

Internal nonlocality in generally dilated HermiticityMinyi Huang ^{1,2,*} and Ray-Kuang Lee ^{3,4,5,6,†}¹*Interdisciplinary Center of Quantum Information, State Key Laboratory of Modern Optical Instrumentation, and Zhejiang Province Key Laboratory of Quantum Technology and Device, Department of Physics, Zhejiang University, Hangzhou 310027, China*²*Department of Mathematical Sciences, Zhejiang Sci-Tech University, Hangzhou 310018, People's Republic of China*³*Institute of Photonics Technologies, National Tsing Hua University, Hsinchu 300, Taiwan*⁴*Department of Physics, National Tsing Hua University, Hsinchu 300, Taiwan*⁵*Center for Quantum Technology, Hsinchu 30013, Taiwan*⁶*Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan*

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According to von Neumann, the global Hamiltonian of the whole universe must be Hermitian in order to keep the eigenvalues real and to construct a self-consistent quantum theory. In addition to the open system approach by introducing environmental degrees of freedom to a small system, a global Hermitian Hamiltonian can also be generated through the dilation from a small Hilbert space. For example, a local non-Hermitian \mathcal{PT} -symmetric system can be simulated with a global Hermitian one by the Naimark dilation. Recently, by introducing local measurements and investigating the correlation functions of outcomes, the internal nonlocality in such dilated Hermitian systems has been revealed, but only for a special case with a twofold structure. In this paper, we extend such a discussion to the generalized case when the twofold structure breaks. The internal nonlocality is discussed with different correlation pictures and the corresponding correlation bounds. Our results provide a device-independent test of the reliability of the simulation in the global Hermiticity.

DOI: [10.1103/PhysRevA.105.052210](https://doi.org/10.1103/PhysRevA.105.052210)**I. INTRODUCTION**

By introducing the environment of infinite free space to an open system, an effective non-Hermitian Hamiltonian can be obtained from a global Hermitian Hamiltonian after eliminating the environmental degrees of freedom [1]. Typically, complex eigenvalues of resonant states are produced due to the coupling between the local subsystem and the macroscopic environment. However, parity-time (\mathcal{PT}) symmetry assumes that the local subsystem can be non-Hermitian but in a parameter regime of real eigenvalues [2]. The symmetry under the combination of time-reversal and parity operations, or more generally an antilinear operation combined with linear operations, can be generalized to the pseudo-Hermiticity [3–6] and anti- \mathcal{PT} symmetry [7,8], with either real or conjugate pairs of complex eigenvalues. Many theoretical and experimental applications of \mathcal{PT} -symmetric systems have been found [9–14] and recently extended to the field of dynamics and topology [15].

Similar to the Feshbach formalism dealing with an effective description [1], \mathcal{PT} -symmetric systems can be viewed as effective models in the sense of open systems. In 2008, Günther and Samsonov showed that a class of unbroken two-dimensional \mathcal{PT} -symmetric Hamiltonians can always be dilated to some four-dimensional Hermitian ones [16]. In fact, by using the dilation techniques, one can simulate any

finite dimensional unbroken \mathcal{PT} -symmetric systems in dilated Hermitian systems [17–20]. By evolving states under the dilated Hermitian Hamiltonians, it is always possible to simulate the evolution of unbroken \mathcal{PT} -symmetric Hamiltonians in subspaces. On the other hand, for broken \mathcal{PT} -symmetric systems, their evolutions can also be simulated by utilizing time-dependent Hermitian Hamiltonians [21].

In the simulation of \mathcal{PT} -symmetric systems, the dilated Hermitian Hamiltonians play an important role, which governs a composite system. By projecting the dilated Hamiltonians to some subsystems, the effect of \mathcal{PT} -symmetric Hamiltonians can be realized [18]. Owing to the non-Hermiticity of \mathcal{PT} -symmetric systems, the dilated Hamiltonians usually bring nonlocal correlations between the subsystems. Recently, by proposing different correlation pictures, the internal nonlocality of these dilated Hamiltonians was discussed [22]. By evaluating the correlations with local measurements in three different pictures, the resulting different expectations of the Bell operator revealed the distinction of the internal nonlocality. Such a result provides the figure of merit to test the reliability of the simulation, as well as to verify a \mathcal{PT} -symmetric (sub)system.

However, the known discussions mainly focus on Günther and Samsonov's special example, depending highly on the special form of the dilated Hamiltonian. In general, such a twofold structure may not exist in a generic dilated Hermitian Hamiltonian. Then how can one have an effective way to verify a more general \mathcal{PT} -symmetric Hamiltonian when the twofold structure breaks? Furthermore, similar to the device-independent test of the state nonlocality [23], can we also

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have a detection-loop-hole-free test of the reliability of the simulation in the global Hermiticity?

In this paper, we propose a generalization of the scenario in Ref. [22]. The correlation pictures are extended in different ways, obtaining the expectations of the Bell operator and their bounds. It is shown that the correlation behaviors are more complex and have alternative features in the general case. A direct reflection of this is for the generic Bell operator expectations. In contrast to the results in Ref. [22], the Bell operator expectations often have some energy shifts in the general case. Moreover, the deviation bounds should be tackled carefully, instead of a simple order relation. This also leads to the conception of a genuine local Hermitian picture in the general case. Interestingly, the energy shifts and the deviation bounds can also help to distinguish the global Hermitian Hamiltonians.

The remainder of this paper is organized as follows. In Sec. II we introduce the preliminaries for the related notions of \mathcal{PT} -symmetric systems, the concept of dilation, and the previously known results on the extraction of internal nonlocality [22]. In Sec. III we propose different correlation pictures for general Hermitian dilations. The expectations of the Bell operator and their bounds are obtained. Section IV concerns the problem of how to distinguish a dilated Hermitian Hamiltonian. In Sec. V we discuss our findings. Finally, we conclude our results in Sec. VI.

II. PRELIMINARIES

A. The concept of dilation

By dilating a time-independent \mathcal{PT} -symmetric Hamiltonian H , we mean that one can find some Hermitian operator $\hat{H} = \begin{bmatrix} H_1 & H_2 \\ H_2^\dagger & H_4 \end{bmatrix}$ and an invertible Hermitian operator τ such that for any vector ψ ,

$$\begin{bmatrix} i\psi' \\ i(\tau\psi)' \end{bmatrix} = \begin{bmatrix} H_1 & H_2 \\ H_2^\dagger & H_4 \end{bmatrix} \begin{bmatrix} \psi \\ \tau\psi \end{bmatrix} = \begin{bmatrix} H\psi \\ \tau H\psi \end{bmatrix}. \quad (1)$$

\hat{H} is called a dilated Hermitian Hamiltonian or a Hermitian dilation of H .

Note that for the first component, $i\psi' = H\psi$. According to the Schrödinger equation,

$$\psi(t) = e^{-itH}\psi(0),$$

an effective \mathcal{PT} -symmetric system is realized.

For an unbroken \mathcal{PT} -symmetric Hamiltonian H , one can prove that such an operator τ always exists and satisfies the following condition:

$$H^\dagger(I + \tau^2) = (I + \tau^2)H. \quad (2)$$

With τ , one can construct different \hat{H} satisfying Eq. (1), among which a typical one is

$$\hat{H} = I_2 \otimes H_1 + i\sigma_y \otimes H_2, \quad (3)$$

$$H_1 = (H\tau^{-1} + \tau H)(\tau^{-1} + \tau)^{-1}, \quad (4)$$

$$H_2 = (H - \tau H\tau^{-1})(\tau^{-1} + \tau)^{-1}. \quad (5)$$

Compared with the general case in Eq. (1), the dilated Hamiltonian \hat{H} in Eq. (3) depends only on H_1 and H_2 . Such a neat

and symmetric form (twofold structure) has some interesting properties. For example, one can prove that the \hat{H} in Eq. (3) has the same eigenvalues as H . For more details of the dilation problem see Refs. [16,18,19].

B. Two-dimensional example

Let us start with the two-dimensional \mathcal{PT} -symmetric Hamiltonian [16,24],

$$H = E_0 I_2 + s \begin{bmatrix} i \sin \alpha & 1 \\ 1 & -i \sin \alpha \end{bmatrix}. \quad (6)$$

The eigenvalues of H are $\lambda_{\pm} = E_0 \pm s \cos \alpha$. Moreover, there exists an exceptional point when $\sin \alpha = \pm 1$ ($\alpha = \pm \frac{\pi}{2}$), in which case the Hamiltonian cannot be diagonalized. When $\alpha \neq \pm \frac{\pi}{2}$, the Hamiltonian H has real eigenvalues and can be diagonalized. Hence, \mathcal{PT} symmetry is unbroken. In particular, when $\sin \alpha = 0$, i.e., $\alpha = 0$ or π , the Hamiltonian is also Hermitian. In the following, we do not consider the case of broken \mathcal{PT} symmetry, since time-independent dilation applies only to the case of unbroken \mathcal{PT} symmetry. We do not consider the Hermitian case since it is trivial.

For the \mathcal{PT} -symmetric Hamiltonian in Eq. (6), a possible way to have the Hermitian dilation \hat{H} is [16,18]

$$\hat{H} = I_2 \otimes H_1 + i\sigma_y \otimes H_2, \quad (7)$$

where

$$H_1 = E_0 I_2 + \frac{\omega_0}{2} \cos \alpha \sigma_x, \quad (8)$$

$$H_2 = i \frac{\omega_0}{2} \sin \alpha \sigma_z, \quad (9)$$

$$\omega_0 = 2s \cos \alpha, \quad (10)$$

and

$$\tau = \frac{1}{\cos \alpha} \begin{bmatrix} 1 & -i \sin \alpha \\ i \sin \alpha & 1 \end{bmatrix}. \quad (11)$$

It can be verified that the above example is a special case of Eqs. (3)–(5). Moreover, \hat{H} has the same eigenvalues as H , with multiplicities of two. According to Eq. (3) or Eq. (7), the dilated Hermitian Hamiltonian \hat{H} is inseparable. That is, \hat{H} cannot be written as a tensor product of two local operators. As a consequence, such a global Hamiltonian \hat{H} can bring nonlocal correlations to the subsystems, which leads to the discussion of nonlocality [22].

C. The internal nonlocality in simulating \mathcal{PT} -symmetric systems

A profound approach to discussing the nonlocality is the CHSH (Clauser, Horne, Shimony, and Holt) scenario [25,26]. In this scenario, there are two observers, Alice and Bob, sharing an entangled state, on which they can perform local measurements. What they want to see is whether the entanglement can bring some nontrivial correlations between the subsystems. Suppose that Alice can make local measurements A_1 and A_2 , whose outcome is denoted by a . Due to the randomness of the local measurement, the outcome a can take different values, e.g., $a \in \{+1, -1\}$. Similarly, Bob can perform two measurements B_1 and B_2 with his outcome

$b \in \{+1, -1\}$. A natural way to see the correlations between the outcomes is to investigate the expectation value of the product ab . For instance, $\langle A_i B_j \rangle = \sum_{ab} ab P(ab|i_j)$ represents the expectation value of ab for given measurements $A_i B_j$, where $P(ab|i_j)$ is the joint probability distribution. In particular, one can calculate the expectation of the following Bell operator:

$$S = B_0 A_0 + B_0 A_1 + B_1 A_0 - B_1 A_1.$$

In the classical setting, one is not concerned with the quantum realization but only a classical (local) description of what Alice and Bob can do. Under this assumption, the probability of Alice and Bob's outcomes does not depend on each other. Thus the joint probability distribution admits a product decomposition of Alice and Bob's marginal probability distributions $p(ab|i_j) = \int p(a|i, v)p(b|j, v)q(v)dv$, where v is some hidden variable with $q(v)$ its distribution. In this case, derivations show that $|\langle S \rangle| \leq 2$. However, in the quantum setting, A_i and B_j correspond to different operators, and the expectation value is $\langle S \rangle = \text{Tr}(S\rho)$, where ρ is the density operator of the entangled state. Now the bound of $|\langle S \rangle|$ is $2\sqrt{2}$. The discrepancy between the two bounds shows the difference between the classical (local) and nonlocal correlations, having a far-reaching influence both theoretically and experimentally. For more details of the standard CHSH inequality, see [25].

In the following, we briefly review a CHSH-like discussion on the nonlocal correlations introduced by the dilated Hermitian Hamiltonian of Eq. (7). Since now the correlations come from the global Hamiltonian rather than an entangled state, we call it *internal nonlocality* to distinguish it from the standard CHSH scenario. Similar to the CHSH's quantum and classical settings giving different Bell operator expectations and bounds, one can also propose different pictures to discuss the internal nonlocality [22].

1. The simulation picture

Suppose Alice and Bob share the dilated Hermitian Hamiltonian \hat{H} in Eq. (7). Similar to the CHSH scenario, they can make local measurements A_i and B_j . Since now we are discussing the correlations introduced by the Hamiltonian, Alice and Bob's "local measurements" are actually local states. Let Alice have the local state $\{|u_+\rangle = u|0\rangle + v|1\rangle\}$ for A_0 and $\{|u_-\rangle = \bar{v}|0\rangle - \bar{u}|1\rangle\}$ for A_1 ; while Bob have two local states $\{|0\rangle\}$ and $\{|1\rangle\}$ for B_0 and B_1 , respectively. Then the expectations of $B_j A_i$ can be calculated as follows:

$$\langle B_0 A_0 \rangle = \text{Tr}(|0\rangle\langle 0| \otimes |u_+\rangle\langle u_+|) \hat{H}, \quad (12)$$

$$\langle B_1 A_0 \rangle = \text{Tr}(|1\rangle\langle 1| \otimes |u_+\rangle\langle u_+|) \hat{H}, \quad (13)$$

$$\langle B_0 A_1 \rangle = \text{Tr}(|0\rangle\langle 0| \otimes |u_-\rangle\langle u_-|) \hat{H}, \quad (14)$$

$$\langle B_1 A_1 \rangle = \text{Tr}(|1\rangle\langle 1| \otimes |u_-\rangle\langle u_-|) \hat{H}. \quad (15)$$

Now, one can further consider the expectation value of the Bell operator:

$$\begin{aligned} \langle B_0 A_0 \rangle + \langle B_0 A_1 \rangle + \langle B_1 A_0 \rangle - \langle B_1 A_1 \rangle \\ = 2E_0 + (\bar{u}v + u\bar{v})\omega_0 \cos \alpha. \end{aligned} \quad (16)$$

For the last deviation term shown in Eq. (16), we have the following bound:

$$|(\bar{u}v + u\bar{v})\omega_0 \cos \alpha| \leq |\omega_0 \cos \alpha| = |2s \cos^2 \alpha|. \quad (17)$$

2. The classical picture

The classical picture means that one skips the details of quantum mechanics but considers only a classical description of what Alice and Bob do. To give such a classical picture, several key points must be emphasized. First, the classical picture should be consistent with the simulation picture. It requires that Alice has a " \mathcal{PT} -symmetric like" subsystem, and the joint measurements of Alice and Bob reveal the characteristics in the global Hamiltonian \hat{H} . A natural consequence is to assume that the measurement results from A_i are just λ_{\pm} , namely, the eigenvalues of the \mathcal{PT} -symmetric Hamiltonian H . Moreover, note that the dilated Hermitian Hamiltonian \hat{H} has the same eigenvalues as the \mathcal{PT} -symmetric Hamiltonian H but with a multiplicity of two. Hence the results of B_i should be 1, such that the correlation functions $B_j A_i$ trivially give the eigenvalues of \hat{H} . Second, the "results" of Alice and Bob are independent, leading to a classical (nonlocal) correlation. In fact, since Bob's results always give 1, apparently the two observers' results and the corresponding probability distributions are independent. Thus, we do have a classical local picture.

To calculate the expectation of the Bell operator, note that $\langle B_j A_i \rangle = \sum_{ab} ab p(ab|i_j)$, where the results $a = \lambda_{\pm}$ and $b = 1$. Like the standard CHSH scenario, one can formally write $p(ab|i_j) = \int p(a|i, \mu)p(b|j, \mu)q(\mu)d\mu$, where μ is a hidden variable with $q(\mu)$ its distribution such that $\int q(\mu)d\mu = 1$. By changing the variable $dv = q(\mu)d\mu$ and denoting $A_i(v) = \sum_a ap(a|i, v)$, $B_j(v) = \sum_b bp(b|j, v)$, one can see that $\langle B_j A_i \rangle = \int B_j(v)A_i(v)dv$, where $\int 1dv = 1$. Unlike the standard CHSH scenario, we use only local states rather than an entangled state, and hence the measurements B_j and A_i are completely independent, without an interaction through v (or μ). Thus one can assume that $A_i(v)$ and $B_j(v)$ are constants independent of v . Moreover, by definition $\int A_i(v)dv = \sum_a ap(a|i)$ and $\int B_j(v)dv = \sum_b bp(b|j) = 1$, hence we see that $A_i(v) = \sum_a ap(a|i)$ and $B_j(v) = 1$. Then

$$\begin{aligned} \langle B_0 A_0 \rangle + \langle B_0 A_1 \rangle + \langle B_1 A_0 \rangle - \langle B_1 A_1 \rangle \\ = \int [B_0(v)(A_0 + A_1)(v) + B_1(v)(A_0 - A_1)(v)] dv \\ = \int [(A_0 + A_1)(v) + (A_0 - A_1)(v)] dv \\ = 2E_0 + \omega_0 (p_+ - p_-), \end{aligned} \quad (18)$$

where $p_{\pm} = p(\lambda_{\pm}|0)$ are the probabilities corresponding to the situations when the results of A_0 are λ_{\pm} . Moreover,

$$|\omega_0(p_+ - p_-)| \leq |\omega_0| = |2s \cos \alpha|. \quad (19)$$

3. Local Hermitian picture

In this picture, we try to give a description of what Alice and Bob do by some Hermitian Hamiltonians \hat{H}_i , which is in a tensor product form of two local Hermitian Hamiltonians. The key concept in this picture is that it should be consis-

tent with the simulation. To this end, $\hat{H}_l = I \otimes H_h$, where $H_h = \lambda_+ |s_+\rangle\langle s_+| + \lambda_- |s_-\rangle\langle s_-|$ and $|s_\pm\rangle$ are two orthogonal states. Apparently, due to the form of \hat{H}_l , the results of Alice's local measurements are λ_\pm , which is the same as the simulation picture. Moreover, the form of \hat{H}' implies that it will not introduce nonlocal correlations between the subsystems.

By replacing the Hamiltonian \hat{H} in Eqs. (12)–(15) with \hat{H}_l , the expectation of the Bell operator is

$$\begin{aligned} & \langle B_0 A_0 \rangle + \langle B_1 A_0 \rangle + \langle B_0 A_1 \rangle - \langle B_1 A_1 \rangle \\ & = 2E_0 + \omega_0 (p_+ - p_-), \end{aligned} \quad (20)$$

where $p_\pm = |\langle u_+ | s_\pm \rangle|^2$.

There are two motivations to consider the local Hermitian picture. The first one is to show the difference between a dilated Hermitian Hamiltonian and a global Hamiltonian which will not bring in nonlocal correlations (thus it cannot be used for simulation). Such a global Hermitian Hamiltonian is necessarily a tensor product of two local Hermitian Hamiltonians. The second motivation is to consider a concrete quantum realization of the classical picture. Since the classical picture is an abstract description of the measurements from the perspective of nonlocal correlations, through the comparison, a quantum realization of the classical picture may give us a deeper understanding on the features of internal nonlocality. In fact, by comparing Eq. (20) with Eq. (16) and Eq. (18), all the expectations in the three pictures contain two terms. The common term $2E_0$ is the sum of the two eigenvalues λ_+ and λ_- , while the other one represents a deviation term. Apparently, the deviations have a relatively simple order relation on their numerical bounds. The classical and local Hermitian pictures have the same form of deviation term, which usually gives a larger bound than the simulation picture. Such a result can help to distinguish the dilated Hermitian Hamiltonian [22].

In the above discussions, the special form of the dilated Hamiltonian \hat{H} implicitly plays a key role, especially in the classical and local Hermitian pictures. It renders a reasonable way to correlate Alice and Bob's subsystems, as well as to establish the connections between the dilated Hamiltonian \hat{H} and the \mathcal{PT} -symmetric Hamiltonian H . Based on this, one can propose the classical and local Hermitian pictures and compare the corresponding Bell operator expectations in different pictures [22].

III. THE GENERAL CASE

If we are considering the general case, \hat{H} may not have such a special form as Eq. (7). Moreover, the dilated Hermitian Hamiltonian \hat{H} may even have eigenvalues different from H . Then can we discuss the internal nonlocality for a general \hat{H} ? In the following, we show that this is possible.

Such a generalization is based on the following observation: If \hat{H} is a Hermitian dilation of a \mathcal{PT} -symmetric Hamiltonian H [i.e., Eq. (1) is valid for \hat{H} and τ], then we have

$$\begin{bmatrix} H_1 & H_2 \\ H_2^\dagger & H_4 \end{bmatrix} \begin{bmatrix} -\tau\psi \\ \psi \end{bmatrix} = \begin{bmatrix} -\tau H^\perp \psi \\ H^\perp \psi \end{bmatrix}, \quad (21)$$

where

$$H^\perp = -H_2^\dagger \tau + H_4, \quad (22)$$

$$H_2 = (H - H_1)\tau^{-1}, \quad (23)$$

$$H_4 = (\tau H - H_2^\dagger)\tau^{-1}. \quad (24)$$

Utilizing Eqs. (1) and (2), one can verify Eqs. (21)–(24) through direct calculations (see the Appendix Sec. A for details). In addition, note that there is some freedom to determine the dilated Hamiltonian \hat{H} . In fact, Eqs. (23) and (24) show that a different Hermitian matrix H_1 usually yields different \hat{H} . Equation (21) also shows that the eigenvalues of the Hamiltonian H^\perp are just the eigenvalues of the dilated Hermitian Hamiltonian \hat{H} .

Equations (1) and (21) show the effect of the Hermitian dilation \hat{H} when it is confined to the subsystems. In fact, Eq. (1) can be written as

$$\hat{H}(|0\rangle|\psi\rangle + |1\rangle|\tau\psi\rangle) = |0\rangle|H\psi\rangle + |1\rangle|\tau H\psi\rangle.$$

By postselecting the ancillary system in state $|0\rangle$, we have

$$\hat{H} : |0\rangle|\psi\rangle \rightarrow |0\rangle|H\psi\rangle.$$

Similarly, Eq. (21) can also be written as

$$\hat{H}(-|0\rangle|\tau\psi\rangle + |1\rangle|\psi\rangle) = -|0\rangle|\tau H^\perp\psi\rangle + |1\rangle|H^\perp\psi\rangle.$$

By postselecting the ancillary system in state $|1\rangle$, we have

$$\hat{H} : |1\rangle|\psi\rangle \rightarrow |1\rangle|H^\perp\psi\rangle.$$

Thus, the effect of \hat{H} can be represented by two Hamiltonians: one is the \mathcal{PT} -symmetric Hamiltonian H , the other is H^\perp .

In particular, it can be verified that if H_1 takes the special form in Eq. (4), then $H^\perp = H$ and the dilated Hermitian Hamiltonian \hat{H} reduce to the special case of Eq. (3). In this special case, we build up connections between \hat{H} and H to discuss the internal nonlocality. For the general case, both H and H^\perp will be connected with \hat{H} . To be more precise, one can assume that Alice is either measuring the Hamiltonian H or H^\perp and the joint measurements of Alice and Bob depict the characteristics of the global Hamiltonian \hat{H} . Similar to the discussion in Sec. II, it is possible to reconstruct the different correlation pictures in the general case.

A. The simulation picture

In the following, we discuss the correlation pictures for general dilated Hamiltonians of the \mathcal{PT} -symmetric Hamiltonian H in Eq. (6). For the convenience of discussion, we specify some notations. Let us denote the special dilated Hamiltonian in (7) by $\hat{H} = \begin{bmatrix} H_1 & H_2 \\ H_2^\dagger & H_4 \end{bmatrix}$, where $H_4 = H_1$. Denote a generally dilated Hermitian Hamiltonian by $\hat{H}' = \begin{bmatrix} H_1' & H_2' \\ (H_2')^\dagger & H_4' \end{bmatrix}$. When confined to the subspaces, the effect of \hat{H}' can be depicted by H and $(H^\perp)'$. Denoting $\hat{H}'' = \hat{H}' - \hat{H}$, we then have $\hat{H}_i'' = \hat{H}_i' - \hat{H}_i$. In particular, we denote

$$H_1'' = \hat{H}_1' - \hat{H}_1 = \begin{bmatrix} a + c & d + ib \\ d - ib & a - c \end{bmatrix}.$$

In a general simulation picture, what Alice and Bob do is the same as the special case. They conduct measurements and calculate the expectation of the Bell operator, which

is given by Eqs. (12)–(15) with \hat{H} replaced by \hat{H}' . Calculations show that the numerical value of the expectation is (see the Appendix Secs. B and C for details)

$$\begin{aligned} & \langle B_0A_0 \rangle + \langle B_0A_1 \rangle + \langle B_1A_0 \rangle - \langle B_1A_1 \rangle \\ & = 2E_0 + 2a + \omega_0''(p_+'' - p_-''), \end{aligned} \quad (25)$$

where

$$\omega_0'' = 2\sqrt{(s \cos^2 \alpha + d)^2 + \frac{(b + b \sin^2 \alpha + 2a \sin \alpha)^2}{\cos^4 \alpha}} + c^2 \quad (26)$$

is the difference of the two eigenvalues of H_4' , $p_{\pm}'' = |\langle u_+ | s_{\pm}'' \rangle|^2$ and $|s_{\pm}'' \rangle$ are the eigenstates of H_4' .

Comparing Eq. (25) with Eq. (16), one can see that now the expectation of the Bell operator has an energy shift $2a$. For the deviation term, we have

$$|\omega_0''(p_+'' - p_-'')| \leq \omega_0''.$$

B. The classical picture

The classical picture gives a generic description of what Alice and Bob do, regardless of the details of realization. The key to this picture is that Alice and Bob's results are independent, only with classical (local) correlations.

To have such a classical picture, we consider the following scenario. Suppose Alice can make two measurements A_0 and A_1 . The results of A_0 are the eigenvalues of H , and the results of A_1 are the eigenvalues of $(H^\perp)'$. However, Alice knows only that one of A_i outputs the eigenvalues of H and the other outputs the the eigenvalues of $(H^\perp)'$. Moreover, we assume that Alice makes measurements in some black box; that is, she is unaware of which measurement she has conducted. Briefly speaking, Alice can only obtain the measurement results but cannot distinguish between A_0 and A_1 . As for Bob, his results are always 1. Thus, their results are independent, implying the correlations are classical (local). Denote the eigenvalues of $(H^\perp)'$ by λ'_{\pm} . The expectation of Bell operator is (see the Appendix Secs. B and C for details)

$$\begin{aligned} & \langle B_0A_0 \rangle + \langle B_0A_1 \rangle + \langle B_1A_0 \rangle - \langle B_1A_1 \rangle \\ & = E_0 + E'_0 + \frac{1}{2}[\omega_0(p_+ - p_-) + \omega'_0(p'_+ - p'_-)], \end{aligned} \quad (27)$$

where

$$E'_0 = \frac{1}{2}(\lambda'_+ + \lambda'_-) = E_0 + \frac{2(a + b \sin \alpha)}{\cos^2 \alpha} \quad (28)$$

and

$$\begin{aligned} \omega'_0 & = \lambda'_+ - \lambda'_- \\ & = 2\sqrt{\left(s + \frac{2d}{\cos^2 \alpha}\right)^2 \cos^2 \alpha + \frac{4c^2}{\cos^2 \alpha} + \frac{4(b + a \sin \alpha)^2}{\cos^4 \alpha}}. \end{aligned} \quad (29)$$

p_{\pm} are the probabilities that the measurement results are λ'_{\pm} . For the deviation term, we have

$$\left| \frac{1}{2}[\omega_0(p_+ - p_-) + \omega'_0(p'_+ - p'_-)] \right| \leq \frac{1}{2}(\omega'_0 + |\omega_0|).$$

C. The local Hermitian and genuine local Hermitian picture

There are different approaches to generalizing the local Hermitian picture, which we call local Hermitian and genuine local Hermitian pictures for the general case.

The local Hermitian picture aims at describing what Alice and Bob do by using local Hermitian Hamiltonians. As was mentioned, when the ancillary system is postselected in $|0\rangle$ or $|1\rangle$, the effect of \hat{H} can be represented by H and $(H')^\perp$, respectively. Hence to be consistent with the simulation, the global Hamiltonian in the local Hermitian picture is

$$\hat{H}'_l = |0\rangle\langle 0| \otimes H_h + |1\rangle\langle 1| \otimes (H^\perp)'_h, \quad (30)$$

where H_h and $(H^\perp)'_h$ are Hermitian Hamiltonians having the same eigenvalues as H and $(H^\perp)'$, respectively. Due to this, when the ancillary system is in the state $|0\rangle$ or $|1\rangle$, the measurement results of \hat{H}'_l are the eigenvalues of H_h or $(H^\perp)'_h$, which is similar to \hat{H}' .

Suppose that $H_h = \lambda_+ |s_+\rangle\langle s_+| + \lambda_- |s_-\rangle\langle s_-|$ and $|s_{\pm}\rangle$ are two orthogonal states. Similarly, $(H^\perp)'_h = \lambda'_+ |s'_+\rangle\langle s'_+| + \lambda'_- |s'_-\rangle\langle s'_-|$ and $|s'_{\pm}\rangle$ are two orthogonal states. Replacing \hat{H} with \hat{H}'_l in Eqs. (12)–(15), the expectation of the Bell operator is (see the Appendix Secs. B and C)

$$\langle B_0A_0 \rangle + \langle B_1A_0 \rangle + \langle B_0A_1 \rangle - \langle B_1A_1 \rangle = 2E_0 + \omega'_0(p'_+ - p'_-), \quad (31)$$

where $p'_{\pm} = |\langle u_+ | s'_{\pm} \rangle|^2$. Apparently, for the deviation term

$$|\omega'_0(p'_+ - p'_-)| \leq \omega'_0.$$

In the special case of Ref. [22], the local Hermitian picture can be viewed as a quantum realization of the classical picture, yielding the same form of the Bell operator expectation. However, Eqs. (27) and (31) show that they often differ in the general case. In particular, the deviation bounds do not have a simple order relation as that in Ref. [22].

To realize the Bell operator expectation in the classical picture by utilizing local Hermitian Hamiltonians, we introduce the genuine local Hermitian picture. The global Hamiltonian is given by

$$\hat{H}'_g = \frac{1}{2}I \otimes (H_h + (H^\perp)'_h). \quad (32)$$

Replacing \hat{H} with \hat{H}'_g in Eqs. (12)–(15), the expectation of the Bell operator is (see the Appendix Secs. B and C)

$$\begin{aligned} & \langle B_0A_0 \rangle + \langle B_1A_0 \rangle + \langle B_0A_1 \rangle - \langle B_1A_1 \rangle \\ & = E_0 + E'_0 + \frac{1}{2}[\omega_0(p_+ - p_-) + \omega'_0(p'_+ - p'_-)], \end{aligned} \quad (33)$$

where $p_{\pm} = |\langle u_+ | s_{\pm} \rangle|^2$ and $p'_{\pm} = |\langle u_+ | s'_{\pm} \rangle|^2$.

Direct calculations show that the deviation term is smaller than

$$\sqrt{\left(\frac{\omega_0}{2}\right)^2 + \left(\frac{\omega'_0}{2}\right)^2 + 2\frac{\omega_0}{2}\frac{\omega'_0}{2}\cos 2\delta}, \quad (34)$$

where δ is some parameter related to the angle of $|s_{\pm}\rangle$ and $|s'_{\pm}\rangle$. In particular, when $\frac{\omega_0}{2}\cos 2\delta = |\frac{\omega_0}{2}|$ (this is possible when $\cos 2\delta = 1$ or -1), the above bound reduces to $\frac{1}{2}(|\omega_0| + \omega'_0)$, which is the same as the classical picture.

IV. DISTINGUISHING THE DILATED HAMILTONIAN \hat{H}'

Suppose we have a set of devices that can produce a dilated Hermitian Hamiltonian and simulate a \mathcal{PT} -symmetric system. One may wonder whether the device is reliable, or if it faithfully realizes the simulation design. Apparently, this question is closely related to whether the dilated Hermitian Hamiltonian is well prepared.

In particular, it is instructive to distinguish between the dilated Hermitian Hamiltonian and the local Hermitian. Take the dilated Hamiltonian \hat{H} in Eq. (7) and $\hat{H}_l = I \otimes H_l$ in the local Hermitian picture in Sec. II as an example. Suppose we want to simulate a \mathcal{PT} -symmetric system, whose effective Hamiltonian is H in Eq. (6). One can use the device to produce a global system whose Hamiltonian is \hat{H} to realize such a simulation in the subsystem. Since a \mathcal{PT} -symmetric system is usually non-Hermitian, the dilated Hermitian Hamiltonian \hat{H} necessarily brings nonlocal correlations to the subsystems.

However, the local Hermitian Hamiltonian $\hat{H}_l = I \otimes H_l$ cannot produce such correlations, although it has similar properties to the dilated \hat{H} when local measurements are conducted. Briefly speaking, to see whether the device is reliable, one needs to distinguish the Hamiltonian it produces from one that cannot bring nonlocal correlations. Note that \hat{H} has the same eigenvalues as \hat{H}_l . Hence one cannot distinguish them only by measurements. However, one can calculate the Bell operator expectations. Indeed, for the special case of Eq. (7), it is shown that the classical and local Hermitian pictures give a larger deviation term than the simulation picture. Thus the expectations in different correlation pictures can help to distinguish the dilated Hermitian Hamiltonian and have potential applications [22].

In the general case, one can also discuss how to distinguish \hat{H}' from \hat{H}'_l . In fact, once the Bell operator expectations differ in the simulation and local Hermitian pictures, one can distinguish between \hat{H}' and \hat{H}'_l . Equations (25) and (31) show that such a difference may come from two parts: one is an energy shift of $2a$, and the other is a different bound of the deviation term.

However, in the general case, the correlation behaviors of the global Hamiltonians are more complex, and generally one may not distinguish \hat{H}' from \hat{H}'_l . In fact, if we take $a = b = c = 0$ and $d = \frac{s(\cos^2 \alpha - \cos^3 \alpha)}{\cos \alpha - 2}$, then Eqs. (26) and (29) show that the simulation picture and the local Hermitian picture give the same form of the Bell operator expectation and deviation bound. Thus one cannot distinguish between them. Such a result is natural in some sense. In fact, \hat{H}'_l in Eq. (30) is not in a tensor product form. Thus it actually brings nonlocal correlations between the subsystems, just like the Hermitian dilation \hat{H} . Hence it is not unexpected that the Bell operator expectations in the two pictures sometimes have the same ranges.

On the other hand, in most cases, such a distinction is possible, e.g., when H and $(H^\perp)'$ have the same eigenvalues or when $d = 0$. In these two cases, one can distinguish between \hat{H}' and \hat{H}'_l , by observing either an energy shift or a smaller deviation bound in the the Bell operator expectation of the simulation picture (see the Appendix Sec. D for details). This result can be viewed as a natural generalization of that in Ref. [22].

One may also discuss the problem for \hat{H}' and \hat{H}'_g . When \hat{H}' and \hat{H}'_g do not have the same eigenvalues, one can distinguish them by making measurements directly. When \hat{H}' and \hat{H}'_g have the same eigenvalues, one can see either an energy shift in the the Bell operator expectations or a smaller deviation bound in the simulation picture, which distinguishes the two types of Hamiltonians.

The above results show that when \hat{H}' and H , or equivalently $(H^\perp)'$ and H , have the same eigenvalues, the Bell operator expectations have better properties and can help in the task of distinguishing \hat{H}' . In fact, since the eigenvalues of H are also the eigenvalues of \hat{H}' , when \hat{H}' and H have different eigenvalues, Alice can obtain more than two outcomes. Such a situation is quite different from the standard CHSH scenario. However, when \hat{H}' and H have the same eigenvalues, Alice obtains exactly two outcomes. This is similar to CHSH's discussion, which partly explains why the Bell operator expectations behave better in this case.

V. DISCUSSION

Compared to the the special case revealed in Ref. [22], here the physical implications behind the general results are discussed. A significant difference exists in deriving the classical pictures. To obtain a classical picture for the general case, one needs an extra assumption that Alice cannot distinguish between the measurements A_i . Such an assumption is not needed in the special case [22].

However, in the general case, due to the fact that H and $(H^\perp)'$ usually have different eigenvalues, there are four outcomes of measurements, which is quite different from the usual CHSH scenario. If we calculate the usual expectation of the Bell operator, that is, if Alice is aware of the details of her measurements, then she can get an expectation value only related to H but irrelevant to $(H^\perp)'$ (see the Appendix Sec. C for details). Intuitively, such a biased value is not suitable for investigating the properties of the global Hamiltonian \hat{H} . For this reason, the extra assumption is needed and gives a more reasonable expectation value. Moreover, such an assumption is implicitly valid for the special Hermitian dilation in Eq. (7), in which case $(H^\perp)' = H$. Only with the same measurement results, Alice cannot distinguish between A_0 and A_1 . Hence such an assumption is natural, and the classical picture will reduce to the special one in Sec. II.

In the special case of Eq. (7), the classical and local Hermitian pictures have the same expectation of the Bell operator. However, in the general case, Eqs. (27), (31), and (33) show that the Bell operator expectation of the classical picture is different from the local Hermitian picture but the same as the genuine local Hermitian picture. The reason is that the form of \hat{H}'_l is not a tensor product. Although we still use the term the "local Hermitian picture" in comparison with [22], it is actually nonlocal, which cannot be described by a classical picture. As mentioned, the form of \hat{H}'_l implies that when the measurement is A_0 (the ancillary system is postselected in $|0\rangle$), the results of Alice's are the eigenvalues of H . When the measurement is A_1 (the ancillary system is postselected in $|1\rangle$), the results of Alice's are the eigenvalues of $(H^\perp)'$. Since H and $(H^\perp)'$ generally have different eigenvalues, Alice

can directly distinguish between A_0 and A_1 by simply reading out the measurement results, contradicting the assumption that Alice cannot distinguish between the measurements A_0 and A_1 in the classical picture. Hence the Bell operator expectation generally differs in the local Hermitian and classical pictures.

To see why the classical and genuine local Hermitian pictures still have the same expectations, note that if Alice mistook A_1 for A_0 , then the Hamiltonian should be

$$\hat{H}_l'' = |0\rangle\langle 0| \otimes (H^\perp)'_h + |1\rangle\langle 1| \otimes H_h.$$

Now, since Alice cannot distinguish between A_i , the Hamiltonian realizing the Bell operator expectation in the classical picture should be $\frac{1}{2}(\hat{H}_l' + \hat{H}_l'') = \hat{H}_g'$, which is just Eq. (32). Hence it is natural that the classical and genuine local Hermitian pictures have the same expectations.

VI. CONCLUSION

In this paper, we investigate the internal nonlocality of generally dilated Hermitian Hamiltonians of \mathcal{PT} symmetry. It is shown that in addition to the \mathcal{PT} -symmetric Hamiltonian H , the effect of a generally dilated Hermitian Hamiltonian can also be characterized by another Hamiltonian H^\perp . Based on this observation, the internal nonlocality is revealed in the general case, even when the twofold structure of the dilated Hamiltonian in Ref. [22] breaks. Different correlation pictures are proposed, and the Bell operator expectations are obtained.

The results in this paper covers that in Ref. [22], giving a natural generalization. However, the correlation behaviors are more complex and have different features in the general case. From the aspect of construction of correlation pictures, the generic classical picture utilized an assumption which is not needed but implicitly valid for the special case. A correlation picture, the genuine local Hermitian picture, is proposed. The Bell operators often have some energy shifts and the deviation bounds are also changed, which do not give a simple order relation as in Ref. [22]. In particular, the Bell operator expectation in the local Hermitian picture can coincide with the simulation picture but differs from the classical picture. It is shown that when the dilated Hermitian and the \mathcal{PT} -symmetric Hamiltonians have the same eigenvalues, the Bell operator expectations have good properties and can help in the task of distinguishing differences. Similar to the device-independent test of the state nonlocality, our results provide a detection-loophole-free test of the reliability of the simulation in a global Hermiticity.

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APPENDIX

A. The properties related to \hat{H} and H^\perp

We show how Eqs. (21)–(24) are obtained. Note that τ is invertible, Eqs. (23) and (24) are direct results of Eq. (1). To show that Eqs. (23) and (24) do give a Hermitian Hamiltonian \hat{H} , we have to show H_4 is Hermitian. In fact, $H_4^\dagger = H_4$ is equivalent to

$$(\tau^{-1})(H^\dagger\tau - H_2) = (\tau H - H_2^\dagger)\tau^{-1}.$$

According to Eq. (23), we know $H_2 = (H - H_1)\tau^{-1}$. Thus, direct calculations show that the above equation is equivalent to

$$H^\dagger(I + \tau^2) = (I + \tau^2)H,$$

which is just Eq. (2). Hence we know that H_4 is Hermitian and \hat{H} is a dilated Hermitian Hamiltonian.

To see Eq. (22), note that Eq. (21) is equivalent to the following equations:

$$-H_1\tau + H_2 = -\tau H^\perp, \quad (\text{A1})$$

$$-H_2^\dagger\tau + H_4 = H^\perp, \quad (\text{A2})$$

in which Eq. (A2) is just Eq. (22). Now to show Eq. (21) is valid, we need to prove only Eq. (A1). Substituting Eqs. (23) and (24) into Eq. (A1), we find that Eq. (A1) is also equivalent to Eq. (2). Thus, Eq. (21) is valid.

It should be noted that Eqs. (3) and (5) can be obtained from Eqs. (23) and (24) when H_1 takes the form in Eq. (4). In fact, by substituting Eq. (4) into Eq. (23), one can obtain H_2 in Eq. (5).

Now to obtain Eq. (3), we need only to show $H_4 = H_1$, which is equivalent to

$$H_1(\tau + \tau^{-1})\tau = H_4(\tau + \tau^{-1})\tau.$$

According to Eqs. (23) and (24), the above equation can be written as

$$H_1(\tau + \tau^{-1})\tau = [\tau H - \tau^{-1}(H^\dagger - H_1)]\tau^{-1}(\tau + \tau^{-1})\tau.$$

Now using Eq. (4) and the fact $(\tau^{-1} + \tau)\tau = \tau(\tau^{-1} + \tau)$, we see that the above equation reduces to

$$\tau^{-1}H^\dagger(\tau^{-1} + \tau) = \tau H\tau^{-1} + \tau^{-1}H\tau^{-1}.$$

However, direct calculations show that this equation can be proved by using Eq. (2). Thus we know that $H_1 = H_4$, and the dilated Hamiltonian \hat{H} in Eq. (3) is indeed a special case when H_1 takes the special form in Eq. (4). In fact, one can further prove that $H^\perp = H$ in this special case. To see this, first, we note that now $H_1 = H_4$. Hence it follows from Eq. (22) that $H^\perp = -H_2^\dagger\tau + H_1$. Thus to show $H^\perp = H$ we need only to prove

$$-H_2^\dagger\tau + H_1 = H,$$

from which we have

$$(-H_2^\dagger\tau + H_1)(\tau^{-1} + \tau) = H(\tau^{-1} + \tau).$$

According to Eqs. (4) and (23), calculations show that the above equation is also equivalent to Eq. (2). Thus we know $H = H^\perp$ in the special case.

To see that the eigenvalues of H^\perp are also the eigenvalues of \hat{H} , let us assume that λ is an eigenvalue of H^\perp and ϕ is an eigenvector. Now Eq. (21) implies that

$$\hat{H} \begin{bmatrix} -\tau\phi \\ \phi \end{bmatrix} = \begin{bmatrix} -\tau H^\perp \phi \\ H^\perp \phi \end{bmatrix} = \lambda \begin{bmatrix} -\tau\phi \\ \phi \end{bmatrix},$$

showing that λ is an eigenvalue of \hat{H} . Similarly, one can show that the eigenvalues of H are also the eigenvalues of \hat{H} . Apparently, if $H^\perp = H$, then \hat{H} has the same eigenvalues as H , with multiplicities two.

B. Some calculations related to \hat{H}'

In this part, we show how the expectations in different correlation pictures are obtained. For the convenience of calculations, denote a general Hermitian dilation Hamiltonian by $\hat{H}' = \begin{bmatrix} H'_1 & H'_2 \\ (H'_2)^\dagger & H'_4 \end{bmatrix}$ and the special Hermitian dilation Hamiltonian in Eq. (7) by $\hat{H} = \begin{bmatrix} H_1 & H_2 \\ H_2^\dagger & H_4 \end{bmatrix}$, where $H_4 = H_1$. Moreover, assume that $H'_i = H_i + H''_i$ and

$$H''_1 = \begin{bmatrix} a+c & d+ib \\ d-ib & a-c \end{bmatrix}.$$

Now we see the effect of H''_1 and note that $H'_1 = H_1 + H''_1$. Then according to Eq. (23),

$$\begin{aligned} H'_2 &= (H - H'_1)\tau^{-1} \\ &= (H - H_1)\tau^{-1} - H''_1\tau^{-1} \\ &= H_2 - H''_1\tau^{-1}. \end{aligned} \tag{A3}$$

According to Eqs. (24) and (A3),

$$\begin{aligned} H'_4 &= (\tau H - H'_2)\tau^{-1} + \tau^{-1}H''_1\tau^{-1} \\ &= H_4 + \tau^{-1}H''_1\tau^{-1} \\ &= H_1 + \tau^{-1}H''_1\tau^{-1}. \end{aligned} \tag{A4}$$

Moreover, Eq. (21) shows that

$$\begin{aligned} (H^\perp)' &= -(H'_2)^\dagger\tau + H'_4 \\ &= -H_2^\dagger\tau + H_4 + \tau^{-1}H''_1(\tau + \tau^{-1}) \\ &= H + \tau^{-1}H''_1(\tau + \tau^{-1}), \end{aligned} \tag{A5}$$

where the last equation holds because $H^\perp = -H_2^\dagger\tau + H_4 = H$.

Direct calculations show that

$$\begin{aligned} &\tau^{-1}H''_1\tau^{-1} \\ &= \begin{bmatrix} \frac{a+c+2b\sin\alpha+(a-c)\sin^2\alpha}{\cos^2\alpha} & \frac{d\cos^2\alpha+i(b+b\sin^2\alpha+2a\sin\alpha)}{\cos^2\alpha} \\ \frac{d\cos^2\alpha-i(b+b\sin^2\alpha+2a\sin\alpha)}{\cos^2\alpha} & \frac{a-c+2b\sin\alpha+(a+c)\sin^2\alpha}{\cos^2\alpha} \end{bmatrix} \end{aligned} \tag{A6}$$

and

$$\begin{aligned} &\tau^{-1}H''_1(\tau + \tau^{-1}) \\ &= \begin{bmatrix} \frac{2(a+c)+2(b+id)\sin\alpha}{\cos^2\alpha} & \frac{2d+2i(b+a\sin\alpha-c\sin\alpha)}{\cos^2\alpha} \\ \frac{2d-2i(b+a\sin\alpha+c\sin\alpha)}{\cos^2\alpha} & \frac{2(a-c)+2(b-id)\sin\alpha}{\cos^2\alpha} \end{bmatrix}. \end{aligned} \tag{A7}$$

If we denote

$$\begin{aligned} A_1 &= \frac{2(a+b\sin\alpha)}{\cos^2\alpha}, \\ A_2 &= \frac{2(b+a\sin\alpha)}{\cos^2\alpha}, \\ C_1 &= \frac{2c+2id\sin\alpha}{\cos^2\alpha} + is\sin\alpha, \\ C_2 &= \frac{2d-2ic\sin\alpha}{\cos^2\alpha} + s, \end{aligned}$$

then

$$(H^\perp)' = (E_0 + A_1)I_2 + \begin{bmatrix} C_1 & C_2 + iA_2 \\ C_2 - iA_2 & -C_1 \end{bmatrix}.$$

The eigenvalues of $(H^\perp)'$ are

$$\begin{aligned} \lambda'_+ &= E_0 + A_1 + \sqrt{C_1^2 + C_2^2 + A_2^2}, \\ \lambda'_- &= E_0 + A_1 - \sqrt{C_1^2 + C_2^2 + A_2^2}. \end{aligned}$$

Accordingly,

$$\begin{aligned} \omega'_0 &= \lambda'_+ - \lambda'_- \\ &= 2\sqrt{\left(s + \frac{2d}{\cos^2\alpha}\right)^2 \cos^2\alpha + \frac{4c^2}{\cos^2\alpha} + \frac{4(b+a\sin\alpha)^2}{\cos^4\alpha}}, \end{aligned}$$

which is just Eq. (29).

Similarly, one can calculate the eigenvalues of H'_4 using Eq. (A4). If we denote

$$\begin{aligned} A'_1 &= \frac{a+2b\sin\alpha+a\sin^2\alpha}{\cos^2\alpha}, \\ A'_2 &= \frac{b+b\sin^2\alpha+2a\sin\alpha}{\cos^2\alpha}, \\ C'_1 &= c, \\ C'_2 &= s\cos^2\alpha + d, \end{aligned}$$

then

$$H'_4 = (E_0 + A'_1)I_2 + \begin{bmatrix} C'_1 & C'_2 + iA'_2 \\ C'_2 - iA'_2 & -C'_1 \end{bmatrix}.$$

Direct calculation shows that the two eigenvalues of H'_4 are

$$\begin{aligned} \lambda''_+ &= E_0 + A'_1 + \sqrt{(C'_1)^2 + (C'_2)^2 + (A'_2)^2}, \\ \lambda''_- &= E_0 + A'_1 - \sqrt{(C'_1)^2 + (C'_2)^2 + (A'_2)^2}. \end{aligned}$$

Accordingly,

$$\begin{aligned} \omega''_0 &= \lambda''_+ - \lambda''_- \\ &= 2\sqrt{(s\cos^2\alpha + d)^2 + \frac{(b+b\sin^2\alpha+2a\sin\alpha)^2}{\cos^4\alpha} + c^2}, \end{aligned}$$

which is just Eq. (26).

C. The calculation of different expectations and bounds in the general case

With the above results, one can calculate the simulation bound. Note that a general dilated Hermitian Hamiltonian \hat{H}' can be written as

$$\hat{H}' = |0\rangle\langle 0| \otimes H'_1 + |1\rangle\langle 1| \otimes H'_4 + |0\rangle\langle 1| \otimes H'_2 + |1\rangle\langle 0| \otimes (H'_2)^\dagger.$$

Denote $H'_4 = \lambda''_+ |s'_+\rangle\langle s'_+| + \lambda''_- |s'_-\rangle\langle s'_-|$, $\omega''_0 = \lambda''_+ - \lambda''_-$. By substituting \hat{H}' into Eqs. (12)–(15), direct calculations show that the simulation bound is

$$\begin{aligned} & \text{Tr}[|0\rangle\langle 0| \otimes H'_1 + |1\rangle\langle 1| \otimes (|u_+\rangle\langle u_+| - |u_-\rangle\langle u_-|)H'_4] \\ &= \text{Tr}H'_1 + \langle u_+|H'_4|u_+\rangle - \langle u_-|H'_4|u_-\rangle \\ &= 2E_0 + 2a + \langle u_+|H'_4|u_+\rangle - \langle u_-|H'_4|u_-\rangle \\ &= 2E_0 + 2a + \omega''_0(p''_+ - p''_-), \end{aligned}$$

which is just Eq. (25). The concrete expression of the Bell operator expectation is

$$\begin{aligned} & \langle B_0A_0\rangle + \langle B_0A_1\rangle + \langle B_1A_0\rangle - \langle B_1A_1\rangle \\ &= 2E_0 + 2a + (\bar{u}v + u\bar{v})(\omega_0 \cos \alpha + 2d) \\ & \quad + \bar{u}v \frac{2i(b + b \sin^2 \alpha + 2a \sin \alpha)}{\cos^2 \alpha} \\ & \quad - u\bar{v} \frac{2i(b + b \sin^2 \alpha + 2a \sin \alpha)}{\cos^2 \alpha} + 2c(|u|^2 - |v|^2). \end{aligned}$$

For the classical picture, the Bell operator expectation is

$$\begin{aligned} & \langle B_0A_0\rangle + \langle B_0A_1\rangle + \langle B_1A_0\rangle - \langle B_1A_1\rangle \\ &= \int [B_0(v)(A_0 + A_1)(v) + B_1(v)(A_0 - A_1)(v)] dv \\ &= \int [(A_0 + A_1)(v) + (A_0 - A_1)(v)] dv, \quad (\text{A8}) \end{aligned}$$

where the last equation holds because the results of B_i are 1. Since the results of A_0 are the eigenvalues λ_\pm , then the above equation gives

$$2E_0 + \omega_0(p_+ - p_-), \quad (\text{A9})$$

where p_\pm are the probabilities that Alice's results are λ_\pm . However, Alice is unaware of the details of the measurements; hence she may mistake A_1 for A_0 . Thus the Bell operator expectation will be calculated by changing A_0 and A_1 in Eq. (A8). Since the results of A_1 are the eigenvalues of $(H^\perp)'$, i.e., λ'_\pm , then the Bell operator expectation will be

$$2E'_0 + \omega'_0(p'_+ - p'_-),$$

where $E'_0 = \frac{1}{2}(\lambda'_+ + \lambda'_-)$ and p'_\pm are the probabilities that the results are λ'_\pm . Now the best Alice can do is to calculate the mean value of the above two results,

$$E_0 + E'_0 + \frac{1}{2}[\omega_0(p_+ - p_-) + \omega'_0(p'_+ - p'_-)],$$

which is just Eq. (27).

We now calculate the Bell operator expectation in the local Hermitian picture. Note that $H_h = \lambda_+ |s_+\rangle\langle s_+| + \lambda_- |s_-\rangle\langle s_-|$ and $(H^\perp)_h = \lambda'_+ |s'_+\rangle\langle s'_+| + \lambda'_- |s'_-\rangle\langle s'_-|$. By replacing \hat{H} with $\hat{H}'_g = |0\rangle\langle 0| \otimes H_h + |1\rangle\langle 1| \otimes (H^\perp)_h$ in Eqs. (12)–(15), direct

calculations show that

$$\begin{aligned} & \langle B_0A_0\rangle + \langle B_1A_0\rangle + \langle B_0A_1\rangle - \langle B_1A_1\rangle \\ &= \text{Tr}(|0\rangle\langle 0| \otimes H_h + |1\rangle\langle 1| \\ & \quad \otimes (|u_+\rangle\langle u_+| - |u_-\rangle\langle u_-|)(H^\perp)_h) \\ &= 2E_0 + \omega'_0(p'_+ - p'_-), \end{aligned}$$

where $p'_\pm = |\langle u_\pm | s'_\pm \rangle|^2$. This is just the result of Eq. (31).

Similarly, one can calculate the Bell operator expectation for the genuine local Hermitian picture. Replacing \hat{H} with $\hat{H}'_g = \frac{1}{2}I \otimes (H_h + (H^\perp)_h)$ in Eqs. (12)–(15), direct calculations show that

$$\begin{aligned} & \langle B_0A_0\rangle + \langle B_1A_0\rangle + \langle B_0A_1\rangle - \langle B_1A_1\rangle \\ &= \langle u_+ | H_h | u_+ \rangle + \langle u_+ | (H^\perp)_h | u_+ \rangle \\ &= E_0 + E'_0 + \frac{1}{2}[\omega_0(p_+ - p_-) + \omega'_0(p'_+ - p'_-)], \end{aligned}$$

where $p_\pm = |\langle u_\pm | s_\pm \rangle|^2$ and $p'_\pm = |\langle u_\pm | s'_\pm \rangle|^2$. This is just the result of Eq. (33).

We now calculate the bound of Eq. (34) in the genuine local Hermitian picture. Note that such a bound is obtained by altering $|u_\pm\rangle$ but fixing $|s_\pm\rangle$ and $|s'_\pm\rangle$ in Eq. (33). Since we are considering the two-dimensional case, one can parametrize the states in a way similar to the Bloch sphere. Assume that $|\langle s_\pm | s'_\pm \rangle| = \cos \delta$, where δ is a parameter characterizing the angle between $|s_\pm\rangle$ and $|s'_\pm\rangle$. Without loss of generality, one may assume that $|s_+\rangle = |0\rangle$ and $|s_-\rangle = |1\rangle$. In addition,

$$\begin{aligned} |u_+\rangle &= \begin{bmatrix} \cos \alpha \\ e^{i\Delta} \sin \alpha \end{bmatrix}, \\ |s'_+\rangle &= \begin{bmatrix} \cos \delta \\ e^{i\Delta'} \sin \delta \end{bmatrix}, |s'_-\rangle = \begin{bmatrix} -\sin \delta \\ e^{i\Delta'} \cos \delta \end{bmatrix}, \end{aligned}$$

where Δ , Δ' , and α are real parameters. Then direct calculations show that

$$\begin{aligned} & \frac{1}{2}[\omega_0(p_+ - p_-) + \omega'_0(p'_+ - p'_-)] \\ &= \frac{\omega_0}{2}(\cos^2 \alpha - \sin^2 \alpha) + \frac{\omega'_0}{2}[\cos^2(\alpha + \delta) - \sin^2(\alpha + \delta) \\ & \quad + \sin 2\alpha \sin 2\delta + \cos(-\Delta + \Delta') \sin 2\alpha \sin 2\delta] \\ &= \cos 2\alpha \left(\frac{\omega_0}{2} + \frac{\omega'_0}{2} \cos 2\delta \right) \\ & \quad + \frac{\omega'_0}{2} \sin 2\delta \cos(-\Delta + \Delta') \sin 2\alpha \\ &\leq \sqrt{\left(\frac{\omega_0}{2} + \frac{\omega'_0}{2} \cos 2\delta \right)^2 + \left[\frac{\omega'_0}{2} \sin 2\delta \cos(-\Delta + \Delta') \right]^2} \\ &\leq \sqrt{\left(\frac{\omega_0}{2} \right)^2 + \left(\frac{\omega'_0}{2} \right)^2 + 2 \frac{\omega_0 \omega'_0}{2} \cos 2\delta}, \quad (\text{A10}) \end{aligned}$$

where the last two inequalities hold due to the Schwartz inequality and the fact that $\cos(-\Delta + \Delta')^2 \leq 1$. When $\frac{\omega_0}{2} \cos 2\delta = |\frac{\omega_0}{2}|$, i.e., equivalently $\cos 2\delta = \pm 1$, Eq. (A10) saturates its largest value.

D. To distinguish the Hamiltonian \hat{H}'

When H and \hat{H}' , or equivalently $(H^\perp)'$ have the same eigenvalues, one can distinguish \hat{H}' from \hat{H}'_l by comparing the Bell operator expectations. First, note that H and $(H^\perp)'$ have the same eigenvalues iff $\lambda'_+ + \lambda'_- = \lambda_+ + \lambda_-$ and $\lambda'_+ - \lambda'_- = |\lambda_+ - \lambda_-|$:

$$E'_0 = E_0, \quad \omega'_0 = |\omega_0|.$$

Thus, according to Eq. (28), we have $a = -b \sin \alpha$. Now, if $a \neq 0$, then Eq. (25) shows that there is an energy shift $2a$ in the simulation picture. However, Eq. (31) shows that such a shift does not exist in the local Hermitian picture. Thus by comparing the Bell operator expectations, one can distinguish \hat{H}' from \hat{H}'_l . Next we consider the case $a = 0$. Since $a = -b \sin \alpha$, we have $b = 0$ ($\sin \alpha = 0$ is the trivial case that H is Hermitian, which is not considered). Now $\omega'_0 = |\omega_0|$ implies that

$$\sqrt{\left(s + \frac{2d}{\cos^2 \alpha}\right)^2 \cos^2 \alpha + \frac{4c^2}{\cos^2 \alpha}} = |s \cos \alpha|. \quad (\text{A11})$$

It follows that

$$c^2 = \frac{\cos^2 \alpha}{4} \left[s^2 \cos^2 \alpha - \left(s + \frac{2d}{\cos^2 \alpha} \right)^2 \cos^2 \alpha \right]. \quad (\text{A12})$$

Note that $c^2 \geq 0$, from Eq. (A12) we have

$$-ds \geq \frac{d^2}{\cos^2 \alpha}.$$

Now we calculate $(\omega'_0)^2 - (\omega''_0)^2$. By substituting Eq. (A12) into Eqs. (26) and (29), as well as using the fact $-ds \geq d^2 / \cos^2 \alpha$, we have

$$\begin{aligned} (\omega'_0)^2 - (\omega''_0)^2 &= 4 \left[\left(s + \frac{2d}{\cos^2 \alpha} \right)^2 \cos^2 \alpha + \frac{4c^2}{\cos^2 \alpha} \right. \\ &\quad \left. - (s \cos^2 \alpha + d)^2 - c^2 \right] \\ &= 4s^2 \cos^2 \alpha - 4(s \cos^2 \alpha + d)^2 - s^2 \cos^4 \alpha \end{aligned}$$

$$\begin{aligned} &+ (s \cos^2 \alpha + 2d)^2 \\ &= 4(s^2 \cos^2 \alpha \sin^2 \alpha - ds \cos^2 \alpha) \\ &\geq 4(s^2 \cos^2 \alpha \sin^2 \alpha + d^2)(-ds \geq d^2 / \cos^2 \alpha) \\ &> 0. \end{aligned}$$

Thus we know $\omega'_0 = |\omega_0| > \omega''_0$; that is, the local Hermitian picture gives a larger deviation bound than the local Hermitian picture.

To summarize, when H and $(H^\perp)'$ have the same eigenvalues, one can distinguish \hat{H}' from \hat{H}'_l by investigating the Bell operator expectation; there is either an energy shift or a smaller range of deviation. In particular, the above discussions generalize the results in Sec. II C, which can be viewed as a special case when $H = (H^\perp)'$.

Another special case is $d = 0$. In this case, Eqs. (26) and (29) show that $\omega'_0 \geq |\omega_0 \cos \alpha|$ and $\omega'_0 \geq |\omega_0|$. By comparing Eqs. (26), (29), and (31) with Eqs. (17), (18), and (20), one can see that when $d = 0$, the simulation, classical, and local Hermitian bounds are usually larger than the special case. Moreover, one can still distinguish \hat{H}' from \hat{H}'_l by utilizing the Bell operator expectations. In fact, when $a \neq 0$, then there is a shift in the Bell operator expectation for the simulation picture. Thus one can immediately distinguish \hat{H}' from \hat{H}'_l . When $a = 0$, by taking $d = 0$ in Eqs. (26) and (29), we see that $\omega'_0 > \omega''_0$; thus the different bounds of deviation can help distinguish \hat{H}' .

One can also discuss the problem for \hat{H}' and \hat{H}'_g . Note that when they have different eigenvalues, one can distinguish between them with measurements. Hence we need to consider only the situation \hat{H}' and \hat{H}'_g that have the same eigenvalues as H . Now without loss of generality, one can rewrite the Hamiltonian \hat{H}' in Eq. (32) as $\hat{H}'_g = I \otimes H_h$, where H_h has the same eigenvalues as H . In this case, the Bell operator expectation of \hat{H}'_g is given by Eq. (20), and the deviation bound is $|\omega_0|$. Equations (20) and (25) show that when $a \neq 0$, one can distinguish \hat{H}' from \hat{H}'_g by the energy shift $2a$. Hence we need to consider only the case $a = 0$. However, the fact that \hat{H}' and H [or equivalently $(H^\perp)'$ and H] have the same eigenvalues also implies that $E_0 = E'_0$ and $|\omega_0| = \omega'_0$. As shown in the above discussion of distinguishing between \hat{H}' and \hat{H}'_l , we know that $|\omega_0| = \omega'_0 > \omega''_0$ in this case. Thus, by comparing the different deviation bounds, one can distinguish \hat{H}' from \hat{H}'_g .

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