time but only depend on the selection of the metric operator η [it will be seen more clearly in the example given in Eq. (64)], and it means that the success probability of this scheme is bounded by the system itself, and the η has to be carefully designed in order to achieve a good balance between the success probability of the simulation and experimental convenience. At the same time, we know that when the non-Hermitian degree is very small, especially when it is small to zero, the system H_S will be Hermitian ($H_S = H_S^\dagger$) and η can be I. Then $\lambda_{\max} = \lambda_{\min} = 1$, the success probability will reach 100% exactly and be always 100%, which can also be verified by the discussions surrounding Eq. (39), and then $\xi = 0$, $\rho_{AS}(t) = |0\rangle_A\langle 0| \otimes \rho_S(t)$, all of which completely meet our physical intuition.

IV. SIMULATING THE DYNAMICS OF A $\mathcal{PT}$-SYMMETRIC SYSTEM WITH A LOCC PROTOCOL BASED ON AN EMBEDDING SCHEME

A. The LOCC protocol based on an embedding scheme

However, reviewing the whole embedding scheme process, we find that some resources are wasted because the part $\xi\rho_S\xi$ in ρ_{AS} in Eq. (22) is thrown away in application, which will inevitably lead to a low success probability of the simulation scheme. In the following, we extract ρ_S from $\xi\rho_S\xi$ with a LOCC protocol. The LOCC protocol can be implemented in three steps as follows (see Fig. 1):

(1) Prepare the initial state $\rho_{AS}(0) = \begin{pmatrix} \rho_S(0) & \rho_S(0)\xi \\ \xi\rho_S(0) & \xi\rho_S(0)\xi \end{pmatrix}$; Alice possesses the auxiliary system (a single qubit), and Bob possesses the simulated system.

(2) Evolve the state $\rho_{AS}(0)$ under the dilated Hermitian Hamiltonian $\hat{H}_{AS}$ for period t, and then $\rho_{AS}(t) = \begin{pmatrix} \rho_S(t) & \rho_S(t)\xi \\ \xi\rho_S(t) & \xi\rho_S(t)\xi \end{pmatrix}$ is obtained.

(3) Alice performs a two-outcome measurement described by measurement operators $\{\Pi_0, \Pi_1\}$ on her qubit (recalling that $\Pi_0 = |0\rangle_A\langle 0| \otimes I_S$, $\Pi_1 = |1\rangle_A\langle 1| \otimes I_S$) corresponding to the results "0" and "1", respectively. After the measurement,

(i) if Alice gets the result "0", the state in Bob's system will become $\rho_S(t)$; then she instructs Bob to do nothing.
(ii) else if Alice gets the result "1", the state in Bob's system will become $\xi\rho_S(t)\xi$; then she instructs Bob to make a recovery operation,

$$R = c\xi^{-1} \quad (0 \leqslant c\xi^{-1} \leqslant 1), \tag{41}$$

to restore it to the state $\rho_S(t)$.

B. The success probability of the LOCC protocol scheme

We now discuss the success probability of the LOCC protocol. In the third step of our LOCC protocol scheme, according to Eq. (38), we have known that the success probability of the projection (postselection) Π_0 is $P_0(t) = \mathrm{Tr}(\rho_S(\mathrm{t}))$. We next calculate the success probability of the projection Π_1:

$$\begin{aligned} P_1(t) &= \mathrm{Tr}(\xi\rho_S(t)\xi) \\ &= \mathrm{Tr}[(\eta - I_S)\cdot\rho_S(t)] \\ &= 1 - \mathrm{Tr}(\rho_S(t)) \\ &= 1 - P_0(t). \end{aligned} \tag{42}$$

Here $P_1(t) = 1 - P_0(t)$ can also be given directly because $\{\Pi_0, \Pi_1\}$ constitutes a set of complete measurement. When Alice gets the result "1", she can make an operation $c\xi^{-1}$ to restore the state $\rho_S(t)$. As we know from Eq. (26a) $\xi = (\eta - I_S)^{\frac{1}{2}}$, so the spectrum of the ξ^{-1} will be $\{1/\sqrt{\lambda_n - 1}\}$. According to the condition of quantum operations, $c^2\xi^{-1\dagger}\xi^{-1} \leqslant 1$, we obtain that $c \leqslant \sqrt{\lambda_{\min} - 1}$, so we can take $c = \sqrt{\lambda_{\min} - 1}$ to maximize the success probability. Therefore, the total success probability of our LOCC protocol becomes

$$\begin{aligned} P_{\mathrm{LOCC}}(t) &= \mathrm{Tr}(\rho_S(t)) + \mathrm{Tr}(c\xi^{-1}\cdot\xi\rho_S(t)\xi\cdot\xi^{-1}c) \\ &= (c^2+1)\mathrm{Tr}(\rho_S(t)) = \lambda_{\min}P_0(t). \end{aligned} \tag{43}$$

The physical meaning of P_{LOCC} is the success probability of simulating $\mathcal{PT}$-symmetric systems with the LOCC protocol, so, in general, P_{LOCC} is not unitary except for some special cases (such as some special time for special states, which can be seen in Fig. 5 in the examples given in Sec. VI).

Then we can obtain the bound of the success probability of our LOCC protocol:

$$\frac{\lambda_{\min}}{\lambda_{\max}} \leqslant P_{\mathrm{LOCC}}(t) \leqslant \frac{\lambda_{\min}}{\lambda_{\min}} = 1. \tag{44}$$

Here $\lambda_{\min}/\lambda_{\max}$ and 1 are the infimum and supremum of the success probability of our LOCC protocol, respectively. Note that neither $\lambda_{\min}/\lambda_{\max}$ nor 1 depends on the selection of the metric operator η, but only on the ratio of the minimum eigenvalue $\lambda_{\min}$ to the maximum eigenvalue $\lambda_{\max}$ of η, which means that this LOCC protocol scheme has more flexibility in the selection of the metric operators η and more adaptability in practical applications than the embedding scheme.

Comparing Eq. (40) with Eq. (44), we can find the fact that this LOCC protocol increases the success probability of the original embedding scheme to $\lambda_{\min}$ ($\lambda_{\min} > 1$) times, and it is worth emphasizing that the infimum of success probability of the original embedding scheme is only $1/\lambda_{\max}$, while it is $\lambda_{\min}/\lambda_{\max}$ in our LOCC protocol; the supremum of success probability of the original embedding method is only $1/\lambda_{\min}$ (it cannot reach 100%, in any case), while it is 100% in our LOCC protocol. This is one of the important proofs of the advantage of our scheme, and can be seen more clearly in the example given in Eq. (67). When the Hamiltonian H_S is Hermitian, the two schemes will be equal because $\eta = I_S, \xi = 0$, and the density operator will be a separable state $\rho_{AS}(t) = |0\rangle_A\langle 0| \otimes \rho_S(t)$. Another advantage of this LOCC protocol is that it does not depend on the special state or time, and the recovery operation $c\xi^{-1}$ is time independent; therefore, this protocol can be conveniently applied in practice.

V. FURTHER STUDY: THE RELATION BETWEEN THE LOWER BOUND OF the SUCCESS PROBABILITY AND THE DEGREE OF NON-HERMITICITY

As we all know, any non-Hermitian operator $H(\vec{\alpha})$ can be decomposed into

$$H(\vec{\alpha}) = H_r(\vec{\alpha}) + iH_i(\vec{\alpha}), \tag{45}$$

where $\vec{\alpha} = (\alpha_1, \alpha_2, \ldots)$ represents the set of parameters (the metric operator can be written as $\eta(\vec{\alpha})$; for convenience, it will be omitted later), $H_r = (H + H^\dagger)/2$ and $H_i = (H - H^\dagger)/2i$ are both Hermitian, and H_r and iH_i represent the Hermitian and non-Hermitian (anti-Hermitian) parts, respectively. We define a quantity d_{nh} to characterize the degree of non-Hermiticity (or anti-Hermitian) as follows:

$$d_{nh} \equiv \frac{\|H_i\|_F}{\|H\|_F} \equiv \frac{\|H - H^\dagger\|_F}{2\|H\|_F} \leqslant \frac{\|H\|_F + \|H^\dagger\|_F}{2\|H\|_F} = 1, \tag{46}$$

where the subscript "F" indicates the Frobenius norm, so we know $d_{nh} \in [0, 1]$; when H is completely Hermitian, $d_{nd} = 0$, and when H is completely anti-Hermitian, $d_{nd} = 1$.

After that, using the matrix vectorization skills mentioned in the Appendix of Ref. [49], i.e., $\overrightarrow{A\cdot X\cdot B} = A\otimes B^{\mathrm{T}}\cdot\vec{X}$, where $\vec{X}$ is constituted by stacking each row of matrix X into a column one by one, and knowing that for any vector $\vec{X}$, $\|\vec{X}\|_F = \|\vec{X}\|_2$, then, according to the property of the norm, we can obtain that

$$\begin{aligned} \|H - H^\dagger\|_F &= \|H - \eta H\eta^{-1}\|_F = \|\overrightarrow{H - \eta H\eta^{-1}}\|_F = \|\vec{H} - \eta\otimes\eta^{\mathrm{T}^{-1}}\vec{H}\|_F = \|(I - \eta\otimes\eta^{\mathrm{T}^{-1}})\vec{H}\|_F \\ &= \|(I - \eta\otimes\eta^{\mathrm{T}^{-1}})\vec{H}\|_2 \leqslant \|(I - \eta\otimes\eta^{\mathrm{T}^{-1}})\|_2\cdot\|\vec{H}\|_2 = \|(I - \eta\otimes\eta^{\mathrm{T}^{-1}})\|_2\cdot\|\vec{H}\|_F = \|(I - \eta\otimes\eta^{\mathrm{T}^{-1}})\|_2\cdot\|H\|_F, \end{aligned} \tag{47}$$

where $\eta = \eta(\vec{\alpha})$. Therefore, according to $\|\eta\|\cdot\|\eta^{-1}\| \geqslant \|\eta\cdot\eta^{-1}\| = \|I\|$ and Eq. (46),

$$d_{nh} \leqslant \frac{1}{2}\|\eta\otimes\eta^{\mathrm{T}^{-1}} - I\|_2 = \frac{1}{2}\|\eta\otimes\eta^{-1} - I\|_2 = \frac{1}{2}\|\lambda(\eta)\otimes\lambda(\eta^{-1}) - I\|_2 = \frac{1}{2}\left(\frac{\lambda_{\max}}{\lambda_{\min}} - 1\right), \tag{48}$$

where $\lambda(\eta)$ represents the diagonal matrix constituted by the eigenvalue of η, and the above derivation uses the Hermitian property of η, i.e., its eigenvalues (marked by λ_i) are real. Then according to Eq. (48), we can get

$$\frac{\lambda_{\min}}{\lambda_{\max}} \leqslant \frac{1}{2d_{nh}+1}, \quad \frac{\lambda_{\max}}{\lambda_{\min}} \geqslant 2d_{nh}+1 \in [1,3],$$
$$\Rightarrow \frac{c_{\text{protocol}}}{\lambda_{\max}} \leqslant \frac{c_{\text{protocol}}}{\lambda_{\min}(2d_{nh}+1)}, \tag{49}$$

where c_{protocol} is the coefficient based on the embedding scheme optimized by a protocol; once the protocol is selected, this coefficient will be determined. It is worth emphasizing that the above result is general; i.e., in a $\mathcal{PT}$-symmetric system (whether broken or not), all the spectrums of its metric operators obey this law: the ratio of the maximum eigenvalue to the minimum eigenvalue of the metric operators must be greater than or equal to two times the degree of non-Hermiticity d_{nh} plus one. The above results are also meaningful for us to understand the spectrum structure of those legitimate metric operators in the simulation of a $\mathcal{PT}$-symmetry-unbroken system. The result of the LOCC protocol given in Eq. (44) also obeys this law.

Therefore, according to the above analysis we can get a conclusion: in the simulation of a $\mathcal{PT}$-symmetry-unbroken system based on the embedding method, once the metric operator η ($\eta > 1$) and the protocol are selected, the lower bound of the success probability will decrease with the degree of non-Hermiticity, d_{nh}. From the derivation process above, we know that we did not assume specific protocols in our derivations, so this conclusion has no dependence on the specific protocol; in other words, this conclusion also holds true in the general protocol.

Then according to the conditions required by the embedding method in the main text $\lambda_i \geqslant 1$, and if we choose $\lambda_{\min} \to 1$, we can get the infimum of success probability of the embedding method according to Eq. (48) and the result of the embedding method given in Eq. (40) in the above section:

$$\frac{1}{\lambda_{\max}} \leqslant \frac{1}{2d_{nh}+1}. \tag{50}$$

We can check that the above conclusion and the result given in Eq. (49) are all true by comparing them with Eq. (64) (the embedding method) and Eq. (66) (the LOCC protocol) in the example given in the next section (for example, we can set $r = s$).

VI. AN EXAMPLE: TWO-DIMENSIONAL $\mathcal{PT}$-SYMMETRIC SYSTEM

In this section, we consider a two-dimensional $\mathcal{PT}$-symmetric system,

$$H_S = \begin{pmatrix} re^{i\theta} & s \\ s & re^{-i\theta} \end{pmatrix}, \quad r, s \in \mathbb{R}, \quad \theta \in [-\pi/2, \pi/2], \tag{51}$$

where $\mathcal{P}$ ($P = \sigma_x$) denotes the parity operator, $\mathcal{T}$ ($T = I$) denotes the time reflection and complex conjugation operator, and θ characterizes the non-Hermiticity of the Hamiltonian H_S (when $\theta = 0$, H_S will be Hermitian, and the non-Hermiticity increases with $|\theta|$). The eigenvalues of H_S are $E_\pm = r\cos\theta \pm \sqrt{s^2 - r^2\sin^2\theta}$, and when $s^2 - r^2\sin^2\theta > 0$, H_S is $\mathcal{PT}$-symmetry unbroken; otherwise, when $s^2 - r^2\sin^2\theta < 0$, H_S is $\mathcal{PT}$-symmetry broken, and then the two eigenvalues are conjugate. According to Eq. (46) we can compute the d_{nh} of H_S,

$$d_{nh} = \frac{r|\sin\theta|}{\sqrt{r^2+s^2}} = \frac{s|\sin\alpha|}{\sqrt{r^2+s^2}} < \frac{r|\sin\theta|}{\sqrt{r^2+r^2\sin^2\theta}}$$
$$= \frac{|\sin\theta|}{\sqrt{1+\sin^2\theta}} \leqslant \frac{1}{2}, \tag{52}$$

where "<" is caused by the constraint of the $\mathcal{PT}$-symmetry-unbroken condition: $s^2 - r^2\sin^2\theta > 0$, and we have set $\sin\alpha = r\sin\theta/s$, so the meaning of α is similar to θ. We can check that when $s = 0$ or $\theta = 0$, H_S is Hermitian and the corresponding $d_{nh} = 0$; when $s = 0$ and $\theta = 0$, H_S is anti-Hermitian and d_{nh}=1.

The normalized standard eigenstates of H_S are

$$|\phi_{s+}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\alpha/2} \\ e^{-i\alpha/2} \end{pmatrix}, \quad |\phi_{s-}\rangle = \frac{i}{\sqrt{2}}\begin{pmatrix} e^{-i\alpha/2} \\ -e^{i\alpha/2} \end{pmatrix}. \tag{53}$$

Then we can get the eigenstates of $H_S^\dagger$ though $H_S^\dagger(\theta) = H_S(-\theta)$ so $H_S^\dagger(\alpha) = H_S(-\alpha)$:

$$|\chi_{s+}\rangle = \frac{1}{\sqrt{2}\cos\alpha}\begin{pmatrix} e^{-i\alpha/2} \\ e^{i\alpha/2} \end{pmatrix}, \quad |\chi_{s-}\rangle = \frac{i}{\sqrt{2}\cos\alpha}\begin{pmatrix} e^{i\alpha/2} \\ -e^{-i\alpha/2} \end{pmatrix}. \tag{54}$$

It can be verified that $\langle\chi_{s_p}|\phi_{s_q}\rangle = \delta_{pq}$, where $p, q \in \{+, -\}$. Then according to Eq. (12), η_s will be

$$\eta_s = \sum_{p=\{+,-\}} |\chi_{s_p}\rangle\langle\chi_{s_p}| = \frac{1}{\cos^2\alpha}\begin{pmatrix} 1 & -i\sin\alpha \\ i\sin\alpha & 1 \end{pmatrix}, \tag{55}$$

where the eigenvectors of η are $|\eta_+\rangle = 1/\sqrt{2}(1, i)^T$ and $|\eta_-\rangle = 1/\sqrt{2}(1, -i)^T$, and the corresponding eigenvalues are $1/(1 - \sin\alpha)$ and $1/(1 + \sin\alpha)$, respectively, so the condition $\eta_s > 1$ does not hold and then Eq. (26a) will have no solution. Therefore, in order to make $\eta > 1$, we take

$$\eta = 2\eta_s = \frac{2}{\cos^2\alpha}\begin{pmatrix} 1 & -i\sin\alpha \\ i\sin\alpha & 1 \end{pmatrix},$$
$$\eta^{-1} = \frac{1}{2}\eta_s^{-1} = \frac{1}{2}\begin{pmatrix} 1 & i\sin\alpha \\ -i\sin\alpha & 1 \end{pmatrix}, \tag{56}$$

and then the corresponding biorthogonal eigenstates of H_S will be $\{|\phi_p\rangle, |\chi_p\rangle\} = \{1/\sqrt{2}|\phi_{s_p}\rangle, \sqrt{2}|\chi_{s_p}\rangle\}$. It is easy to know the maximum (minimum) eigenvalue of η is $\lambda_{\max(\min)} = 2/(1 \mp |\sin\alpha|)$, so $\eta > 1$, and then

$$\xi = \sqrt{\eta - 1} = \frac{1}{\cos\alpha}\begin{pmatrix} 1 & -i\sin\alpha \\ i\sin\alpha & 1 \end{pmatrix},$$
$$\xi^{-1} = \frac{1}{\sqrt{\eta - 1}} = \frac{1}{\cos\alpha}\begin{pmatrix} 1 & i\sin\alpha \\ -i\sin\alpha & 1 \end{pmatrix}, \tag{57}$$

where we can see $\xi = 1/2\cos\alpha\,\eta$ and $\xi^{-1} = 2/\cos\alpha\,\eta^{-1}$ in a two-dimensional system, and we need to note that there is usually no such simple correspondence in the higher-dimensional cases. Thereafter, according to Eqs. (29) and (30), we can give the Hermitian dilation of H_S directly:

$$\begin{aligned}\hat{H}_{AS} &= I_A \otimes (r\cos\theta I_A + s\cos^2\alpha\sigma_x) - s\cos\alpha\sin\alpha\sigma_y \otimes \sigma_z \\ &= I_A \otimes (\sqrt{r^2 - s^2\sin^2\alpha}\, I_A + s\cos^2\alpha\sigma_x) \\ &\quad - s\cos\alpha\sin\alpha\sigma_y \otimes \sigma_z \\ &= V \cdot I_A \otimes E_S \cdot V^\dagger,\end{aligned} \tag{58}$$

where the matrix $E_S = \mathrm{diag}(E_+, E_-)$, and V can be

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 0 & 0 \\ \cos\alpha & -\cos\alpha & \sin\alpha & -\sin\alpha \\ -i\sin\alpha & i\sin\alpha & i\cos\alpha & -i\cos\alpha \\ 0 & 0 & i & i \end{pmatrix}. \tag{59}$$

It is worth noting that if we rewrite $r\cos\theta$ as E_0, then the Hamiltonian $\hat{H}_{AS}$ in Eq. (58) will be the same as the "H_S" below Eq. (12) in Ref. [32]. After that, according to Eq. (20), the $U_{AS}(t)$ will be

$$U_{AS}(t) = V \cdot I_A \otimes e^{-iE_S t} \cdot V^\dagger. \tag{60}$$

For the convenience of calculation, we use the CQM framework, and we assume Ω_S is in one of the eigenstates of η^{-1}, i.e., $\Omega_S = |\eta_+\rangle\langle\eta_+| = 1/2\,(1, i)^T \cdot (1, i)^*$; then the initial state $\rho_S = \eta^{-1/2}\Omega_S\eta^{-1/2} = \frac{1-\sin\alpha}{4}\begin{pmatrix} 1 & -i \\ i & 1\end{pmatrix}$. According to Eq. (36), we can get

$$\begin{aligned} h &= W \cdot E_S \cdot W^\dagger, \\ U_h(t) &= e^{-iht} = W \cdot e^{-iE_S t} \cdot W^\dagger, \end{aligned} \tag{61}$$

where $W = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1\end{pmatrix}$. Then according to Eqs. (35) and (33) we obtain that

$$\begin{aligned}\Omega_S(t) &= U_h(t) \cdot \Omega_S \cdot U_h^\dagger(t) \\ &= \begin{pmatrix} \sin^2 x & -i\sin x\cos x \\ i\sin x\cos x & \cos^2 x \end{pmatrix},\end{aligned} \tag{62a}$$

$$\begin{aligned}\rho_S(t) &= \eta^{-\frac{1}{2}} \cdot \Omega_S(t) \cdot \eta^{-\frac{1}{2}} \\ &= \frac{1}{4}\begin{pmatrix} 1 - \cos\alpha\cos 2x - \sin\alpha\sin 2x & i(\sin\alpha - \sin 2x) \\ -i(\sin\alpha - \sin 2x) & 1 + \cos\alpha\cos 2x - \sin\alpha\sin 2x \end{pmatrix},\end{aligned} \tag{62b}$$

where $x = st\cos\alpha + \pi/4$, and the parameter r is contained in α. Thus according to Eq. (38) we get the success probability,

$$P_0(t) = \mathrm{Tr}(\eta^{-1}\Omega_S(t)) = \frac{1 - \cos(2st\cos\alpha)\sin\alpha}{2}, \tag{63}$$

where P_0 is the function of α and t. Therefore, we can get the bound

$$\frac{1 - |\sin\alpha|}{2} \leqslant P_0(t) \leqslant \frac{1 + |\sin\alpha|}{2}, \tag{64}$$

where $\frac{1-|\sin\alpha|}{2}$ and $\frac{1+|\sin\alpha|}{2}$ are just the infimum $1/\lambda_{\max}$ and the supremum $1/\lambda_{\min}$ respectively derived in Eq. (40). We can check that this result meets the result in Eq. (50). By observing the above equation, it is obvious that when $t = k\pi/s\cos\alpha$, $k \in \mathbb{Z}$, $P_0 = (1 - \sin\alpha)/2$, which is just the infimum $1/\lambda_{\max}$ (or supremum $1/\lambda_{\min}$) in Eq. (40), and when $t = (2k+1)\pi/2s\cos\alpha, k \in \mathbb{Z}$, $P_0 = (1 + \sin\alpha)/2$, which is the supremum $1/\lambda_{\min}$ (or infimum $1/\lambda_{\max}$), and we can see the success probability P_0 oscillates periodically with time t between the infimum and the supremum, and the oscillation period is $\pi/s\cos\alpha$. It is worth noting that the infimum and the supremum depend on the special selection of η, and when $\alpha = 0$, i.e., $\theta = 0$, then the Hamiltonian H_S in Eq. (51) will be Hermitian. We intuitively know that the success probability of the simulation should be 100%, but according to Eq. (63) above, $P_0 = 1/2$, which is caused by η should have been chosen as $\eta = I$; then the infimum and the supremum will be both 100%.

Figure 2 shows the three views of the relation between the success probability and time t and parameter α, and Fig. 2(a) is the overall figure. From these figures, we can clearly see the periodic characteristics of the success probability curve. From Fig. 2(c), we can see that when the non-Hermiticity that can be characterized by $|\alpha|$ [when r, s are fixed; see Eq. (52)] becomes smaller, the success probability of the simulation, P_0, will be more stable. This case can also be understood from the infimum and supremum of Eq. (63), and even when $\alpha = 0$, P_0 will remain unchanged; from the above analysis, we know this phenomenon is caused by the system becoming Hermitian. From Fig. 2(d), we can see that P_0 shows a periodical change with time t and $P_0(\alpha)$ is symmetric with $P_0(-\alpha)$ about $P_0 = 1/2$, which can also be understood by Eq. (63). Figure 2(b) also shows some regular structures, which can be seen more clearly in Fig. 3. From Fig. 3, we can clearly see that P_0 oscillates with t sinusoidally, and the amplitude decreases with the increase of $|\alpha|$, but the oscillation period increases with $|\alpha|$. Next, according to Eqs. (62a) and (22), we obtain $\rho_{AS}(t) = \begin{pmatrix} \rho_S(t) & \rho_S(t)\xi \\ \xi\rho_S(t) & \xi\rho_S(t)\xi \end{pmatrix}$, where ξ was given in Eq. (57). Then according to the condition $c \leqslant \sqrt{\lambda_{\min} - 1}$ we can take $c = \sqrt{\lambda_{\min} - 1} = \frac{\cos\frac{\alpha}{2} - |\sin\frac{\alpha}{2}|}{\cos\frac{\alpha}{2} + |\sin\frac{\alpha}{2}|}$, and then according to Eq. (41) we can use the following recovery operation to restore the state $\rho_S(t)$:

$$\begin{aligned} R &= \sqrt{\lambda_{\min} - 1}\,\xi^{-1} \\ &= \frac{\cos\frac{\alpha}{2} - |\sin\frac{\alpha}{2}|}{\cos\alpha(\cos\frac{\alpha}{2} + |\sin\frac{\alpha}{2}|)}\begin{pmatrix} 1 & i\sin\alpha \\ -i\sin\alpha & 1 \end{pmatrix},\end{aligned} \tag{65}$$

where R is a measurement operator.

Then according to Eqs. (43) and (63), we can obtain that

$$P_{\mathrm{LOCC}}(t) = \lambda_{\min}P_0(t) = \frac{1 - \cos(2st\cos\alpha)\sin\alpha}{1 + |\sin\alpha|}, \tag{66}$$

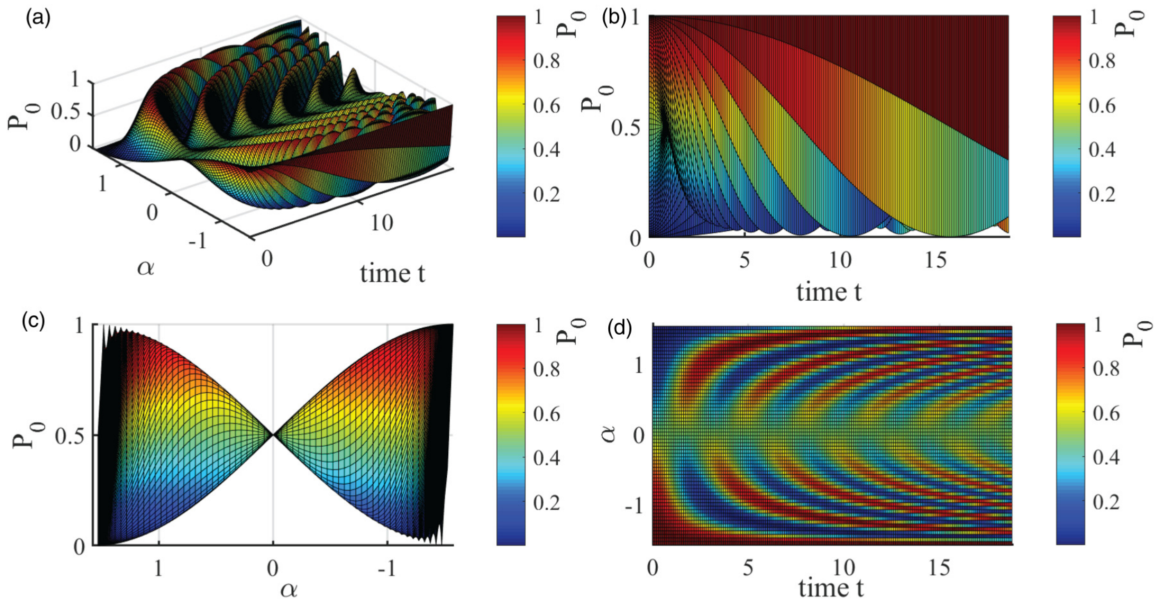

FIG. 2. The success probability P_0 of the embedding scheme in a two-dimensional system (s, t have the energy dimension and time dimension, respectively, and their units can be determined by $st = \hbar$; we set $s = 1$ here). (a) The relation between the success probability and time t and parameter α, (b) the front view, (c) the side view, and (d) the vertical view.

and it is easy to check that

$$\frac{1-|\sin\alpha|}{1+|\sin\alpha|} \leqslant P_{\text{LOCC}} \leqslant \frac{1-|\sin\alpha|}{1-|\sin\alpha|} = 1. \tag{67}$$

We can check that this result meets Eq. (49). By comparing Eqs. (66) and (67) with Eqs. (63) and (64), we can verify that this LOCC protocol scheme increases the success probability of the simulation to $\lambda_{\min}$ times, which can be seen by comparing Fig. 5 with Fig. 3 and Fig. 4(d) with Fig. 2(d). Comparing Fig. 4(c) with Fig. 2(c), we can find that the infimum of the success probability of this LOCC protocol can be increased to 100% with the decreases of $|\alpha|$, but the original embedding scheme can only be increased to $1/2$, which means the LOCC protocol scheme is more in line with physical reality than the original embedding scheme. Meanwhile, the LOCC protocol scheme does not depend on the special selection of the metric operator η as seriously as the embedding scheme but on the ratio $\lambda_{\min}/\lambda_{\max}$; in other words, the LOCC protocol scheme

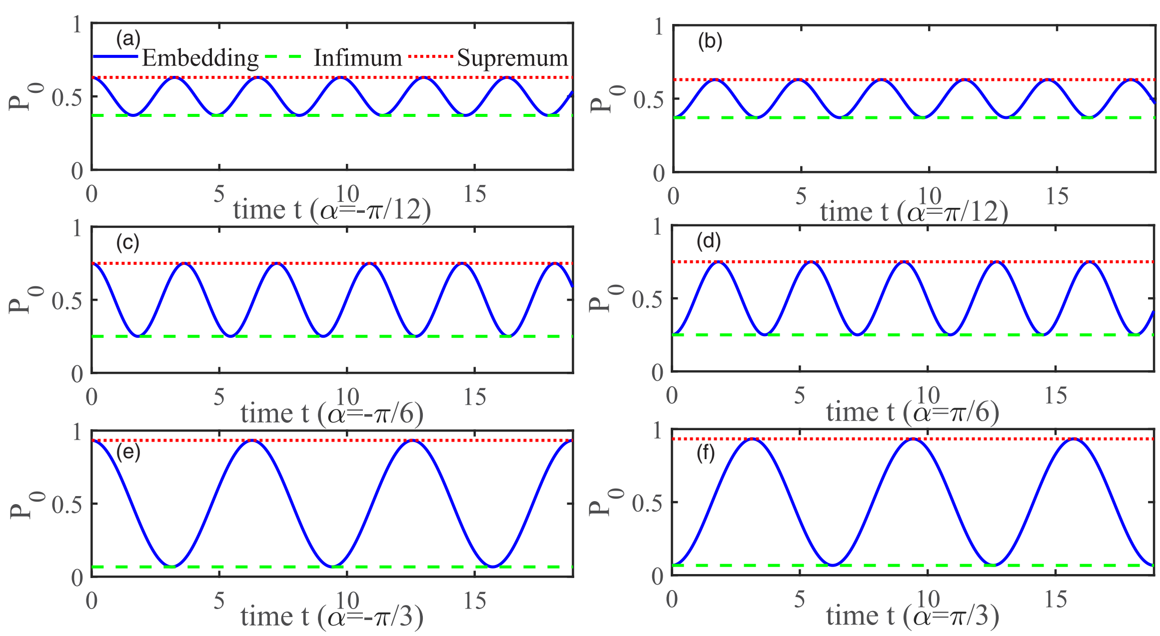

FIG. 3. The success probability P_0 of the embedding scheme in a two-dimensional system with different α (s, t have the energy dimension and time dimension, respectively, and their units can be determined by $st = \hbar$; we set $s = 1$ here), and the corresponding infimum (green dashed line) and supremum (red dotted line). (a–f) The cases under different parameters α.

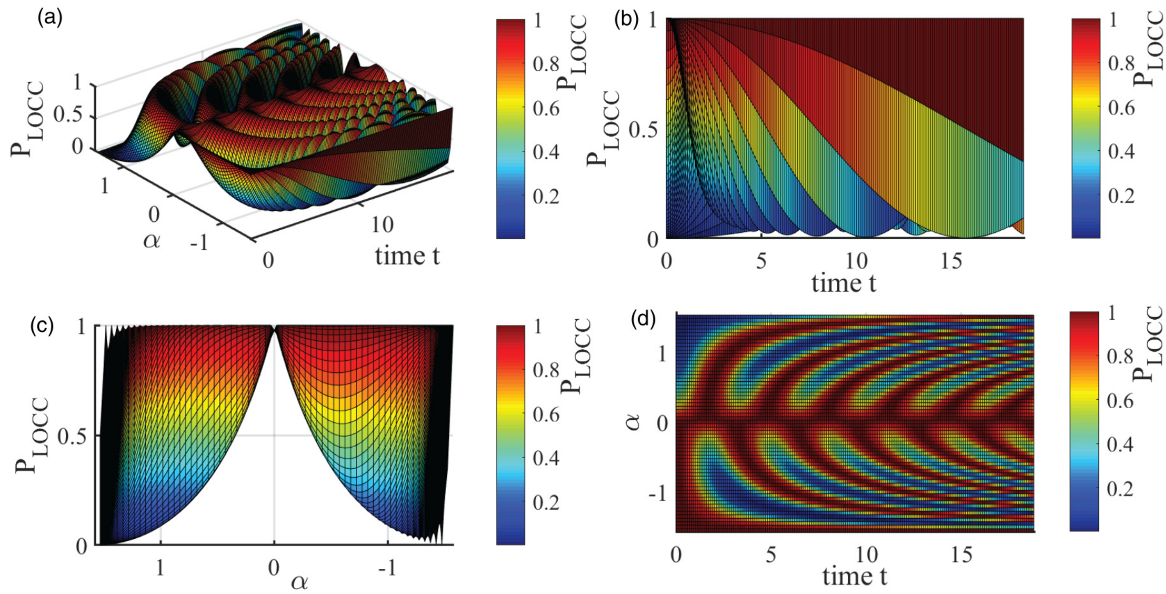

FIG. 4. The success probability P_{LOCC} of the LOCC protocol scheme in a two-dimensional system (s, t have the energy dimension and time dimension, respectively, and their units can be determined by $st = \hbar$; we set $s = 1$ here). (a) The relation between the success probability and time t and parameter α, (b) the front view, (c) the side view, and (d) the vertical view.

has less dependence on but more flexibility in the selection of η and more adaptability in practical applications than the embedding scheme.

VII. CONCLUSIONS AND DISCUSSIONS

In this work, by clarifying some common confusions in the simulation of a $\mathcal{PT}$-symmetric system, we naturally extend the embedding simulation scheme of the $\mathcal{PT}$-symmetry-unbroken system from a pure-states case to a mixed-states case, and then we analyze the key but usually neglected problem of success probability, and give a concise bound. Based on the above analyses and derivations, we find the embedding scheme is usually not effective enough because some resources are wasted. Therefore, we propose a LOCC protocol scheme based on the embedding scheme to simulate the $\mathcal{PT}$-symmetry-unbroken system more effectively. Both the embedding scheme and the LOCC protocol scheme need only one qubit as an auxiliary system to simulate the dynamics of any arbitrary finite-dimensional $\mathcal{PT}$-symmetric system in the $\mathcal{PT}$-unbroken phase. Our LOCC protocol scheme has at least three main advantages over the embedding scheme: (1) it

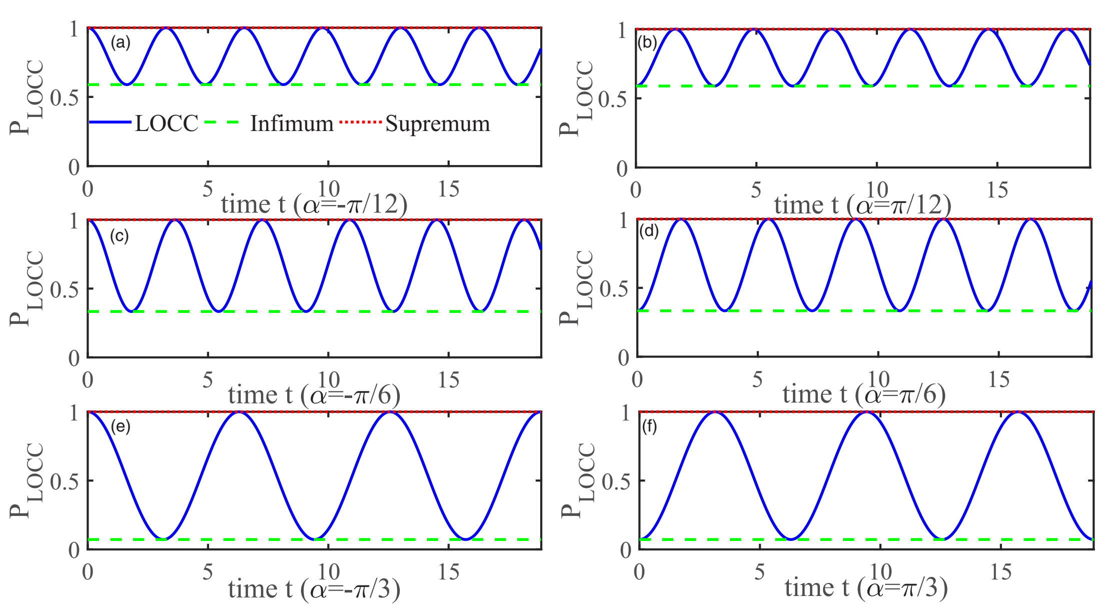

FIG. 5. The success probability P_{LOCC} of the LOCC protocol scheme in a two-dimensional system with different α (s, t have the energy dimension and time dimension, respectively, and their units can be determined by $st = \hbar$; we set $s = 1$ here), and the corresponding infimum (green dashed line) and supremum (red dotted line). (a–f) The cases under different parameters α.

increases the success probability to $\lambda_{\min}$ ($\lambda_{\min} > 1$) times, (2) it has less dependence on but more flexibility in the special selection of the metric operator η and more adaptability in practical applications, and (3) it is more in line with our physical intuition than the embedding scheme. We then further study the relation between the lower bound of the success probability and the degree of non-Hermiticity, and give a general lower bound that does not depend on the specific protocol.

In addition, we also noticed the work of Huang *et al.* regarding the simulation of an arbitrary $\mathcal{PT}$-symmetric system including the broken case using the generalized embedding scheme and weak measurement [66]. However, it seems that this scheme cannot be directly extended to the LOCC protocol scheme in the broken case of a $\mathcal{PT}$-symmetric system because the metric operator may not be positive.

Finally, we go back and try to discuss the physical or philosophical meaning behind the embedding scheme and the LOCC protocol scheme. According to the analyses of the embedding scheme and its success probability above in Sec. III, we can find this fact: For a low-dimensional observer in the subspace of dilated higher-dimensional $\hat{H}_{AS}$, i.e., the space of the $\mathcal{PT}$-symmetric system H_S, the event that the state $\rho_S(0)$ evolves to the state $\rho_S(t)$ will happen determinately; however, from the perspective of a higher-dimensional observer located in the higher-dimensional space of $\hat{H}_{AS}$ and dominated by the CQM, this event will happen casually. More specifically, this event happens with probability $P_0(t)$, while in another branch, ρ_S evolves to $\xi\rho_S(t)\xi$ with $1 - P_0(t)$, while the low-dimensional observer imprisoned in the low-dimensional space of H_S and dominated by the $\mathcal{PT}$-QM is not able to discover this truth except for communicating with the higher-dimensional observer.

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APPENDIX A: THE DETAILS OF THE EMBEDDING PROCESS

According to the derivation process between Eq. (24) and Eq. (30), especially Eq. (25), and recalling the operation rules of the symbol "$\circ$" defined above Eq. (20), i.e., $(B\cdot C)\circ\rho = (BC)\cdot\rho\cdot(C^\dagger B^\dagger) = B\circ C\circ\rho$, we know that

$$\begin{aligned}\hat{H}_{AS}\circ\rho_{AS} &= \begin{pmatrix} H_1 & H_2 \\ H_2^\dagger & H_4\end{pmatrix}\circ(|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\circ\rho_S \\ &= \left[\begin{pmatrix} H_1 & H_2 \\ H_2^\dagger & H_4\end{pmatrix}\cdot(|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\right]\circ\rho_S \\ &= \begin{pmatrix} H_1 + H_2\xi \\ H_2^\dagger + H_4\xi\end{pmatrix}\circ\rho_S \\ &= \begin{pmatrix} H_S \\ \xi\cdot H_S\end{pmatrix}\circ\rho_S \\ &= [(|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\cdot H_S]\circ\rho_S \\ &= (|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\circ H_S\circ\rho_S. \end{aligned} \tag{A1}$$

Repeating the above derivation process, we can obtain that

$$\begin{aligned}\hat{H}^2_{AS}\circ\rho_{AS} &= \hat{H}_{AS}\circ\hat{H}_{AS}\circ\rho_{AS} \\ &= \hat{H}_{AS}\circ[(|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\cdot H_S]\circ\rho_S \\ &= [(|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\cdot H_S\cdot H_S]\circ\rho_S \\ &= (|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\circ H_S^2\circ\rho_S. \end{aligned} \tag{A2}$$

Therefore, we can get

$$\hat{H}^n_{AS}\circ\rho_{AS} = (|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\circ H_S^n\circ\rho_S, \quad n\in\mathbb{N}, \tag{A3}$$

if we set $\rho_S = \rho_S(0)$, $\rho_{AS} = \rho_{AS}(0)$. Then according to the Taylor expansion formula

$$\begin{aligned}\rho_{AS}(t) &= U_{AS}(t)\circ\rho_{AS}(0) \\ &= e^{-it\hat{H}_{AS}}\circ\rho_{AS}(0) \\ &= \left(\sum_n \frac{-it\hat{H}^n_{AS}}{n!}\right)\circ\rho_{AS}(0) \\ &= (|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\circ\left(\sum_n\frac{-itH_S^n}{n!}\right)\circ\rho_S(0) \\ &= (|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\circ e^{-itH_S}\circ\rho_S(0) \\ &= (|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\circ\mathcal{U}_S(t)\circ\rho_S(0) \\ &= (|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\circ\rho_S(t), \end{aligned} \tag{A4}$$

where $U_{AS} = e^{-it\hat{H}_{AS}}$, $\mathcal{U}_S(t) = e^{-itH_S}$, and $\rho_S(t) = \mathcal{U}_S(t)\circ\rho_S(0) = \mathcal{U}_S(t)\cdot\rho_S(0)\cdot\mathcal{U}_S^\dagger(t)$. Finally, we can get

$$\begin{aligned}\mathcal{M}_0[\rho_{AS}(t)] &= \mathcal{M}_0[(|0\rangle_A\otimes I_S + |1\rangle_A\otimes\xi)\circ\rho_S(t)] \\ &= \rho_S(t). \end{aligned} \tag{A5}$$

APPENDIX B: EXPLANATIONS OF THE RATIONALITY OF THE INTRODUCED ρ_S AND THE LEGITIMACY OF THE DENSITY OPERATOR ρ_{AS}

First, we prove the rationality of the introduced ρ_S [ρ_S can be $\rho_S(0)$ or $\rho_S(t)$]. According to Eqs. (18) and (19), we can get

$$\begin{aligned}\rho_S &= \rho_{\mathcal{PT}}\cdot\eta^{-1} \\ &= \eta^{\frac{1}{2}}\cdot\rho_c\cdot\eta^{\frac{1}{2}}, \end{aligned} \tag{B1}$$

where η is the metric operator, which is always positive in the $\mathcal{PT}$-symmetry-unbroken case and in fact $\eta > 1$ in our assumption of the main text (in the $\mathcal{PT}$-symmetry-broken case, η may not be positive [16,24,45]), and ρ_c is a legal density operator as we have known in the main text, i.e., ρ_c is a positive-semidefinite operator. And from Eq. (B1), we know ρ_S is Hermitian. Therefore, we assume that for any vector $|x\rangle$, which is an arbitrary state (vector), and $|y\rangle = \eta^{\frac{1}{2}}|x\rangle$, it is obvious that

$$\langle x|\rho_S|x\rangle = \langle y|\rho_c|y\rangle \geqslant 0, \tag{B2}$$

so ρ_S is a positive-semidefinite operator. However, according to Eqs. (19) and (25a), $\mathrm{Tr}(\rho_S) \leqslant \mathrm{Tr}(\eta\rho_S) \equiv 1$, so it is actually an unnormalized density operator (hence Hermitian operator) with $\mathrm{Tr}(\rho_c) \equiv 1$. Note that all the density operators (ρ_c) and unnormalized density operators (ρ_S) are Hermitian in the framework of CQM, while the density operators ($\rho_{\mathcal{PT}}$) are non-Hermitian in the framework of $\mathcal{PT}$-QM.

Then ρ_S can be seen as a normalized form of the density operator $\rho_{S\,\mathrm{normalized}}$:

$$\rho_{S\,\mathrm{normalized}} = \frac{\mathrm{Tr}_A(\prod_0 \rho_{AS})}{\mathrm{Tr}_{AS}(\prod_0 \rho_{AS})} = \frac{\rho_S}{\mathrm{Tr}(\rho_S)}, \tag{B3}$$

where $\mathrm{Tr}(\rho_{S\,\mathrm{normalized}}) = 1$, and because we have proved ρ_S is a positive-semidefinite operator (and obviously Hermitian), $\rho_{S\,\mathrm{normalized}}$ is a legal density operator. In addition, the probability of getting the result "0" corresponding to the measurement Π_0 is $P_0 = \mathrm{Tr}_{AS}(\prod_0 \rho_{AS}) = \mathrm{Tr}(\rho_S)$. As we all know, in a practical experiment, both $\rho_{S\,\mathrm{normalized}}$ and P_0 can be obtained, so ρ_S can also be obtained. The unnormalized density matrix ρ_S actually absorbs the probability P_0. It is worth noting that when $\rho_S(0)$ evolves to $\rho_S(t)$, their traces are not equal in general, and the probability P_0 will change from $P_0(0) = \mathrm{Tr}(\rho_S(0))$ to $P_0(t) = \mathrm{Tr}(\rho_S(t))$ [in the embedding method, we always have $P_0(t) \leqslant 1$ according to Eq. (38)]. Therefore, replacing the normalized state $\rho_{S\,\mathrm{normalized}}$ with the unnormalized state ρ_S will provide a lot of convenience in expressing and calculating probability [such as Eqs. (38) and (43)] and meet the usage requirements. On the premise of no misunderstanding, we usually default that the two are equivalent and only strictly distinguish them when calculating probability (the normalization often occurs when calculating probability), and this is a very common practice (such as Eqs. (13) and (18) in Ref. [30], and Eqs. (36)–(38) in Ref. [31]). In particular, Eqs. (14) and (15) in Ref. [32] are just a special case of our case (pure state and just the two-dimensional case), and it is worth noting that the embedding method can also be realized experimentally in Ref. [62].

In summary, the introduction of the unnormalized density operator ρ_S is not only reasonable, but also experimentally feasible.

Next, we prove the legitimacy of ρ_{AS} [ρ_{AS} can be $\rho_{AS}(0)$ or $\rho_{AS}(t)$]. According to Eq. (19), ρ_S can be expressed as

$$\rho_S = \sum_{mn} \rho_{c_{mn}} |\phi_m\rangle\langle\phi_n|, \tag{B4}$$

where the matrix element $\rho_{c_{mn}}$ is also the matrix element of ρ_c under its complete orthogonal bases $\{|n\rangle\}$, which can be seen from Eq. (18). Then we assume $|\nu_n\rangle = (|0\rangle_A \otimes I_S + |1\rangle_A \otimes \xi)|\phi_n\rangle$, and according to Eq. (9) we know

$$\begin{aligned}\langle\nu_m|\nu_n\rangle &= \langle\phi_m|(\langle 0| \otimes I_S + \langle 1| \otimes \xi) \\ &\quad\cdot (|0\rangle_A \otimes I_S + |1\rangle_A \otimes \xi)|\phi_n\rangle \\ &= \langle\phi_m|\eta|\phi_n\rangle \\ &= 0,\end{aligned} \tag{B5}$$

where $\eta = \xi^2 + I_S$. That means $\{|\nu_n\rangle\}$ can form a set of orthogonal bases. (In fact, $|\phi_n\rangle$ is n dimensional, but $|\nu_n\rangle$ is $2n$ dimensional, so the base $\{|\nu_n\rangle\}$ is incomplete; however, we can add another n suitable bases to construct the complete orthogonal bases. In this way, all the other matrix elements are zero except the element occupied by $\rho_{c_{mn}}$.) Then, according to Eqs. (22) and (26a), we can get

$$\begin{aligned}\rho_{AS} &= (|0\rangle_A \otimes I_S + |1\rangle_A \otimes \xi)\rho_S(\langle 0| \otimes I_S + \langle 1| \otimes \xi) \\ &= \sum_{mn} \rho_{c_{mn}} |\nu_m\rangle\langle\nu_n|,\end{aligned} \tag{B6}$$

where the matrix elements $\rho_{c_{mn}}$ are just the same as the matrix elements of ρ_c, which is a legal density operator, and it is obvious $\mathrm{Tr}(\rho_{AS}) \equiv 1$ according to Eq. (25a), so ρ_{AS} is also obviously a legal density operator. Therefore, when we set $\rho_{AS}(0) = \rho_{AS}$, according to Eq. (32) and Appendix A, $\rho_{AS}(t) = e^{-it\hat{H}_{AS}} \cdot \rho_{AS}(0) \cdot e^{it\hat{H}_{AS}}$ is also a legal density operator, i.e., a positive-semidefinite (hence Hermitian) operator with unit trace.

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