Dynamics simulation based on density operator and numerical analysis of arbitrary time-dependent $\mathcal{PT}$-symmetric system and the influence of quantum noises

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$\mathcal{PT}$-symmetric system has attracted extensive attention in recent years because of its unique properties and applications. How to simulate $\mathcal{PT}$-symmetric system in traditional quantum mechanical system not only has basic theoretical significance, but also has practical application value. We propose a dynamics simulation scheme of arbitrary time-dependent $\mathcal{PT}$-symmetric system based on density operator. Based on that, we further study the influence of quantum noises on the simulation results with the technique of vectorization of density operator and matrixization of superoperators (VDMS), and we show the depolarizing (Dep) noise is the most fatal and should be avoided as much as possible. Meanwhile, we also give a numerical analysis of the above works. By theoretical analysis and numerical calculation, we find the problem of chronological product may have to be solved not only in numerical calculation, but also even in experiment, because the delayed higher-dimensional Hamiltonian is usually time-dependent. And the solution of chronological product problem is actually one of the key factors to the accuracy of dynamics simulation of the time-dependent $\mathcal{PT}$-symmetric system, and even the most key factor. We prove that the trusted duration of numerical calculation is actually bounded by the critical time $T_c$ of convergence of Magnus series, while the implemented duration of experimental running is actually bounded by the critical time $T_c$ of legitimacy of dilation method.

I. INTRODUCTION

That all physical observables including Hamiltonians must be Hermitian operators has long been seen as one of axioms in conventional quantum mechanics (CQM) [1], because Hermitian operators have real eigenspectrums as we all know. However, Bender et al. found that some non-Hermitian Hamiltonians, which are parity-time ($\mathcal{PT}$)-reversal symmetric, may also have real eigenspectrums in 1998 [2], and then established the $\mathcal{PT}$-symmetric quantum mechanics ($\mathcal{PT}$-QM) [3–5]. In last two decades, $\mathcal{PT}$-symmetry theory has developed rapidly [6,13], and aroused wide attentions [14,15]. The phenomenon related to $\mathcal{PT}$ symmetry exists widely, not only in classical system, such as optical lattices [16], microcavities [17] and circuits [18], but also in quantum system, such as strongly correlated many-body systems [19], quantum critical spin chains [20], and ultracold atoms [21]. In addition, $\mathcal{PT}$-symmetric system also shows practical values in quantum sensors [22,24], which can use the sensitivity of $\mathcal{PT}$-symmetric system near the exceptional points (EPs) to amplify small signals. In particular, it is worth noting that, with the increasing interest in $\mathcal{PT}$-symmetric systems, some new phenomena have emerged [23,26], which are impressive because they seem to conflict with theory of conventional quantum mechanics or theory of relativity, such as the instantaneous quantum brachistochrone problem [15,27,31], the deterministical discrimination of nonorthogonal quantum states [35,36], and the violation of no-signaling principle [37,42]. However, some anomalies actually come from not knowing how to simulate $\mathcal{PT}$-symmetric system in conventional quantum system, for instance, if the discarded probabilities during the simulation of $\mathcal{PT}$-symmetric system are considered, the no-signaling principle will still hold [43]. Therefore, finding a way to simulate $\mathcal{PT}$-symmetric system in conventional quantum system has not only practical value, but also theoretical significance.

At present, there are at least three technical routes to simulate $\mathcal{PT}$-symmetric system, and all of them can be realized in experiments [24,44,45]. The method of linear combination of unitaries (LCU) [46], can be used to simulate various time-independent non-Hermitian $\mathcal{PT}$-symmetric systems in discrete time, whether it is in unbroken or broken phase [32,44,46,47] and even anti-$\mathcal{PT}$-symmetric systems [48]. The method of weak measurement [49], can also be used to simulate various time-independent unbroken and broken $\mathcal{PT}$-symmetric systems in restricted continuous time under the condition of weak interaction by a weak measurement. The methods based on embedding or dilation theory [43,45,50], can be used to simulate the dynamics of unbroken time-independent $\mathcal{PT}$-symmetric system (in pure-sates case [43] or mixed-states case [50]) in unrestricted continuous time with only one qubit as a auxiliary system.
What deserves special attention is that in 2019, Wu et al. proposed a general simulation scheme of dynamics of time-dependent (TD) arbitrary \( \mathcal{PT} \)-symmetric system based on pure-state vector in open system using dilation, and realized it with a single nitrogen-vacancy center in diamond \[55\]. Specifically, their method is performed by dilating a general TD \( \mathcal{PT} \)-symmetric Hamiltonian into a higher dimensional TD Hermitian one with the help of a auxiliary qubit system, and evolving the sate in the dilated Hermitian system for a period of time, then performing a fixed projection measurement on the auxiliary system, after that, the remained main system is equivalent to going through the evolution process govern by the \( \mathcal{PT} \)-symmetric Hamiltonian. However, the dilated Hamiltonian is usually time-dependent, which means the system is actually an open quantum system. As we all know, in an open quantum system, the influence of quantum noises in the environment is inevitable so that they have to be considered \[51\]. The time evolution of an open quantum system interacting with memoryless environment can be described by the Lindblad master equation \[51\]–\[52\], which is usually based on the density operator (matrix) rather than the sate vector. In addition, as we all know, a pure state may evolve to mixed state under the quantum noises, so the theory based on pure-state vector can not conveniently deal with the question related to mixed states, then the tool of pure-state vector may be failed, in this situation, the density operator will also be a better tool.

Motivated mainly by the work of Wu et al. in Ref.\[45\] and our previous work in Ref.\[50\], in this paper, we generalize the work of Wu et al. based on dilation from the pure-state vector case to the mixed-state density operator case with the tool of density operator, and provide more mathematical and physical completeness. Based on that, we are able to deal with problems of open quantum systems using the vectorization of density operator and matrixization of superoperators (VDMS) technique. Then we study the influence of quantum noises to the dynamics of time-dependent arbitrary \( \mathcal{PT} \)-symmetric system, meanwhile, we also give a numerical analysis. It is worth noting that it is not a trivial progress for generalizing the quantum state form pure-state vector to mixed-state density operator in the simulation of \( \mathcal{PT} \)-symmetric system, and the difficulty mainly comes from the flexibility of characterizing quantum states in \( \mathcal{PT} \)-symmetric systems and the uncertainty of mapping it to high-dimensional quantum states in conventional quantum systems \[53\]–\[55\]. In the numerical analysis, we find that the trusted duration of numerical calculation is actually bounded by the critical time \( T_c \) of convergence of Magnus series, this phenomenon occurs because the dilated higher-dimensional Hamiltonian is usually time-dependent, the chronological product problem may have to be dealt with, so the Magnus series have to be calculated \[54\]–\[56\], which may diverge when \( t \to T_c \); meanwhile, the implemented duration of experimental running is actually bounded by the critical time \( T_c \) of legitimacy of dilation method, this phenomenon occurs because when \( t \to T_c \), the energy may diverge. In fact, the problem of chronological product may have to be solved not only in numerical calculation, but also even in experiment, because the dilated \( \hat{H}_{AS}(t) \) has to be parameterized in advance by numerically calculating the chronological product caused by \( H_S(t) \) needed to be dilated. We also find that the solution of the problem of chronological product is one of the key factors to the accuracy of dynamics simulation of the TD \( \mathcal{PT} \)-symmetric system, and even the most key factor. In addition, when considering the influence of quantum noises, we find the depolarizing (Dep) noise (channel) is the most fatal to the simulation of \( \mathcal{PT} \)-symmetric system among three kinds of quantum noise we considered and should be avoided as much as possible. It is worth noting that when the system considered is \( \mathcal{PT} \)-symmetry unbroken, the results of simulations of this work are consist with our previous results in Ref.\[50\], and when the sate considered is pure state, the results of this work are consist with the theoretical results given in Ref.\[45\]. In a summary, this work provides a general theoretical framework based on density operator to analytically and numerically analyze the dynamics of time-dependent arbitrary \( \mathcal{PT} \)-symmetric system and the influence of quantum noises.

The rest of this paper is organized as follows. In Sec.\[II\] we give some necessary basic theories of \( \mathcal{PT} \)-symmetric system. In Sec.\[III\] we give an universal Hermitian dilation method of non-Hermitian Hamiltonians with density operators, and based on that, we give an universal simulation scheme of the dynamics of TD arbitrary \( \mathcal{PT} \)-symmetric system. To be able to solve problems in open quantum system, we vectorize density operators and matrixize the Liouvilian superoperators in Sec.\[IV\]. In Sec.\[V\] we give an example of two-dimensional \( \mathcal{PT} \)-symmetric system, and numerically analyze its dynamics, meanwhile, we also consider the influence of three kinds of quantum noise. In Sec.\[VI\] we give conclusions and discussions. In addition, we make Appendix A to show the details of the delated Hamiltonians, and make Appendix B to introduce the problem of chronological product at the end of this paper.

## II. THEORETICAL PREPARATIONS

Given a \( n \)-dimensional non-Hermitian \( \mathcal{PT} \)-symmetric Hamiltonian \( \mathcal{H} \), the parity operator \( \mathcal{P} \) and time reversal operator \( \mathcal{T} \), where \( \mathcal{T} \) is an anti-linear operator, and \( \mathcal{H}, \mathcal{P}, \mathcal{T} \) denote their matrix representation, respectively. They have the following properties:

\[
\mathcal{P}^2 = I, \mathcal{T} \mathcal{T}^* = I, \mathcal{PT} = \mathcal{T} \mathcal{P}
\]

\[
\mathcal{PT} \mathcal{T}^* = \mathcal{H} \mathcal{PT},
\]  

(1)

where \( \mathcal{T}^* \) denotes complex conjugate of \( \mathcal{T} \), and it occurs because \( \mathcal{T} \) is an anti-linear operator. If \( \mathcal{H} \) is similar to a real diagonal matrix, \( \mathcal{H} \) will be \( \mathcal{PT} \)-symmetric unbroken,
otherwise, $H$ is called $PT$-symmetry broken if and only if it satisfies either of these two conditions \cite{6,7,50,57}: (1) it cannot be diagonalized, (2) it has complex eigenvalues that appear in complex conjugate pairs.

For a time-independent $PT$-symmetry $H$, there is a time-independent operator $\eta$ satisfy that:

$$\eta H = H^\dagger \eta,$$  \hspace{1cm} (2)

where $\eta$ is called the metric operator of $H$, and it is a reversible Hermitian operator, when $H$ is $PT$-symmetry unbroken, it can be completely positive. The metric operator is usually not unique, for instance, if $\eta$ is a metric operator of $H$, so is $\eta r$ ($r \in \mathbb{R}$). The above Eq. (2) is also referred to as the pseudo-Hermiticity relation, and $H$ is also referred to as pseudo-Hermitian Hamiltonian \cite{6,58}. All $PT$-symmetric Hamiltonians belong to pseudo-Hermitian \cite{6}

The elements of $PT$-QM in the unbroken phase of $H$ can be represented by biorthogonal basis of $H$: \{$|\chi_n, a\rangle, |\phi_n, a\rangle\}$, and they have the properties as follows \cite{6}:

$$\langle \chi_n, a | \phi_n, b \rangle = \delta_{mn} \delta_{ab}, \hspace{1cm} (3a)$$

$$H |\phi_n, a\rangle = E_n |\phi_n, a\rangle, \hspace{1cm} H^\dagger |\chi_n, a\rangle = E_n |\chi_n, a\rangle, \hspace{1cm} (3b)$$

$$\sum_n \sum_{a=1}^{d_n} |\chi_n, a\rangle \langle \phi_n, a| = \sum_{a=1}^{d_n} |\phi_n, a\rangle \langle \chi_n, a| = I, \hspace{1cm} (3c)$$

$$|\chi_n, a\rangle = \eta |\phi_n, a\rangle, \hspace{1cm} (3d)$$

$$\eta = \sum_n \sum_{a=1}^{d_n} |\chi_n, a\rangle \langle \chi_n, a|, \hspace{1cm} (3e)$$

$$\eta^{-1} = \sum_n \sum_{a=1}^{d_n} |\phi_n, a\rangle \langle \phi_n, a|, \hspace{1cm} (3f)$$

where $d_n$ is the degree of degeneracy of the eigenvalue $E_n$, and $a$ and $b$ are degeneracy labels, and $|\phi_k\rangle$s ($|\chi_k\rangle$s) are usually not orthogonal to each other. The possible real coefficients before $\eta$ have been absorbed into the biorthogonal basis. For convenience, we set $d_n = 1$ hereafter. If we recorded that $\Phi = \{|\phi_1\rangle, \ldots, |\phi_n\rangle\}$, $\Xi = \{|\chi_1\rangle, \ldots, |\chi_n\rangle\}$, $E = \text{diag}(E_1, \ldots, E_n)$, then according to Eqs. (3) we will get \cite{6,50}:

$$\Phi^{-1} H \Phi = E, \hspace{1cm} \Xi^{-1} H^\dagger \Xi = E \hspace{1cm} (4)$$

Through the positive Hermitian metric operator $\eta$, the representations of quantum observable $O$ under the framework of CQM and the framework of $PT$-QM can be connected by a similar transformation, i.e., the Dyson map \cite{59,60}:

$$O_c = \eta^{\frac{1}{2}} \cdot O_{PT} \cdot \eta^{-\frac{1}{2}}, \hspace{1cm} (5)$$

where $O_c$ is the observable in $PT$-QM framework, $O_{PT}$ is the corresponding observable in CQM. Similarly, there is a relation between the quantum state $\rho_c$ in CQM and the state $\rho_{PT}$ in $PT$-QM:

$$\rho_c = \sum_{mn} \rho_{c mn} |m\rangle \langle n| \Leftrightarrow \rho_{PT} = \sum_{mn} \rho_{c mn} |\phi_m\rangle \langle \chi_n|, \hspace{1cm} (6)$$

where $\{|m\rangle\}$ is a mutual orthogonal basis in CQM, and $\rho_c$ and $\rho_{PT}$ are connected by the Dyson map given above in Eq. (5). Therefore, there is a fixed relation between the quantum states (unnormalized) $\rho_S$ in the framework of CQM and the quantum states $\rho_{PT}$ in the framework of $PT$-QM \cite{50}:

$$\rho_S = \rho_{PT} \cdot \eta^{-1} = \sum_{mn} \rho_{c mn} |\phi_m\rangle \langle \phi_n|, \hspace{1cm} (7)$$

where $\rho_S$ can be normalized by $\text{Tr}(\eta \rho_S) = 1$. Clarifying the relation between the density operator in $PT$-QM and the density operator in CQM is an important step to extend the dynamics simulation scheme of $PT$-symmetric system from pure state to mixed state \cite{50}.

Now we introduce the concept of $\eta$-inner product \cite{6,50}:

$$\langle \psi_1, | \psi_2 \rangle_\eta \equiv \langle \psi_1 | \psi_2 \rangle_\eta := \langle \psi_1 | \eta | \psi_2 \rangle \hspace{1cm} \forall |\psi_1\rangle, |\psi_2\rangle \in L(\mathcal{H}), \hspace{1cm} (8)$$

where $L(\mathcal{H})$ denotes Hilbert space, and $\eta$ is a reversible Hermitian metric operator of this $\eta$-inner space, especially in the unbroken phase of $PT$-QM, it can be a positive operator \cite{6}.

If the non-Hermitian $PT$-symmetric system $H(t)$ is time-dependent, considering two evolving states $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$, we assume that they satisfy the Schrödinger-like equation:

$$\frac{d|\psi(t)\rangle}{dt} = -iH(t)|\psi(t)\rangle. \hspace{1cm} (9)$$

According to the probability conservation in the inner product space defined in the Eq. (3), we can obtain that

$$\frac{d}{dt} \langle \psi_1(t) | \psi_2(t) \rangle_{\eta(t)} = \langle \psi_1(t) | \eta(t) | \psi_2(t) \rangle = \langle \psi_1(t) | -i\eta(t) H(t) + iH^\dagger(t) \eta(t) + \eta(t) | \psi_2(t) \rangle = 0, \hspace{1cm} (10)$$

where we have recorded the differential operator $\frac{d}{dt}$ as the symbol $\cdot$. Then we can get the result:

$$\eta'(t) = i[\eta(t) H(t) - H^\dagger(t) \eta(t)] \hspace{1cm} (11)$$

The above Eq. (11) is referred to the time-dependent (TD) pseudo-Hermiticity relation, $\eta(t)$ is the time-dependent (TD) metric operator in its corresponding inner space \cite{59,60}. It is worth noting that when $H$ is
time-independent, and \( \eta(t) \) can be time-independent so that \( \eta' = 0 \), and then the TD pseudo-Hermiticity relation given above in Eq. (11) will be reduced to the pseudo-Hermiticity relation given in Eq. (2).

The solution of Eq. (11) can be obtained as:

\[
\eta(t) = T e^{-i \int_0^t H^{(1)}(\tau) d\tau} \eta(0) T e^{-i \int_0^t H(\tau) d\tau},
\]

(12)

where \( T \) is time-ordering operator and \( \overline{T} \) is the anti-time-ordering operator, moreover, \( \eta(0) \) can be arbitrary Hermitian operator. If we take \( \eta(0) > 0 \), then there must exist a period of time \( T_\eta \) make \( \eta(t) > 0 \) with \( t \in [0,T_\eta] \).

In addition, according to Eq. (10), if we set \( |\psi(t)\rangle_1 = |\psi(t)\rangle_2 = |\psi(t)\rangle \), and \( \rho_S(t) = |\psi(t)\rangle \langle \psi(t)| \), then we know:

\[
\frac{d \text{Tr}[\rho_S(t)\eta(t)]}{dt} = \frac{d \text{Tr}[\rho_{PT}(t)]}{dt} = 0.
\]

(13)

Here \( \rho_{PT}(t) \equiv \rho_S(t)\eta(t) \) can be seen as a quantum state in TD \( \mathcal{PT} \)-QM, and can be normalized by \( \text{Tr}[\rho_{PT}(t)] = \text{Tr}[\rho_S(t)\eta(t)] = 1 \). The form of \( \rho_{PT}(t) \) can be easily generalized, and can be mapped to a quantum state \( \rho_c(t) \) in (TD) CQM through a time-dependent (TD) similar transformation, i.e., the TD Dyson map similar to Eq. (5) in (TD) CQM through a time-independent (TD) similar transformation, i.e., the TD Dyson map similar to Eq. (5) 60:

\[
O_c(t) = \eta^\frac{1}{2}(t) \cdot O_{PT}(t) \cdot \eta^{-\frac{1}{2}}(t),
\]

(14)

and \( \rho_c(t) \) is similar to Eq. (6):

\[
\rho_c(t) = \sum_{mn} \rho_{c,mn}(t) \langle m(t)| \langle n(t)| \Leftrightarrow \rho_{PT}(t) = \sum_{mn} \rho_{c,mn}(t) \langle \phi_m(t)| \langle \chi_n(t)|,
\]

\[
= \sum_{mn} \rho_{c,mn}(t) \langle \phi_m(t)| \langle \phi_n(t)| \cdot \eta(t),
\]

(15)

where \( \rho_c(t) \) is a quantum state in CQM with the TD orthogonal basis \( \{ |m(t)\rangle \} \), which is a TD mutual orthogonal basis in CQM, and \( \{ |\phi(t)\rangle, |\chi(t)\rangle \} \) is a TD biorthogonal basis in \( \mathcal{PT} \)-QM, and \( |\chi(t)\rangle = \eta(t)|\phi(t)\rangle \). Therefore, if we take \( \eta(0) > 0 \) given in Eq. (11), similar to Eq. (6), we can obtain that

\[
\rho_S(t) = \rho_{PT}(t) \cdot \eta^{-1}(t)
\]

\[
= \sum mn \rho_{c,mn}(t) \langle \phi_m(t)| \langle \phi_n(t)|,
\]

(16)

which means on the promise that \( \eta(t) > 0 \), we can always find an unnormalized quantum state \( \rho_S(t) \) in TD CQM corresponding to a quantum state \( \rho_{PT}(t) \) in TD \( \mathcal{PT} \)-QM (refer to Appendix B in Ref. 50 for the proof that \( \rho_S \) is actually an unnormalized state in (TD) CQM). According to the relation between the unnormalized state of \( \rho_S(t) \) in TD CQM and quantum state \( \rho_{PT}(t) \) in TD \( \mathcal{PT} \)-QM given above in Eq. (16), we know that once \( \eta(t) \) is known (given, or calculated), for the purpose of simulation, \( \rho_S \) can be used to represent \( \rho_{PT} \). It is worth noting that the two are actually different in the physical sense, because they are not satisfied with similarity transformation. Fortunately, for a simulation task, it is not necessary to pursue the absolute equivalence of the two physical meanings, but only to ensure that their form is appropriate and can be realized physically 50. The Eq. (16) is actually the prerequisite for the implementation of the dilation method based on density operator we will discuss next.

III. UNIVERSAL HERMITIAN DILATION METHOD OF NON-HERMITIAN HAMILTONIANS WITH DENSITY OPERATORS

One of methods to simulate the dynamics of \( \mathcal{PT} \)-symmetric system is to find a dilated higher-dimensional Hermitian system (marked by "AS", where "A", "S", "AS" represents the auxiliary system, the main system used to generate the dynamics of the non-Hermitian system, and the composite system, respectively), which obey the von Neumann equation (it reduces to the Schrödinger equation when restricted to pure-state vectors), to simulate the dynamics of non-Hermitian system, which obey the von Neumann-like equation (Schrödinger-like equation in pure-state vector). We assume the evolution equation (the von Neumann-like equation) of unnormalized state \( \rho_S \) that has been mentioned in Eq. (16) is (hereafter, we set \( \hbar = 1 \)) 26 63 61 62:

\[
\frac{d \text{Tr}[\rho_S(t)]}{dt} = -i[H_S(t), \rho_S(t)],
\]

\[
= -i[H_S(t)\rho_S(t) - \rho_S(t)H_S(t)],
\]

(17)

where \( H_S(t) \) is non-Hermitian Hamiltonian in the system \( S \) and can be \( \mathcal{PT} \)-symmetric Hamiltonian, for generality, we assume it is time-dependent, so the time-independent Hamiltonian can be regraded as a special case of it. \( \rho_S(t) \) is an unnormalized state in the system \( S \) at time \( t \), its normalized form is

\[
\rho_{SN}(t) = \frac{\rho_S(t)}{\text{Tr}[\rho_S(t)]},
\]

(18)

where \( \rho_{SN}(t) \) is a legal quantum state (i.e., a positive-semidefinite operator with unit trace) actually measured in the experiment, and \( P_0(t) \equiv \text{Tr}[\rho_{SN}(t)] \) represents the corresponding probability of the measured state in system \( S \) is located in \( \rho_{SN}(t) \) at the time moment \( t \). Because both \( P_0(t) \) and \( \rho_{SN}(t) \) can be measured in an experiment, \( \rho_S(t) \) can be used to represent \( \rho_{SN}(t) \), and this practice meet the common usage 28 30 45 50. The the probability \( P_0(t) \) is actually absorbed in the unnormalized density matrix \( \rho_S(t) \). (see the Ref. 50 and its Appendix B for details). Without misunderstanding, we assume that they are equivalent and are strictly distinguished only when calculating probability. It should be noted that since \( H_S \) is non-Hermitian, \( \text{Tr}[\rho_S(t)] \) is usually not constant, and may be greater than one so that loses its
where \( \hat{\rho} \) is a Hermitian Hamiltonian in the system \( AS \), and \( \rho_{AS}(t) \) is the density operator in this system.

We assume that

\[
\rho_{AS}(t) = \begin{bmatrix} I_S & \rho_S(t) \cdot I_S \end{bmatrix},
\]

where \( \begin{bmatrix} I_S \\ \xi(t) \end{bmatrix} = |0\rangle_A \otimes I_S + |1\rangle_A \otimes \xi(t) \), and we can see that the state \( \rho_{AS}(t) \) is usually an entanglement state.

Meanwhile, we assume

\[
\hat{H}_{AS}(t) = \begin{bmatrix} H_1(t) & H_2(t) \\ H_2^\dagger(t) & H_4(t) \end{bmatrix},
\]

where \( H_1(t), H_2(t), H_4(t) \) are all operators, and it is obvious that \( H_1^\dagger(t) = H_1(t), H_4^\dagger(t) = H_4(t) \), i.e., they are Hermitian, because \( \hat{H}_{AS}(t) \) is Hermitian.

Then according to the probability conservation principle, we know that

\[
\frac{d}{dt}[\rho_{AS}(t)] = \frac{d}{dt}[\rho_S(t) + \xi(t)\rho_S(t)\xi(t)]
\]

\[
= \frac{d}{dt}[\langle \xi(t)\xi(t) + I_S \rangle\rho_S(t)]
\]

\[
= \frac{d}{dt}[\langle M(t) \rangle \rho_S(t)]
\]

\[
= \text{Tr}[M'(t)\rho_S(t) + M(t)\rho_S(t)]
\]

\[
= \text{Tr}\{M'(t)\rho_S(t) - iM(t)\}H_S(t)\rho_S(t) - \rho_S(t)H_S^\dagger(t)\}
\]

\[
= \text{Tr}\{[M'(t) - iM(t)H_S(t) - H_S^\dagger(t)M(t)]\rho_S(t)\}
\]

\[
= 0,
\]

(22)

where we have made

\[ M(t) = \xi^\dagger(t)\xi(t) + I_S. \]

It is obvious that \( M(t) \) is Hermitian and \( M(t) > I_S \), so \( M(t) \) is reversible. For the convenience, we set

\[
\text{Tr}[\rho_{AS}(t)] = \text{Tr}[M(t)\rho_S(t)] = 1.
\]

Then according to Eq. (22), we get the result

\[
M'(t) = -i[H_S^\dagger(t)M(t) - M(t)H_S(t)].
\]

(25)

It is worth noting that the above Eq. (25) has the same form with Eq. (11), so this relation can also be a TD pseudo-Hermiticity relation, which can replace the (time-independent) pseudo-Hermiticity relation like \( H_S^\dagger M \neq MH_S \) [27]. In general, \( M'(t) \neq 0 \), so \( H_S^\dagger(t)M(t) \neq M(t)H_S(t) \), which means \( M(t) \) is not the metric operator of \( H_S(t) \), but only the TD metric operator of the inner space where \( H_S \) is located, and under this metric operator \( H_S(t) \), the probability is conserved. \( M(t) \) is actually the metric operator of TD pseudo-Hermitian Hamiltonian \( h_S(t) \) that will be introduced next.

Then multiplying left and right sides of the above Eq. (25) by \( M^{-1}(t) \), we can get

\[
iM^{-1}(t)M'(t)M^{-1}(t) = M^{-1}(t)H_S^\dagger(t) - H_S(t)M^{-1}(t).
\]

(26)

If we record

\[
K(t) = H_S(t)M^{-1}(t) + \frac{i}{2}M^{-1}(t)M'(t)M^{-1}(t),
\]

(27)

then according to the above Eq. (26), we will find \( K^\dagger = K \), which means \( K(t) \) is Hermitian. The introduction of the operator \( K(t) \) will be very beneficial to our following work. We then introduce a new Hamiltonian \( h_S(t) \):

\[
h_S(t) \equiv K(t)M(t) = H_S(t) + \frac{i}{2}M^{-1}(t)M'(t)M^{-1}(t) = \frac{1}{2}H_S(t) + \frac{1}{2}M^{-1}(t)H_S^\dagger(t)M(t),
\]

(28)

where the Eq. (25) is used in the derivation. Obviously, \( h_S(t) \) is non-Hermitian. At the same time, it is easy to verify that

\[
M(t)h_S(t) = h_S^\dagger(t)M(t),
\]

(29)

which is pseudo-Hermiticity relation mentioned in Eq. (2), and that means that \( h_S(t) \) is actually pseudo-Hermitian Hamiltonian, and \( M(t) \) is actually its metric operator. As we have known in Eq. (23), \( M(t) > I_S \), so according to above Eq. (29), there is a similar transformation make

\[
h_{\text{phys}}(t) \equiv M^\frac{1}{2}(t) \cdot h_S(t) \cdot M^{-\frac{1}{2}}(t) = M^{-\frac{1}{2}}(t) \cdot M(t)h_S(t) \cdot M^{-\frac{1}{2}}(t) = h_{\text{phys}}^\dagger(t),
\]

(30)

which means \( h_{\text{phys}}(t) \) is a Hermitian operator with real eigenspectrum and can be a legal observable in physical, so \( h_S(t) \) is also a legal observable with real eigenspectrum [14] [15] [59] [63]. Unfortunately, the meaning of \( M(t) \) has not been revealed in Ref. [45].

By solving the Eq. (25), we obtain that

\[
M(t) = T e^{-i \int_0^t H_S^\dagger(\tau)d\tau} M(0) T e^{i \int_0^t H_S(\tau)d\tau},
\]

(31)

where \( M(0) \) can be any Hermitian operator except that the condition \( M(0) > I_S \) is satisfied. The above Eq. (31) is
also obtained in Ref.[45]. It is worth noting that, if we take \( M(0) = \eta(0) > 1 \) given in Eq. (12), then \( M(t) \) will be \( \eta(t) \). This means that \( M(t) \) is actually an TD metric operator like \( \eta(t) \) given in Eq. (12). In addition, when \( H_S \) is given, some eigenvalues of \( M(t) \) may be decreases with time in some cases, such as in the \( PT \)-symmetry broken phase of \( H_S \), so we can defined a critical time \( T_1 \) of legitimacy that make \( M(t) \) legal, i.e., \( M(t) > I_S \) when \( t \in [0, T_1) \), while when \( t = T_1 \), at least one of eigenvalues of \( M(T_1) \) become one. It should be noted that \( T_1 \) may be infinite in some cases, such as in the \( PT \)-symmetry unbroken phase of \( H_S \). In addition, in the cases that \( T_1 \neq \infty \), \( T_1 \) will depend on the initial setting of \( M(0) \), in general, \( T_1 \) will increase with \( M(0) \), a big enough \( T_1 \) can always be obtained by scaling \( M(0) \) to meet the requirement of experiment or numerical calculation tasks.

It is worth noting that when the system is \( PT \)-symmetry unbroken, there must be a metric operator \( \eta \) that satisfies \( \eta > 1 \), then \( M(0) \) can be chosen as \( M(0) = \eta \), after that

\[
M(t) = T e^{-i \int_0^t H^\dagger(\tau) d\tau} \eta T e^{i \int_0^t H(\tau) d\tau} = \eta \cdot T e^{-i \int_0^t H^\dagger(\tau) d\tau} \cdot T e^{i \int_0^t H(\tau) d\tau} = \eta, \tag{32}
\]

which means \( M(t) \) will be metric operator and time-independent.

We must point out that when \( H_S \) is time-dependent, the problem of chronological product will have to be considered so the convergence of \( M(t) \) have to be considered in numerical calculation [54, 56], and we will see the adverse effect of the chronological product problem on the numerical calculation in our examples in Sec[V].

Specifically, for an arbitrary TD linear operator (matrix) \( A(t) \), its chronological product problem \( Y(t) = T \exp \left( \int_0^t A(s) ds \right) Y(0) \) has a sufficient but unnecessary convergence conditions:

\[
\int_0^{T_c} \|A(s)\|_2 ds < \pi, \tag{33}
\]

where \( \|A(s)\|_2 \) denotes 2-norm of \( A(s) \). The above integral converges completely only in the interval \( t \in [0, T_c) \) (see more details in Appendix [B]), and \( T_c \) is the critical time of convergence, and it depends only on the operator \( A \) itself. This brings a difficulty to numerical calculation, the critical time \( T_c \) actually bounds how long the numerical calculations we can perform, because before time \( T_c \), the results can be completely trusted, while after time \( T_c \), the results can only be trusted empirically at most. We will see that in the example given in Sec[V].

By the above Eq.(20), we establish a map between \( \rho_S(t) \) and \( \rho_{AS}(t) \), now we try to establish the map between \( H_S(t) \) and \( H_{AS}(t) \), specifically, we need to find the solutions of \( H_1(t), H_2(t), H_4(t) \).

Substituting the Eqs. (20) and (17) into the Eq.(19), we obtain that

\[
\begin{align*}
\frac{d \rho_{AS}(t)}{dt} &= \left[ 0 \; \xi(t) \right] \cdot \rho_{S}(t) \cdot [I_S \; \xi(t)] + \left[ I_S \; \xi(t) \right] \cdot \rho_{0} \cdot [I_S \; \xi(t)] + \left[ I_S \; \xi(t) \right] \cdot \rho_{S} \cdot [0 \; \xi(t)] \\
&= -i \left\{ \left[ I_S \; \xi(t) \right] \cdot \rho_{S}(t) \cdot [I_S \; \xi(t)] - \left[ I_S \; \xi(t) \right] \cdot \rho_{S}(t) \cdot [H_1(t) \; H_2(t)] \; H_4(t) \xi(t) - i \xi(t) \right\} \\
&= -i \left\{ \left[ H_1(t) \; H_2(t) \right] \; I_S \; \xi(t) - \left[ I_S \; \xi(t) \right] \cdot \rho_{S} \cdot [I_S \; \xi(t)] \; \left[ H_1(t) \; H_2(t) \right] \; H_4(t) \xi(t) \right\} \\
&= -i \left\{ H_1(t) + H_2(t) \xi(t) \; H_4(t) \xi(t) \right\} \rho_{S} \cdot [I_S \; \xi(t)] - \left[ I_S \; \xi(t) \right] \cdot \rho_{S} \cdot [H_1(t) + \xi(t) H_2(t) + \xi(t) H_4(t)]. \tag{34}
\end{align*}
\]

According to the above Eq.(34), we can get the following relation

\[
\begin{align*}
H_1(t) + H_2(t) \xi(t) &= H_S(t), \tag{35a} \\
H_2(t) + H_4(t) \xi(t) &= i \xi(t) + (\xi(t) H_S(t). \tag{35b}
\end{align*}
\]

Observing the above equations, we know that the solutions of \( H_1(t), H_2(t), H_4(t) \) are not unique, and \( H_1 \) can be chosen as the unique variable, therefore, we can add a gauge in order to obtain the unique solutions. However, the value of \( H_1 \) is artificially chosen in Ref.[45], so some unique properties of the resulting dilated \( H_{AS} \) may be masked, we will see that in our Sec[V] and especially in Fig.[1] we will see the eigenspectrum of \( H_{AS} \) actually have symmetric property, and \( H_{AS} \) obtained in Ref.[45] is actually the result of the application of a symmetric gauge. We then provide more mathematical completeness.

By observing the Eq.(21), we know that the Hilbert space of \( H_{AS}(t) \) is 2n-dimensional, however, the Hilbert space of \( \rho_{S} \) defined in the Eq.(20) is just n-dimensional,
consequently, similar to the Eq.(20), we can assume that

\[ \rho_{AS}^+(t) = \begin{bmatrix} -\xi^\dagger(t) & \rho_S(t) \cdot [-\xi(t) \cdot IS] \\ IS & [\xi(t) \cdot \rho_S(t) \cdot \xi(t) - \rho_S(t) \rho_S(t) \rho_S(t) \rho_S(t)] \end{bmatrix}. \]  

(36)

It is easy to check that \( \text{Tr}[\rho_{AS}(t) \rho_{AS}^+(t)] = 0 \), which means that the space of \( \rho \) and \( \rho_{AS}^+ \) are mutually orthogonal, then we know that \( \rho \) and \( \rho_{AS}^+ \) are located in two different orthogonal subspaces in the space where \( H_{AS}(t) \) is located. Therefore, we can adopt the following symmetric gauge (there are also some other valid gauges:\ref{40}, \ref{58}, \ref{60}):

\[ \frac{d\rho_{AS}^+(t)}{dt} = -i[\hat{H}_{AS}(t), \rho_{AS}^+(t)]. \]  

(37)

With this gauge, according to the probability conservation principle again, similar with Eq.(22), we can also derive another relation between \( M(t) \) and \( \xi(t) \) as following:

\[ M(t) = \xi(t)\xi^\dagger(t) + IS, \]  

(38)

where \( M(t) \) has been given in the Eq.(31). Comparing the Eq.(38) with the Eq.(23), we get

\[ \xi(t)\xi^\dagger(t) = \xi^\dagger(t)\xi(t), \]  

(39)

which means \( \xi(t) \) will be a normal operator under the symmetric gauge in the Eq.(37), so, for convenience, we make \( \xi(t) \) Hermitian, and then

\[ \xi(t) = [M(t) - IS]^{\frac{1}{2}}. \]  

(40)

At the same time, by adopting the similar method with the Eq.(34), we can obtain the following relation:

\[ -H_1(t)\xi^\dagger(t) + H_2(t) = -i\xi^\dagger(t) - \xi(t)H_S(t) \]  

(41a)

\[ -H_2(t)\xi^\dagger(t) + H_4(t) = H_S(t). \]  

(41b)

Then multiplying the Eq.(35a) right by \( \xi(t) \) and substituting it to the Eq.(41a), we can obtain

\[ H_2(t) = [-i\xi'(t) + H_S(t)\xi(t) - \xi(t)H_S(t)]M^{-1}(t) \]
\[ = K(t)\xi(t) - \xi(t)K(t) - \frac{i}{2}[\xi'(t)M^{-1}(t) + M^{-1}(t)\xi'(t)], \]  

(42)

it is obvious that \( H_2(t) \) is anti-Hermitian. The details of the derivation is given in Appendix A.

Then in the similar way like above, multiplying the Eq.(35b) right by \( \xi(t) \) and substituting it to the Eq.(41b), we can obtain

\[ H_4(t) = [i\xi'(t)\xi(t) + \xi(t)H_S(t)\xi(t) + H_S(t)]M^{-1}(t) \]
\[ = K(t) + \xi(t)K(t)\xi(t) + \frac{i}{2}[\xi'(t)\xi(t)M^{-1}(t) - M^{-1}(t)\xi(t)\xi'(t)]] \]
\[ = H_4(t). \]  

(43)

\( H_4(t) \) is Hermitian obviously. The details of the derivation is given in Appendix A.

Next, according to the Eq.(42) and the Eq.(35a), the result as follows will be obtained:

\[ H_1(t) = H_S(t) - H_2(t)\xi(t) \]
\[ = H_S(t) - [-i\xi'(t) + H_S(t)\xi(t) - \xi(t)H_S(t)] \]
\[ = H_S(t) - M^{-1}(t) \cdot \xi(t) \]
\[ = [i\xi'(t)\xi(t) + \xi(t)H_S(t)\xi(t) + H_S(t)]M^{-1}(t) \]
\[ = K(t) + \xi(t)K(t)\xi(t) + \frac{i}{2}[\xi'(t)\xi(t)M^{-1}(t) - M^{-1}(t)\xi(t)\xi'(t)] \]
\[ = H_4(t). \]  

(44)

Consequently, according to the Eq.(44) and the Eq.(42) we can easily get

\[ H_1(t) + iH_2(t) \]  

\[ \]  

\[ H_1(t) - iH_2(t) \]  

\[ \]  

\[ \text{where } M(t) = \xi^2(t) + IS = [IS \pm i\xi(t)] \cdot [IS \mp i\xi(t)]. \]  

\[ H_1(t) + iH_2(t) \text{ and } H_1(t) - iH_2(t) \text{ are both Hermitian.} \]
Finally, according to the Eq. (21), we obtain the final form of $\hat{H}_{AS}(t)$:

$$\hat{H}_{AS}(t) = \mathcal{S} \otimes H_1(t) + i \sigma_y \otimes H_2(t)$$

$$= |+\rangle \langle +| \otimes [H_1(t) + i H_2(t)]$$

$$+ \mathcal{S} \otimes H_1(t) - i H_2(t)],$$

(46)

where $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A + |1\rangle_A), |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A - i|1\rangle_A)$ are the eigenvalues of $\sigma_y$ corresponding to the eigenvalues of $+1, -1$, respectively. The equation above has a similar form to the result of pure-state case given in Ref. [45] (see Eqs.(19)-(21) in their Supplementary Materials), and the differences are mainly caused by they actually use the basis $\{|-\rangle, -i|+\rangle\}$, while we use the basis $\{|0\rangle, |1\rangle\}$. According to Eq. (46), we can find $\hat{H}(t)$ is highly symmetric under the symmetric gauge of $\mathcal{S}$, and use only one single qubit as its auxiliary system. We have to point out that, whether in experiments or numerical calculations, as long as we use a time-dependent $\hat{H}_{AS}$ given above in Eq. (46), it may be inevitable to solve the problem of chronological product. The reason for the numerical calculation situation is obvious, while in the experiment, $\hat{H}_{AS}(t)$ has to be parameterized in advance by numerically calculating $M(t)$ given in Eq. (31), which needs to numerically computing the chronological product caused by $H_S(t)$, so it usually needs to deal with the problem of chronological product unless any two moments of $\hat{H}_{AS}(t)$ are commute to each other (such as the case of $H_S$ is time-independent and $PT$-symmetry unbroken, then $M(0)$ can be chosen as its metric operator $\eta$ just like the case in Eq. (32) [45]). In fact, the solution of the problem chronological is one of the key factors to the accuracy of dynamics simulation of the TD $PT$-symmetric system, and even the most key factor. We will see the impact of the chronological product on simulation accuracy more clearly in Fig. 3 and Fig. 4 in our example given in Sec. V.

For the convenience of expression, we define the "o" operation like $\mathcal{C} [\hat{A}] = \mathcal{C}_1 [\hat{A}]^\dagger$. After that, looking back Eqs. (17) and (19), their solution can be expressed as:

$$\rho_S(t) = \rho_S(0) \equiv \mathcal{S} \mathcal{T} \mathcal{E}^{-i \int_0^t H_S(\tau)d\tau} \circ \rho_S(0),$$

(47a)

$$\rho_{AS}(t) = \rho_{AS}(0) \equiv \mathcal{S} \mathcal{T} \mathcal{E}^{-i \int_0^t H_{AS}(\tau)d\tau} \circ \rho_{AS}(0),$$

(47b)

where $\hat{H}_{AS}(t)$ has been obtained in Eq. (46), and $\mathcal{U}_S$ is the non-unitary evolution operator related to the non-Hermitian Hamiltonian $H_S$, while $U_{AS}$ is the unitary evolution operator related to the Hermitian Hamiltonian $H_{AS}$. We will call the method of obtaining $\rho_{AS}(t)$ through Eq. (47b) the dilation method, while we call the method of first obtaining $\rho_S$ according to Eq. (47a) and then combining it into $\rho_{AS}$ by Eq. (20) the combination method. The difference between two methods is that there is no need to calculate the delayed Hamiltonian $H_{AS}$ for latter while only need to calculate $M(t)$ given in Eq. (31) and $\xi(t)$ given in Eq. (40). The error of the numerical calculation between the dilation method and the combination method can be defined as follows:

$$\Delta_\rho(t) = \|\rho_{AS,\text{dilation}}(t) - \rho_{AS,\text{combination}}(t)\|_2,$$

(48)

where $\rho_{AS,\text{dilation}}(t)$ denotes the result calculated by the dilation method, while $\rho_{AS,\text{combination}}(t)$ denotes the result calculated by combination method.

We define the measurement operator: $\Pi_k = |k\rangle_A \langle k| \otimes I_S, k \in \{0, 1\}$, and the map $\mathcal{M}_0$: $\mathcal{M}_0[\rho_{AS}] = \text{Tr}_A[\Pi_k \circ \rho_{AS}]$. Therefore, the Eq. (47b) can be mapped to the Eq. (47a) by the map $\mathcal{M}_0$, experimentally, by performing a projection measurement $\prod_0 \equiv |0\rangle_A \langle 0|$ on the auxiliary qubit:

$$\mathcal{M}_0[\rho_{AS}(t)] = \rho_S(t) = \mathcal{T} e^{-i \int_0^t H_S(\tau)d\tau} \circ \rho_S(0),$$

(49)

which means we can simulate the non-unitary evolution (the dynamics) of non-Hermitian system $H_S$ in the higher-dimensional system $\hat{H}_{AS}$. It is worth noting that the map $\mathcal{M}_0$ is realized by a fixed projection measurement (post-selection) $\prod_0 \equiv |0\rangle_A \langle 0|$, which is time-independent, so it will be easy to be realized in experiment [45]. However, the success of this process $\mathcal{M}_0$ is probabilistic, and the corresponding success probability $P_0(t)$ is

$$P_0(t) = \text{Tr}[\rho_S(t)].$$

(50)

Obviously, in general, $P_0(t) < 1$. After the map $\mathcal{M}_0$, the state in main system $S$ will be $\rho_{SN}(t)$ in Eq. (18) with success probability $P_0(t)$ given above. It is worth mentioning that the success probability may be optimized by technical means, such as using the local-operations-and-classical-communication (LOCC) protocol scheme proposed in Ref. [50], which may be of significance for experiment.

In particular, when $H_S$ is $PT$-unbroken and time-independent, according to the result of Eq. (32), we can take the operator $M(t) \equiv \eta$, where $\eta$ is a positive metric operator and $\eta > 1$, and then according to the Eqs. (27), (41), (42) and (43), $K, H_1, H_2, H_4$ will all be time-independent, specifically, according to Eqs. (4), they will become [43, 49, 50]:

$$M(t) \equiv \eta \Rightarrow \xi = (\eta - I_S)^{\frac{1}{2}},$$

(51a)

$$K \equiv H_S \cdot \eta^{-1} \equiv \Phi \cdot E_S \cdot \Phi^\dagger,$$

(51b)

$$H_1 = H_S \eta^{-1} + \xi H_S \eta^{-1} \xi = \Phi E_S \Phi^\dagger + \xi \cdot \Phi E_S \Phi^\dagger \cdot \xi,$$

(51c)

$$H_2 = H_S \eta^{-1} \xi - \xi H_S \eta^{-1} = \Phi E_S \Phi^\dagger \cdot \xi - \xi \cdot \Phi E_S \Phi^\dagger = -H_2^\dagger,$$

(51d)

$$H_4 = H_S \eta^{-1} + \xi H_S \eta^{-1} \xi = \xi^{-1} (H_S \eta^{-1} + \eta H_S - H_S - H_S^\dagger) \xi^{-1} + H_S \eta^{-1} = H_1.$$
where $\Phi, \eta$ are given in Eqs.(4). They are the same as the results we obtained in Ref.[50]. Therefore, according to Eq.(45), $H_1 \pm iH_2$ will also become time-independent:

$$H_1 + iH_2 = (I_S - i\xi)\Phi \circ E_S = \Phi_+ \circ E_S, \quad (52a)$$

$$H_1 - iH_2 = (I_S + i\xi)\Phi \circ E_S = \Phi_- \circ E_S, \quad (52b)$$

where $\Phi_{\pm} = (I_S \mp i\xi)$. At the same time, the dilated higher-dimensional system $\hat{H}_{AS}$ will also become time-independent, and according to the result of Eq.(46):

$$\hat{H}_{AS} = I_A \otimes H_1 + i\sigma_y \otimes H_2$$

$$= I_A \otimes (H_S\eta^{-1} + i\xi H_S\eta^{-1} \xi) + i\sigma_y \otimes (H_S\eta^{-1} \xi - \xi H_S\eta^{-1})$$

$$= V_{AS} \circ [I_A \otimes E_S], \quad (53)$$

where

$$V_{AS} = \frac{1}{\sqrt{2}}[(I_A + i\sigma_x) \otimes I_S - i(\sigma_y + \sigma_z) \otimes \xi] \cdot I_A \otimes \Phi$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} \Phi_+ & i\Phi_- \\ i\Phi_+ & \Phi_- \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} (I_S - i\xi)\Phi & i(I_S + i\xi)\Phi \\ i(I_S - i\xi)\Phi & (I_S + i\xi)\Phi \end{pmatrix}$$

is an unitary operator, while $V_{AS}$ is not unique. This is also the result in Ref.[50]. From the above Eq.(53), it can be found that the degeneracy of higher-dimensional dilated system $\hat{H}_{AS}$ is twice that of lower-dimensional $\mathcal{PT}$-symmetric system $H_S$.

### IV. Vectorization of Density Operator and Matrizization of Liouvillian Superoperators in Open Quantum System

The evolution equation of an open quantum system with a Markovian approximation (i.e., memoryless) can be expressed by Lindblad master equation [52] (we set $\hbar = 1$ hereafter):

$$\frac{d\rho_{AS}(t)}{dt} = \mathcal{L}\rho_{AS}(t) = -i[\hat{H}, \rho_{AS}(t)] + \sum_{\mu} \mathcal{D}[\Gamma_{\mu}]\rho_{AS}(t), \quad (54)$$

where $\rho_{AS}(t)$ is the density operator of the system, $\Gamma_{\mu}$ is the jump operator, $\mathcal{L}$ is the Liouvillian superoperator, and $\mathcal{D}[\Gamma_{\mu}]$ is the dissipator associated with the $\Gamma_{\mu}$, which is used to describe the dissipation:

$$\mathcal{D}[\Gamma_{\mu}] \rho_{AS}(t) = \Gamma_{\mu} \rho_{AS}(t) \Gamma_{\mu}^\dagger - \frac{\Gamma_{\mu}^\dagger \Gamma_{\mu}}{2} \rho_{AS}(t) - \rho_{AS}(t) \frac{\Gamma_{\mu}^\dagger \Gamma_{\mu}}{2}. \quad (55)$$

The operator-sum representation is a convenient tool to describe the open system, various models of decoherence and dissipation in open quantum systems have been widely studied, such as amplitude damping (AD) channel model, phase damping (PD) channel model, and depolarizing (Dep) channel. In some cases of simple decoherence (such as the case of Hamiltonian $H = 0$), these channel models have a concise form in the framework of operator-sum representation, however, when the Hamiltonian gets complicated just like the one in Eq.(46), the application of the operator-sum representation will be indirect and inconvenient. Therefore, the vectorization of density operator and matrixization of superoperators (VDMS) technique may be a more convenient tool (see the Appendix of Ref.[52] for details).

We adopt VDMS technique to carry out Kraus decomposition of density operator in matrix basis $\{|\alpha\rangle, |\beta\rangle, \alpha, \beta = 1, 2, \cdots, n\}$ [53]. In this VDMS technique, a matrix $A$ can be mapped to $\hat{A}$ by stacking all the rows of the matrix $A$ to a column in order

$$A = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} \rightarrow \hat{A} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix},$$

so the density operator $\rho$ will be mapped to the vector $\hat{\rho}$, and the superoperators $A[^\dagger] = A[^\dagger]B$ will be mapped into a matrix, which can be recorded as $\hat{A}[^\dagger] = A[^\dagger]B[^\dagger]$. Meanwhile, give the matrix $B$

$$B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix},$$

in the vectorization technique, the Hilbert-Schmidt inner product can be introduced:

$$\langle B|A \rangle = |b_1^* b_2^* b_3^* b_4^* \rangle \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} = \text{Tr}[B[^\dagger]A], \quad (56)$$

where $|A\rangle, \langle B|$ are actually the $\hat{A}, \hat{B}[^\dagger]$ mentioned above. From this point of view, it is easy to find the vector of $\rho_{AS}$ given in Eq.(20), and $\rho_{AS}[^\dagger]$ given in Eq.(36) will still be mutually orthogonal.

Therefore, the Lindbald superoperator $\mathcal{L}$ in Eq.(54) will be mapped to

$$\overline{\mathcal{L}}(t) = -i[\hat{H}_{AS}(t) \otimes I - I \otimes \hat{H}_{AS}(t)]$$

$$+ \sum_{\mu} [\Gamma_{\mu} \otimes \Gamma_{\mu}^* - \frac{\Gamma_{\mu}^\dagger \Gamma_{\mu}}{2} - \frac{\Gamma_{\mu} \Gamma_{\mu}^\dagger}{2}], \quad (57)$$

where the superscript $T$ denotes the transpose operation, while the symbol “*” denotes the conjugate operation. After that the Eq.(19) will be mapped to

$$\frac{d\hat{\rho}_{AS}(t)}{dt} = \overline{\mathcal{L}}(t)\hat{\rho}_{AS}(t), \quad (58)$$
and then we can get the solution of the above equation:

\[ \tilde{\rho}_{AS}(t) = T e^{i \tilde{Z}(\tau) d\tau} \tilde{\rho}_{AS}(0), \]

(59)

where \( T \) is the time-ordering operator mentioned above in the Eq. (12), and \( \tilde{\rho}_{AS}(0) \) is the vector representation of the initial density operator \( \rho_{AS}(0) \). In general, the dilated \( \hat{H}_{AS}(t) \) is time-dependent, so \( \tilde{Z} \) will also be time-dependent, so the problem of chronological product may also have to be dealt with (see more details in Appendix B and our example given in Sec. V).

V. AN EXAMPLE: 2-DIMENSIONAL \( \mathcal{PT} \)-SYMMETRIC SYSTEM

In this section, we analyze an example: 2-dimensional \( \mathcal{PT} \)-symmetric system:

\[ H_S = \begin{bmatrix} r e^{i\theta} & s \\ s & r e^{-i\theta} \end{bmatrix}, r, s \in \mathbb{R}, \theta \in [-\pi/2, \pi/2], \]

(60)

\( \theta \) can be understood as the parameter characterizing the degree of non-Hermiticity of the Hamiltonian \( H_S \), and the degree of non-Hermiticity will increase with \( |\theta| \) (when \( \theta = 0 \), \( H_S \) will be Hermitian, when \( \theta = \pi/2 \), \( H_S \) will be anti-Hermitian, see Sec. V in Ref. [45] for details). The eigenvalues of \( H_S \) are \( E_k = r \cos \theta \pm \sqrt{s^2 - r^2 \sin^2 \theta} \), and when \( s^2 - r^2 \sin^2 \theta > 0 \), \( H \) is \( \mathcal{PT} \)-symmetry unbroken, otherwise, when \( s^2 - r^2 \sin^2 \theta < 0 \), \( H \) is \( \mathcal{PT} \)-symmetry broken, then the two eigenvalues are complex conjugate.

The results of pure-state vector case has been given in Ref. [45], to facilitate comparison with the results in Ref. [45], we set the \( \theta = \pi/2, s = 1 \), which make \( H_S \) have the same form as in Ref. [45], and set \( M(0) = 5I_S \) given in Eq. (31). We set the initial density operator of pure state case as \( \rho_S(0) = \frac{1}{3} |0\rangle_S \langle 0| \), which correspondings to the initial state \( |0\rangle_S \) in Ref. [45], and the coefficient \( \frac{1}{3} \) is required by Tr\[|\rho_{AS}\rangle \langle \rho_{AS}| \equiv 1 \) according to Eq. (24). We set the initial density operator of mixed state case as \( \rho_{S,\text{mixed}}(0) = \frac{1}{30} \begin{bmatrix} 4 & 1 \\ 1 & 2 \end{bmatrix} \), this case can not be described by the pure-state vector used in Ref. [45]. Under this parameter configuration, the system is in the \( \mathcal{PT} \)-symmetry unbroken phase, and the eigenvalues of \( H_S \) will be \( E_{\pm} = \pm \sqrt{1 - r^2} \). In addition, according to Eq. (16) and Eq. (33), the critical time \( T_{\text{dilation}} \) of convergence given below Eq. (31), which is used to represent how long the trusted numerical calculation task of the dilation method through Eq. (49) can continue, can be calculated to be \( T_{\text{dilation}} \approx 3.52 \) according to Eq. (64) given later.

A. The effectiveness of the density operator tool and the eigenspectrums of Hamiltonians before and after dilation

The eigenvalues of \( \mathcal{PT} \)-symmetric Hamiltonian \( H_S \) \((E_{\pm})\) and the eigenvalues of its dilated Hermitian Hamiltonian \( H_{AS} \) \((E_1, E_2, E_3, E_4, \text{arranged in descending order}) \) are given in Fig. (a). Fig. (a) is about the \( \mathcal{PT} \)-symmetric unbroken phase \((r = 0.6, E_{\pm} = \pm \sqrt{1 - 0.6^2} = \pm 0.8) \) will be conjugate complex numbers, which is exactly what \( \mathcal{PT} \)-symmetry theory predicts [6], while Fig. (b) is about the broken phase \((r = 1.4, E_{\pm} = \pm \sqrt{1 - 1.4^2} = \pm 0.98i) \). From the Fig. (a), we can see \( E_{\pm} \) remain unchanged, while \( E_1 \) and \( E_2 \) oscillate around \( E_+ \) and \( E_3 \) and \( E_4 \) oscillate around \( E_- \) and change periodically with time \( t \) (in this case, the critical time \( T_i \) of legitimacy given below Eq. (33) under the setting \( r = 0.6 \) is infinite). Meanwhile, \( E_3 \) and \( E_4 \) are symmetric about \( E = 0 \) (black dashed line). From the Fig. (b), we can see that \( E_k \)'s \((k = 1, 2, 3, 4) \) are also symmetric about \( E = 0 \) (black dashed line), which is similar as the case of unbroken phase. In fact, the symmetry in the case of unbroken and broken phase is caused by the symmetric gauge adopted in Eq. (37). However, the periodicity oscillation of \( E_k \)'s are destroyed, and \( E_k \)'s increase (decrease) monotonically.

![Graph A](image1.png)

**FIG. 1.** The eigenvalues of \( \mathcal{PT} \)-symmetric Hamiltonian \( H_S \) (green curves with small circles or boxes, \( E_{\pm} = \pm 0.8 \)) and the eigenvalues of its dilated Hermitian Hamiltonian \( \hat{H}_{AS} \) (curves with other colors, \( E_1, E_2, E_3, E_4 \)). (a) \( \mathcal{PT} \)-symmetry unbroken phase \((r = 0.6, T_i = \infty) \). (b) \( \mathcal{PT} \)-symmetry broken phase, \( E_\pm = \pm 0.98i \) \((r = 1.4, T_i \approx 0.604) \).
with time $t$. Especially, when $t \to T_1$ (the critical time $T_1$ of legitimacy under the setting $r = 1.4$ is about 0.604), $E_1$ ($E_2$) will increase (decrease) sharply to infinity, which is caused by one of eigenvalues of $M(t)$ given in Eq. (61) tend to zero. In this situation, the energy of system $H_{AS}$ may diverge, and can not be realized by an experiment. In a summary, the critical time $T_1$ of convergence actually bounds the duration of implemented experimental running.

We also characterize the evolution using the renormalized population $P_{N0}(t)$ of state $\rho_S(0)$ in main system $S$ [45]. In this case, the renormalized population $P_{N0}(t)$ can be obtained by

$$P_{N0}(t) = \frac{\text{Tr}[0_{S(t)} \cdot \rho_S(t)]}{\text{Tr}[\rho_S(t)]} = \frac{0_{S(t)} \cdot 0_{S}}{P_0(t)},$$

where $P_0(t) = \text{Tr}[\rho_S(t)]$ has been given below Eq. (18). The result based on the pure-state vector has been given analytically in Ref. [45] as follows:

$$P_{N0}(t) = \begin{cases} 
\frac{|e^{\sqrt{-t} r} - e^{-\sqrt{-t} r}|^2}{(r+1)^2}, & r \neq 1 \\
\frac{|e^{\sqrt{-t} r} - e^{-\sqrt{-t} r}|^2 + |e^{-\sqrt{-t} r} - e^{\sqrt{-t} r}|^2}{(r+1)^2 + 4}, & r = 1.
\end{cases}$$

According to Eq. (47a) and above Eq. (61), we can calculate the renormalized population $P_{N0}(t)$ under the initial density operator $\rho_S(0)$. To verify the effectiveness of density operator method in Sec. III, we take $r = 0.6$ and draw the Fig 2. The green curve is drawn according to analytical results based on the pure-state vector given in the above Eq. (62), while the blue doted curve is drawn according to Eqs. (47a) and (61), and we can find their results are completely consistent, which means that our results based on the density operator compatible the pure-state vector case, just as we intuitively think.

It should be pointed out that the Hamiltonian $H_S$ in this example is time-independent, so the chronological product problem can be avoid in the calculation of $M(t)$ according to Eq. (61), so the blue doted curve is able to match green curve so well in Fig 2.

**B. The influence of three kinds of quantum noise generated in main system**

In the experimental simulation of $\mathcal{PT}$-symmetric system dynamics, the quantum state will inevitably be disturbed by quantum noises, especially if the state is entangled, the influence of the noises may be more serious so that have to be studied carefully. In this section, we introduce the three common quantum noise channel models and using the VDMS technique mentioned in Sec. IV to characterize the Lindblad master equation corresponding to them. We only consider the situation that the noise acts on the main system space (similarly, the situation acting on the auxiliary system can also be considered). Based on that, we analysis their effects on the simulation of $\mathcal{PT}$-symmetric system dynamics.

In AD channel, and PD channel mentioned blow Eq. (55), there is only one jump operators (for convenience, all parameters of decay rate have been set to $\gamma$):

$$\Gamma_{AD} = \sqrt{\gamma} \sigma^S = \sqrt{\gamma} |0\rangle_S \langle 1|, \Gamma_{PD} = \sqrt{\gamma} \sigma^S_z;$$

while in Dep channel, there are three jump operators: $\Gamma_{Depk} = \sqrt{\gamma} \sigma^S_k$, where $k = x, y, z, \{\sigma^S_k\}$ are Pauli operators, and subscript $S$ indicates it acts on the main system, and the complete form of any operator $X$ with different superscripts is $X^S = I_A \otimes X^S, X^A = X^A \otimes I_S$.

Considering the system $\hat{H}_{AS}(t)$ used to simulate the $\mathcal{PT}$-symmetric system dynamics in Eq. (46), and substituting jump operators into Eq. (57), we obtain that

![FIG. 2. Comparisons of the results for 2-dimensional $\mathcal{PT}$-symmetric dynamics simulation (unbroken phase) between the method based on pure-state vector (green curve) and the method based on density operator (blue doted curve) ($\theta = \pi/2, s = 1, r = 0.6$). Both X and Y axes are dimensionless. In this case, the system is in $\mathcal{PT}$-symmetry unbroken phase.](image-url)
Specifically, in the calculation, the operator system $\mathcal{AS}$ by Magnus series given in Eq.(B4) in Appendix B, 

$$
\mathcal{T}_{\text{AD}}(t) = -i[H_{\text{AD}}(t) \otimes I_S - I_{\text{AD} \otimes H_{\text{AS}}^T(t)}] + \gamma \left[ |0\rangle_S \langle 1|_S \otimes (|0\rangle_S \langle 1|)^*_{S} - \frac{1}{2} |1\rangle_S \langle 1|_S \otimes I_S - I_S \otimes \frac{(|1\rangle_S \langle 1|)^*}{2} \right],
$$

$$
\mathcal{T}_{\text{PD}}(t) = -i[H_{\text{PD}}(t) \otimes I_S - I_{\text{PD} \otimes H_{\text{AS}}^T(t)}] + \gamma [\sigma^\gamma \otimes (\sigma^\gamma)^*_{\gamma} - I_S \otimes I_S],
$$

$$
\mathcal{T}_{\text{Dep}}(t) = -i[H_{\text{Dep}}(t) \otimes I_S - I_{\text{Dep} \otimes H_{\text{AS}}^T(t)}] + \gamma \sum_{k=x,y,z} [\sigma^k \otimes (\sigma^k)^* - I_S \otimes I_S],
$$

(63a, 63b, 63c)

where $\hat{H}_{\text{AD}}(t)$ is the dilated Hamiltonian in Eq.(46), $I_S$ and $I_S$ represent the identity operator in the composite system $AS$ and the main system $S$, respectively.

Specifically, we calculate Eqs.(63) and Eqs.(47) to (49) by Magnus series given in Eq.(B4) in Appendix B,

$$
\Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t),
$$

(64)

where $\Omega_1, \Omega_2, \Omega_3$ are Magnus series of first, second and third orders given in Eq.(49) (see Appendix B for details), and only first three order are used in this example. Specifically, in the calculation, the operator $\mathcal{A}(t)$ given in Eq.(B1) can be replaced by $-i\mathcal{H}_{\text{AD}}(t)$ obtained in Eq.(46), and $\mathcal{T}_{\text{AD}}(t), \mathcal{T}_{\text{PD}}(t), \mathcal{T}_{\text{Dep}}(t)$ given in Eqs.(63).

Based on the density operator, we are able to consider the effect of quantum noise on the simulation of the dynamics of $\mathcal{PT}$-symmetric system $\mathcal{H}_S$. The critical time of convergence of $T_c^{\text{simulation}} \approx 3.52, T_c^{\text{PT}} \approx 1.58, T_c^{\text{PD}} \approx 1.50, T_c^{\text{Dep}} \approx 1.38$ mentioned below Eq.(63) according to Eq.(49). Eqs.(63) and Eq.(61), we can calculate the renormalized population $P_{N_0}(t)$ under AD, PD, Dep channel and no noise, respectively. Under the parameter settings of Fig.3, the critical time of legitimacy mentioned below Eq.(61) $T_1 = \infty$ because in the $\mathcal{PT}$-symmetry unbroken phase of $\mathcal{H}_S$, all eigenvalues of $\mathcal{H}_S$ are real.

The relation between the renormalized population $P_{N_0}$ and time $t$ is given in Figs.3. The Figs.3(a) to 3(c) is related to Magnus series from first order to expansion to third order according to Eq.(47b) and Eqs.(63). At first, we focus on the cases of no noise, which are related to the green curves (combination method) and blue dotted curves (dilation method) in the Figs.3. Comparing Fig.3(a), Fig.3(b) with Fig.3(c), we find blue dotted curves in the left side of truncated bar will be more and more closer to the corresponding green curves with the calculated order of Magnus series increases, which shows that the results obtained by the dilation method given in Eq.(49) are more and more closer to the results obtained by combination method given in Eq.(47a), which can be understood as the theoretical value because of the $\mathcal{H}_S$ given in Eq.(60) is time-independent so that the chronological product problem in Eq.(47a) can be avoided. This point can be seen more clearly from the error curves calculated by Eq.(48) in the left side of the truncated line (they are related to the convergence time $T_c$ discussed below Eq.(63) in Fig.3 to 3(f)). From the error curves in the left side of the truncated line, we can see that the error is reduced on the whole with the order of Magnus series increases, and the error is no more than 0.05 in the case of calculated Magnus series to third order (Fig.3(f)). This result prove that the solution of the problem chronological product is one of the key factors to the accuracy of dynamics simulation of the TD $\mathcal{PT}$-symmetric system based on the dilation method, and even the most key factor.

Now we focus on the right side of truncated bar (line) in each curves. However, from Fig.3(a) to 3(b), we can see that the blue dotted curve gets closer to the green curve, while from Fig.3(b) to Fig.3(c), it becomes further from the green curve, the same phenomenon can also be seen in the mixed state case in Fig.4(a). It can be understood more clearly from Fig.3(d) to Fig.3(f), and Fig.4(b). This phenomenon is caused by Magnus series expanded in the nonconvergent region ($t > T_c$). In general, in the convergence region, expanding the Magnus series to the second or third order can meet the requirements of numerical calculation.

Now we focus on the effects of quantum noises on the renormalized population $P_{N_0}$. From Fig.3(a) to 3(c), we can find in the complete convergence region, the curves related to Dep channel drops rapidly, and faster than the cases of AD, PD channels, which is caused by the tendency of Dep channel that transform any quantum state into a maximal mixed state, where $P_{N_0}$ will keep 1/2. The similar phenomenon can also be seen in mixed state density operator case in Fig.4 where we have set the density operator of mixed sate as $\rho_{N_0}(0) = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$. Meanwhile, in the initial short time, the red curves related to AD channel almost coincides with the cyan curves related to PD channel, while after a long time, they separate form each other. The similar phenomenon can also be seen in Fig.4. However, this phenomenon is accidental because the initial pure-state density operator $\rho_S(0) = \frac{1}{4} |0\rangle_S \langle 0|_S$ is just located on the eigenstate (steady state, or fixed point of superoperator of the channel ) of the dissipation terms of AD channel given in Eq.(63a) and PD channel given in Eq.(63b), so their roles can be ignored in a short time, and only the left terms containing $H_{\text{AD}}(t)$ play the roles, while in the long run, the evolution state $\rho_S(t)$ is far away from the initial pure state $|0\rangle_S$, so it can be affected by the dissipation terms that the roles of dissipation terms can not be ignored.
FIG. 3. The effects of quantum noises on the dynamics of simulation of $\mathcal{PT}$-symmetry unbroken system under the initial state of pure state density operator ($\gamma = 0.25, \theta = \pi/2, s = 1, r = 0.6$). Both $X$ and $Y$ axes are dimensionless. (a-c) Renormalized population $P_{N0}$ under Magnus series from expansion to first order to expansion to third order according to Eq.(49) and Eqs.(63). The linestyles (doted curve) and colors associated with each noise (including no noise) are represented differently. The small vertical dashed line on each curve is a truncated bar related to convergence, and we have set their color to be same as the corresponding curves. Due to the convergence problem of chronological product, the curves in the left side of truncated bar are absolutely convergent, so they can be completely trusted, while the curves in the right side are not necessarily convergent, and can only be used as a reference. The linestyles of each curves on both sides of the bar are set to be different, but the color same. (d-e) The errors between the green curves and the blue doted curves corresponding to subfigures (a-c).
Compared with the case of mixed state, we can understand this phenomenon more clearly. From Fig.[3] we can see that in a short time, all the curves including noise and no noise cases rise, which are the results driven by Hamiltonian $\hat{H}_{AS}(t)$. However, the case of AD channel rises faster than all other curves, because AD channel has a tendency to change all states to the state $|0\rangle$, which will contribute the renormalized population $\rho_{N0}$ (more strictly, $|0\rangle$ is the fixed point (steady state) of AD channel $[52,64]$.

The effects of quantum noises on the dynamics of simulation of $\mathcal{PT}$-symmetry broken system under the initial state of pure-state density operator $\rho_S = \frac{1}{2} |0\rangle_S \langle 0|$ are given in Fig.[5] and the renormalized population $\rho_{N0}$ is calculated to the third order of Magnus series. The Magnus series always converges during simulation time ($t \in [0,T_l]$) because $T_l \approx 0.604 < T_c$ (including noises case and no-noise case), then the legitimacy will be lost after the critical time $T_l$. From Fig.[5]a we can see that all curves decrease monotonically, which are caused by the eigenvalues of $H_S$ will be complex number, so dissipative terms will appear in the evolution operator $e^{-iH_S t}$. In addition, the blue curve and the green curve almost completely coincide in the whole interval $t \in [0, T_l]$, which can be seen more clearly in the error diagram given in Fig.[5]b, which shows a high accuracy.

VI. CONCLUSIONS AND DISCUSSIONS

In this work, we generalized the results of Wu et al. in Ref.$[45]$, which are based on dilution method, from the pure-state vector case to the mixed-state case with the help of density operator, and provided a general theoretical framework based on density operator to analytically and numerically analyze the dynamics of TD arbitrary $\mathcal{PT}$-symmetric system and the influence of quantum noises. We make conclusions from the perspective of analytical analysis and numerical analysis, respectively.

At first, from the perspective of analytical analysis, more physical completeness was provided. In the process of derivation, we discussed the physical meaning of $M(t)$ ignored in Ref.$[45]$. Specifically, we proved that $M(t)$ is not the metric operator of $\mathcal{PT}$-symmetric system $H_S$, but the TD metric operator of $M(t)$-inner space, which satisfy probability conservation. Meanwhile, we also gave a Hamiltonian $\hat{H}_{S}(t)$ related to $M(t)$, and proved it actually is a physical observable, because it can be mapped to the Hermitian Hamiltonian $H_{phys}$, which has a real spectrum, through a TD similar transformation, i.e., the TD Dyson map. In addition, more mathematical completeness was also provided by us. Specifically, in the derivation, we obtained the dilated Hamiltonian $\hat{H}_{AS}(t)$ by attaching a symmetric gauge instead of artificially assigning a value to the free variable as in Ref.$[45]$. As a result, the hidden symmetry of the eigenspectrum of the dilated Hamiltonian $\hat{H}_{AS}(t)$ was able to be revealed. It is worth noting that when the system considered is $\mathcal{PT}$-symmetry broken, the results of dynamics simulation of this work are consist with our previous results in Ref.$[50]$, and when the state considered is pure state, the results of this work are consist with the theoretical results given in Ref.$[45]$. Because the dilated system $\hat{H}_{AS}(t)$ is actually located in an open quantum system, the influence of environment will be inevitable, we introduced the tool of VDM to solve the Lindblad master equation under three kinds of quantum noise, then the influence of quantum noises can be studied in the dynamics simulation of $\mathcal{PT}$-symmetric system.

Then, from the perspective of numerical analysis, we pointed out that the trusted duration of numerical calculation is actually bounded by the critical time $T_c$ of convergence of Magnus series, this phenomenon occurs because the dilated higher-dimensional Hamiltonian $\hat{H}_{AS}(t)$ is usually time-dependent, the chronological product problem have to be solved, and the Magnus series have to be calculated, which may diverge when $t > T_c$ (see Fig.[3]a)-(c)). Meanwhile, the implemented duration of experimental running is actually bounded by the critical time $T_l$ of legitimacy of dilation method, this phenomenon occurs because when $t \rightarrow T_l$, at least one of eigenvalues of $M(t)$ given in Eq.(31) will be close to one, then the corresponding eigenvalue of $\xi(t)$ given in Eq.(40) will be close to zero, so the energy may diverge (see Fig.4(a)). In fact, the problem of chronological has to be solved not only in numerical calculation, but also even in experiment, because $\hat{H}_{AS}(t)$ has to be parameterized in advanced by calculating chronological product. We also found that the solution of the problem chronological product is one of the key factors to the accuracy of dynamics simulation of the TD $\mathcal{PT}$-symmetric system based on the dilation method, and even the most key factor. When considering the influence of quantum noises, according to the results of numerical calculation in our example, we knew the depolarizing noise is the most fatal to the dynamics simulation of $\mathcal{PT}$-symmetric system among three kinds of quantum noise we considered and should be avoided as much as possible.

Finally, we have to mention that in Sec VI, we actually gave an example of time-independent Hamiltonian rather that TD Hamiltonian, just like in Ref.$[45]$, for the purpose of facilitate display and comparison. However, the method of analysis and calculation is universal, and what needs additional attention is only to be careful about the convergence of chronological product when calculating $M(t)$ given in Eq.(31), which has been avoid in our example.

VII. ACKNOWLEDGEMENTS

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FIG. 4. The effects of quantum noises on the dynamics of simulation of $\mathcal{PT}$-symmetry unbroken system ($\gamma = 0.25, \theta = \pi/2, s = 1, r = 0.6$) under the initial state of mixed-state density operator. Both $X$ and $Y$ axes are dimensionless. (a) Renormalized population $P_{N0}$ under Magnus series from expansion to first order to expansion to third order according to Eq.(49) and Eqs.(63). The linestyles (dotted curve) and colors associated with each noise (including no noise) are represented differently. The small vertical dashed line on each curve is a truncated bar related to convergence, and we have set their color to be same as the corresponding curve. Due to the convergence problem of chronological product, the curves in the left side of truncated bar are absolutely convergent, so they can be completely trusted, while the curves in the right side are not necessarily convergent, and can only be used as a reference. The linestyles of each curves on both sides of the bar are set to be different, but the color same. (b) The error between the green curve and the blue dotted curve corresponding to (a).

FIG. 5. The effects of quantum noises on the dynamics of simulation of $\mathcal{PT}$-symmetry broken system ($\gamma = 0.25, \theta = \pi/2, s = 1, r = 1.4$) under the initial state of pure-state density operator. Both $X$ and $Y$ axes are dimensionless. (a) Renormalized population $P_{N0}$ under Magnus series expansion to third order according to Eq.(49) and Eqs.(63). The linestyles (dotted curve) and colors associated with each noise (including no noise) are represented differently. The curve converges in the whole time interval. (b) The error between the green curve and the blue dotted curves corresponding to (a).
Appendix A: Derivations of $H_2(t)$ and $H_4(t)$

Here we drive $H_2(t)$, $H_4(t)$ expressed by the operator $K(t)$ in the main text. First of all, we know

$$M'(t) = (\xi^2(t) + I)' = \xi'(t)\xi(t) + \xi(t)\xi'(t), \quad (A1)$$

\[H_2(t) = [-i\xi'(t) + H_S(t)\xi(t) - \xi(t)H_S(t)]M^{-1}(t)\xi(t)
= -i\xi'(t)M^{-1}(t) + H_S(t)M^{-1}(t)\cdot \xi(t) - \xi(t)H_S(t)M^{-1}(t)
= -i\xi'(t)M^{-1}(t) + [K(t) - \frac{i}{2}M^{-1}M'(t)M^{-1}(t)]\xi(t) - \xi(t)[K(t) - \frac{i}{2}M^{-1}M'(t)M^{-1}(t)]
= K(t)\xi(t) - \xi(t)K(t) - \frac{i}{2}[2\xi'(t)M^{-1}(t) + M^{-1}(t)M'(t)\xi(t)\xi(t)M^{-1}(t) - M^{-1}(t)[\xi'(t)\xi(t) + \xi(t)\xi'(t)]M^{-1}(t)]
= K(t)\xi(t) - \xi(t)K(t) - \frac{i}{2}[2\xi'(t)M^{-1}(t) - M^{-1}(t)[M(t) - I]M^{-1}(t)]
= K(t)\xi(t) - \xi(t)K(t) - \frac{i}{2}\xi'(t)M^{-1}(t) - M^{-1}(t)\xi'(t). \quad (A2)\]

In the similar way above, according to Eq. (43),

$$H_4(t) = [i\xi'(t)\xi(t) + \xi(t)H_S(t)\xi(t) + H_S(t)]M^{-1}(t)
= i\xi'(t)\xi(t)M^{-1}(t) + H_S(t)M^{-1}(t) + \xi(t)H_S(t)M^{-1}(t)\xi(t)
= i\xi'(t)\xi(t)M^{-1}(t) + K(t) - \frac{i}{2}M^{-1}M'(t)M^{-1}(t) + \xi(t)[K(t) - \frac{i}{2}M^{-1}M'(t)M^{-1}(t)]\xi(t)
= K(t) + \xi(t)K(t)\xi(t) + \frac{i}{2}M^{-1}(t)[2M(t)\xi'(t)\xi(t) - \xi'(t)\xi(t) + \xi(t)\xi'(t)] - \xi(t)[\xi'(t)\xi(t) + \xi(t)\xi'(t)]M^{-1}(t)
= K(t) + \xi(t)K(t)\xi(t) + \frac{i}{2}M^{-1}(t)[2M(t)\xi'(t)\xi(t) - \xi'(t)\xi(t) + \xi(t)\xi'(t)] - \xi(t)[\xi'(t)\xi(t) + \xi(t)\xi'(t)]M^{-1}(t)
= K(t) + \xi(t)K(t)\xi(t) + \frac{i}{2}M^{-1}(t)[M(t)\xi'(t)\xi(t) + \xi(t)\xi'(t)]M^{-1}(t)
= K(t) + \xi(t)K(t)\xi(t) + \frac{i}{2}[\xi'(t)\xi(t)M^{-1} - M^{-1}(t)\xi'(t)]. \quad (A3)\]

Appendix B: Problem of chronological product

Considering a matrix differential equation [54]:

$$Y'(t) = A(t)Y(t), \quad Y(t_0) = Y_0, \quad (B1)$$

where $A(t)$ is a known time-dependent matrix, $Y_0$ is the initial value of $Y(t)$, and $Y(t)$ is the matrix to be solved.
The formal solution of above equation is [55, 56]:

\[ Y(t) = \mathcal{T} \exp \left( \int_{t_0}^{t} A(s) ds \right) Y_0, \quad (B2) \]

where \( \mathcal{T} \) is the time-ordering operator. For arbitrary two time \( t_1 \) and \( t_2 \) \((t_1 \neq t_2)\), in general, \([A(t_1), A(t_2)] \neq 0\), then \( e^{A(t_1)+A(t_2)} \neq e^{A(t_1)} \cdot e^{A(t_2)} \), the symbol \( \mathcal{T} \) can not be ignored. When \([A(t_1), A(t_2)] = 0\) for arbitrary two time \( t_1 \) and \( t_2 \), especially when \( A \) is time-independent, the symbol \( \mathcal{T} \) can be ignored.

The Eq. (B2) can be expressed as [56]:

\[ Y(t) = \exp \left( \Omega(t, t_0) \right) Y_0, \quad (B3) \]

where \( \Omega(t) \) can be written as the sum of series:

\[ \Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t). \quad (B4) \]

Magnus point out that differential of \( \Omega \) with respect to \( t \) can be written as:

\[ \Omega' = \frac{\text{ad}_\Omega}{\exp (\text{ad}_\Omega) - 1} A, \quad (B5) \]

so the solutions of above equation constitute Magnus expansion, or Magnus series.

The term \( \Omega_n \) can be obtained by \( S_n^{(j)} \), which can be obtained by the following recursive formula:

\[ S_n^{(j)} = \sum_{m=1}^{n-j} \left[ \Omega_m, S_{n-m}^{(j-1)} \right], \quad 2 \leq j \leq n - 1 \]
\[ S_n^{(1)} = [\Omega_{n-1}, A], \quad S_n^{(n-1)} = \text{ad}_{\Omega_{n-1}}^{(n-1)}(A), \quad (B6) \]

where \( \text{ad}_\Omega \) is a shorthand for an iterated commutator, and

\[ \text{ad}_\Omega^0 A = A, \quad \text{ad}_\Omega^{k+1} A = \left[ \Omega, \text{ad}_\Omega^k A \right]. \quad (B7) \]

Therefore, we can get

\[ \Omega_1(t) = \int_0^t A(t_1) dt_1 \]
\[ \Omega_2(t) = \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [A(t_1), A(t_2)] \]
\[ \Omega_3(t) = \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \cdot \]
\[ \cdot ([A(t_1), [A(t_2), A(t_3)]], [A(t_3), [A(t_2), A(t_1)]]) \]
\[ \Omega_4(t) = \frac{1}{12} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4 \cdot \]
\[ \cdot ([A(t_1), [A(t_2), [A(t_3), A(t_4)]]) + [A_1, [A_2, [A_3, A_4]]] + [A_1, [A_2, [A_3, A_4]]] + [A_2, [A_3, [A_4, A_1]]]). \quad (B9) \]

It is worth noting that the Magnus series in Eq. (B4) may diverge [56], and a sufficient condition for it to converge for \( t \in [0, T] \) is:

\[ \int_0^T \|A(s)\|_2 ds < \pi, \quad (B10) \]

where \( \|A\|_2 \) denotes 2-norm of \( A \).
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