Quantifying the nonclassicality of pure dephasing

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The characterization, explanation, and quantification of quantumness, in particular the discrimination from classicality in terms of classical strategies, lie at the heart of quantum physics. Dephasing processes, caused by the information exchange between a quantum system and its environment, play a central role in that respect, as they control the transition between the quantum and the classical realm. Recently, it is shown that dephasing dynamics itself can exhibit classical or nonclassical traits, depending on the nature of the system-environment correlations and the related (im)possibility to simulate these dynamics with
Hamiltonian ensembles—the classical strategy. Here we propose to extend this classification towards quantifying the nonclassicality of pure dephasing dynamics. In the spirit of Wigner’s function, we generalize Hamiltonian ensembles to encompass quasi-probability distributions comprising negative values. Based on Lie algebra representations, Fourier transforms on groups, and root space decompositions, we demonstrate that quasi-probability distributions are faithful representations of pure dephasing dynamics; moreover, we show how to retrieve these quasi-probability distributions. This allows us to quantify process-nonclassicality time-independently, in terms of the deviations of the corresponding quasi-probability distributions from legitimate (non-negative) probability distributions. We exemplify our method along qubit, qutrit, and qubit-pair pure dephasing.

The boundary between the quantum and the classical world has always been a fundamental issue in quantum mechanics. An operationally viable way to demonstrate the genuine quantum nature of an experiment relies on the impossibility to mimic certain statistical properties of interest by using a “classical strategy”. According to this logic, the quantum nature of an experiment is only convincingly demonstrated if the experimental statistics cannot be mimicked by the classical strategy; thus excluding any loophole to explain the statistics with a classical model.

For example, under the assumptions of realism and locality, Bell derived an inequality for correlations between the statistics of measurements on a bipartite system. Whenever the inequality is violated, one cannot reproduce the correlations by using a local hidden variable model, the latter serving as the classical strategy for mimicking the measurement statistics. Another important
paradigm is the quantumness of a boson field, which is formulated in terms of the Wigner function or the Glauber-Sudarshan $P$ representation. Whenever these functions exhibit negative values, the classical explanation in terms of a probability distribution over phase space fails to represent the boson field.

Following this spirit, one may ask for a classical strategy to frame the “quantumness” of open system dynamics. This question has been addressed in different ways. In some approaches, specific properties of system states, e.g., Wigner functions with negativities, violation of Leggett-Garg inequality, or non-stochasticity of dynamical processes are identified as indicators of nonclassicality and monitored during the temporal evolution. While operational in nature, these approaches lack a dedicated reference to the presence of an environment, a defining component of open quantum systems.

Alternatively, we thus propose to take the presence or absence of quantum correlations between system and environment as a signature for the quantum nature of the open system dynamics. As was shown recently, such presence or absence of nonclassical system-environment correlations is intimately linked to the (im)possibility to simulate the open system dynamics with a Hamiltonian ensemble (HE), which may thus serve as the classical strategy to witness the nonclassicality of the open system dynamics. HEs, which are also used to describe disordered quantum systems, attribute to each member of a collection of (time-independent) Hamiltonians a probability of occurrence, giving rise to an effective average dynamics.

Finding a simulating HE certifies that the open dynamics is classical. The nonexistence of
a simulating HE, on the other hand, can be proven by the necessity to resort to a HE that exhibits Hamiltonians accompanied by negative quasi-distributions, as was shown in \ref{14} for the example of an extended spin-boson model. Given its existence and uniqueness, such a quasi-distribution featuring negative probabilities may, in turn, lay the ground to promote the mere witness of non-classicality into a full-fledged measure, weighing the negative contributions.

Here we introduce such measure of nonclassicality for \textit{pure dephasing} dynamics, i.e., we focus on situations where dephasing constitutes the sole dynamical agent. Besides the fundamental relevance for the quantum-to-classical transition \cite{15,16,17}, this may, e.g., characterize quantum memories, which, while designed to preserve quantum states, are exposed to environmental dephasing. Classicality of the dynamics, reflected by the existence of a simulating HE, can then be related to the in-principle possibility to correct errors caused by the HE \cite{18}.

More generally, analyzing (pure) dephasing is essential for the improvement of quantum technologies, as it constitutes one of the main obstacles in the fabrication and manipulation of quantum information devices \cite{19,20,21,22,23,24,25,26,27,28,29,30}. Different implementations for the simulation of controlled pure dephasing \cite{24,26} and its mitigation \cite{27,28,29,30} exist. Other experiments highlight the potential of decoherence or pure dephasing to contribute positively to certain quantum information tasks, such as entanglement stabilization \cite{32} or entanglement swap \cite{33}.

To introduce our nonclassicality measure, we recast arbitrary pure dephasing dynamics into a canonical HE form, based on Lie algebra representations and the Fourier transforms on groups. In this canonical representation, each HE is composed of the same canonical set of Hamiltonians,
such that the accompanying (quasi-)probability distribution fully characterizes the HE. Depending on the dynamics, this (normalized) distribution is either non-negative or partly negative. Let us remark that one can interpret the resulting HE as a generalized random phase model.

We prove that such canonical representation exists for all pure dephasing dynamics. Moreover, we prove that the representation can always be restricted to commuting member Hamiltonians, which renders the corresponding distribution unique, promoting it to a faithful representation of the pure dephasing dynamics. This then allows us to unambiguously quantify the nonclassicality of arbitrary pure dephasing dynamics in terms of the variational distance between its corresponding distribution and the nearest positive one, i.e., classical distribution. To further underscore the viability of this measure, we demonstrate its convexity under the mixing of two pure dephasing dynamics.

We elaborate our ideas by retrieving quasi-probability distributions for qubit, qutrit, and qubit-pair pure dephasing dynamics. Along this, a systematic procedure to retrieve (quasi-)distributions for pure dephasing, relying on Lie algebra representations and root space decompositions, is outlined.

**Results**

**Averaged dynamics of Hamiltonian ensembles.** A HE \( \{ (p_\lambda, \tilde{H}_\lambda) \}_\lambda \) is a collection of Hermitian operators \( \tilde{H}_\lambda \) acting on the same system \([4,34]\), where each member Hamiltonian is drawn according to the probability distribution \( p_\lambda \geq 0 \). A system \( \rho_0 \), isolated from any environment, is sent into a
unitarily-evolving channel $\rho_\lambda(t) = \hat{U}_\lambda \rho_0 \hat{U}_\lambda^\dagger$, with $\hat{U}_\lambda = \exp[-i\hat{H}_\lambda t/\hbar]$ for a chosen $\hat{H}_\lambda$ according to $p_\lambda$. Then, the dynamics of the averaged state $\overline{\rho}(t)$ is given by the unital map

$$\overline{\rho}(t) = \mathcal{E}_t\{\rho_0\} = \int p_\lambda \hat{U}_\lambda \rho_0 \hat{U}_\lambda^\dagger d\lambda.$$ (1)

Even though each single realization $\rho_\lambda(t)$ evolves unitarily, the averaged state $\overline{\rho}(t)$ exhibits incoherent behavior. A seminal and intriguing example is a single qubit subject to spectral disorder with HE given by $\{(p(\omega), \hbar \omega \hat{\sigma}_z/2)\}_\omega$, then the averaged dynamics describes pure dephasing:

$$\bar{\rho}(t) = \begin{bmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \phi(t) \\ \rho_{\downarrow\uparrow} \phi^*(t) & \rho_{\downarrow\downarrow} \end{bmatrix},$$ (2)

with the dephasing factor $\phi(t) = \int p(\omega)e^{-i\omega t}d\omega$ being the Fourier transform of the probability distribution $p(\omega)$.

The pure dephasing in Eq. (2) is a consequence of the commuting member Hamiltonian $\hbar \omega \hat{\sigma}_z/2$ in the ensemble. Each Hamiltonian induces a unitary rotation about the $z$-axis of the Bloch sphere at angular velocity $\omega$. This gives rise to an intuitive interpretation of pure dephasing in terms of random phases: each component rotates at different angular velocity $\omega$ and hence possesses its own time-evolving phase. Consequently the phase of the averaged system gradually blurs out.

Note that $p(\omega)$ is the probability distribution of the angular velocity and qualitatively characterizes the “randomness” of the random phase. Whenever $p(\omega)$ is specified, the dynamics is uniquely determined via the Fourier transform in Eq. (2). This is also in line with our classification
of such pure dephasing as classical \cite{14} since it is a statistical mixture of rotations at different angular velocity. Meanwhile, the experimental simulation of pure dephasing is implemented in a similar spirit \cite{24,25,26}.

**Canonical Hamiltonian-ensemble representation.** Although \( p(\omega) \) is particularly representative for characterizing qubit pure dephasing, it is obvious that, in general cases with non-commuting or higher dimensional member Hamiltonians \( \hat{H}_\lambda \), the Fourier transform in Eq. (2) is not applicable. We are therefore spurred to explore the canonical Hamiltonian-ensemble representation (CHER) as a generalized representation of an averaged dynamics.

To fully understand the CHER, we first observe that, since both \( \hat{H}_\lambda \) and density matrices \( \rho \) are Hermitian, they are elements in the Lie algebra \( \text{u}(n) = \text{u}(1) \oplus \text{su}(n) \), which are spanned by the identity \( \{ \hat{I} \} \) and \( \{ \hat{L}_m \}_m \) of \( n^2 - 1 \) traceless Hermitian generators, respectively. Then \( \hat{H}_\lambda \in \text{u}(n) \) is a linear combination

\[
\hat{H}_\lambda = \lambda_0 \hat{I} + \sum_{m=1}^{n^2-1} \lambda_m \hat{L}_m = \lambda_0 \hat{I} + \vec{\lambda} \cdot \vec{\hat{L}},
\]

where \( \lambda_0 \in \mathbb{R} \) and \( \vec{\lambda} = \{ \lambda_m \}_m \in \mathbb{R}^{n^2-1} \). And so does \( \rho \).

Since the dynamics is a linear map acting on \( \rho \), invoking to the adjoint representation (see **Methods** and Supplementary Note 1), we can assign each generator \( \hat{L}_m \) a linear map (i.e., endomorphism) \( \hat{L}_m \mapsto \tilde{L}_m \in \mathfrak{gl}(\text{u}(n)) \), with its action \( \tilde{L}_m(\bullet) = [\hat{L}_m, \bullet] \) been defined in terms of the commutator.

With the above mathematical setup, given a HE \( \{ (p_\lambda, \hat{H}_\lambda) \}_\lambda \), one can consider the probability
distribution $p_\lambda$ as a CHER of an averaged dynamics $\mathcal{E}_t$, in the sense that Eq. (1) can always be recast into a Fourier transform from $p_\lambda$, on a locally compact group $\mathcal{G}$ characterized by the parameter space $\lambda = \{\lambda_0, \vec{\lambda}\}$, to the dynamical linear map $\mathcal{E}_t(\tilde{L})$:

$$\mathcal{E}_t(\tilde{L}) = \int_{\mathcal{G}} p_\lambda e^{-i\lambda \tilde{L} t} d\lambda. \quad (4)$$

Note that we have set $\hbar = 1$ for symbolic abbreviation. Additionally, we can also express $\rho = \{n^{-1}, \vec{\rho}\}$ in the same manner as Eq. (3), the action of $\mathcal{E}_t$ on $\rho$ is then the usual matrix multiplication $\mathcal{E}_t(\rho) = \mathcal{E}_t(\tilde{L}) \cdot \rho$ (see Supplementary Note 2 for the proof of Eq. (4)).

We emphasize that the translation from Eq. (1) into Eq. (4) is not only a formal mathematical correspondence, but also provides physical insights into the nature of HE and the process nonclassicality, in the sense that an HE can be conceived as a generalized random phase model. In such interpretation, different components rotate about different axes, defined by the generators $\{\hat{L}_m\}_m$. Moreover, $p_\lambda$ is the distribution function of the random rotations over the $n^2$-dimensional Euclidean space and therefore relevant in characterizing the dynamics via Eq. (4).

**HE simulation and process nonclassicality.** So far we have discussed the averaged dynamics of an isolated system, in the absence of any environment, governed by a HE. Conversely, to discuss the nonclassicality of an open system dynamics reduced from a system-environment arrangement, we should construct a simulating $\{(\varphi_\lambda, \hat{H}_\lambda)\}_\lambda$ for a given unital dynamics.

An autonomous system-environment arrangement is characterized by a time-independent total Hamiltonian $\hat{H}_T$ and evolves unitarily with $\hat{U}_T = \exp[-i\hat{H}_T t]$. We have shown that if the
total system $\rho_T(t) = \hat{U}_T \rho_T(0) \hat{U}_T^\dagger$ remains at all times classically correlated between the system and its environment, displaying neither quantum discord nor entanglement, then the reduced system dynamics $\rho_S(t) = \mathcal{E}_t(\rho_S(0)) = \text{Tr}_E[\rho_T(t)]$ can be described by a time-independent HE equipped with a legitimate (i.e., non-negative and normalized to unity) probability distribution.

However, given exclusively the knowledge on the reduced system dynamics $\mathcal{E}_t$, it is impossible to fully verify the correlations between the system and its environment. Counter-intuitively, even if we have limited access to the system alone, the emergence of nonclassical correlations can be witnessed, whenever one has no way to simulate the dynamics with any HEs equipped with a legitimate probability distribution. Such impossibility to simulate arises from the buildup of nonclassical correlations. On the other hand, if such simulation is possible, one can explain $\mathcal{E}_t$ as a classical random phase model. We therefore define the negative values of the quasi-distribution $\wp_\lambda$ within the simulating HE as an indicator of process nonclassicality.

Existence and uniqueness of the CHER for pure dephasing. Here we promote the $\wp_\lambda$ within the simulating HE as a CHER for a reduced system dynamics. In particular, by further investigating the underlying algebraic structures, we can show that such CHER for pure dephasing is even faithful, provided diagonal member Hamiltonians. More precisely, for any pure dephasing dynamics, there always exists a unique simulating HE of diagonal member Hamiltonians, equipped with either a legitimate or quasi-distribution.

The proof will become intelligible only after introducing our procedure to find the CHER below. We postpone it to Supplementary Note 8.
Since $\varphi_\lambda$ is a distribution function over the parameter space of diagonal member Hamiltonians, along with the Fourier transform on the group $G$ in Eq. (4), this endows the CHER with a geometric interpretation of pure dephasing in terms of generalized random phase model. Consequently, the CHER is particularly competent in characterization of the nonclassicality of pure dephasing.

**The nonclassicality measure for pure dephasing dynamics.** Having characterized the HE simulation of pure dephasing and its representation, we are now ready to propose the measure of nonclassicality of dynamics. The measure aims to provide an operational quantification on the nonclassicality of a pure dephasing dynamics. Due to the existence and uniqueness, every pure dephasing $\mathcal{E}_t$ can be assigned a unique (quasi-)distribution $\varphi_\lambda$. We emphasize that it is the distribution $\varphi_\lambda$ which gives the characterization of the nonclassicality: unless they correspond to legitimate probabilities, no HE exists for the exact simulation.

The nonclassicality measure for a dynamics $\mathcal{E}_t$ assigned with a unique (quasi-)distribution $\varphi_\lambda$ is as follows,

$$\mathcal{N}\{\mathcal{E}_t\} = \inf_{p_\lambda} D(\varphi_\lambda, p_\lambda), \text{ with } D(p_\lambda, p'_\lambda) = \int_G \frac{1}{2} |p_\lambda - p'_\lambda| d\lambda,$$

(5)

where the infimum runs over all classical probability distributions $p_\lambda$ over the parameter space $G$ of the diagonal member Hamiltonians. The variational distance $D(p_\lambda, p'_\lambda)$ has an operational meaning as the single-shot distinguishability: it quantifies the highest success probability of distinguishing two probabilistic systems $p_\lambda$ and $p'_\lambda$, such that $p_{\text{success}} = [1 + D(p_\lambda, p'_\lambda)]/2.$
The measure proposed in Eq. (5) contains advantages and useful properties for the quantification. First, the measure has a clear operational meaning. It tells how well a dynamics $E_i$ can be simulated by an HE. The possibility of making success or failure in the simulation with an HE can be found. Second, the measure is monotonic that the larger it is, the harder a classical simulation is. This follows from the fact that the classical dynamics of pure dephasing forms a convex set, i.e., their probabilistic mixture is also classical. The proof is presented in Supplementary Note 3. It is noteworthy that the convexity can be constructed by considering (quasi-)probabilities of dynamics, but not dynamics per se. Finally, we also note that the measure shares some similarities with the quantification of non-Markovianity.

In what follows, we consider the nonclassicality of pure dephasing dynamics on a single qubit reduced from the extended spin-boson with a relative phase between the coupling constants, i.e., $g_{2,k} = g_{1,k}e^{i\phi}$. The quasi-distribution $\mathcal{P}_{X_{\omega}}(X)$ represents the single qubit pure dephasing and, consequently, its nonclassicality varies with $\varphi$. The results are shown in Fig. .

**Retrieval of the (quasi-)distribution.** Given a HE, it is, in principle, straightforward to calculate the averaged dynamics of an isolated system, according to Eq. (1) [or, equivalently, to Eq. (4)]. Nevertheless, the solution to the inverse transform of Eq. (4), i.e., retrieval of the (quasi-)distribution within the simulating HE for a given reduced dynamics, is formidable in general, in contrast to the conventional inverse Fourier transform. Consequently, to establish a systematic procedure to find the CHER of pure dephasing dynamics is very desirable.

In view of the qubit pure dephasing in Eq. (2), to simulate any higher dimensional pure
dephasing dynamics, we focus on the traceless and diagonal member Hamiltonian such that \( \hat{H}_\lambda = \lambda \hat{L} \) belongs to the Cartan subalgebra (CSA) \( \mathfrak{H} \) of \( \mathfrak{su}(n) \) (see Methods). The tracelessness is due to the fact that the trace plays no role in describing the dynamics. Additionally, since the adjoint representation preserves the structure of commutator, the adjoint representation of \( \mathfrak{H} \) is also a CSA of \( \mathfrak{sl}(\mathfrak{u}(n)) \). We therefore have the following commutativity \( [\lambda \hat{L}, \lambda' \hat{L}] = 0 \iff [\lambda \tilde{L}, \lambda' \tilde{L}] = 0 \).

It should be noted that, even if \( \lambda \hat{L} \in \mathfrak{H} \) can be chosen to be diagonal, \( \lambda \tilde{L} \) itself may not necessarily be diagonal as well since the generators of \( \mathfrak{u}(n) \) are not the suitable bases for diagonalizing it. As we will see below, the diagonalization of the adjoint representation is a critical step to the retrieval of the (quasi-)distribution for pure dephasing.

Furthermore, the conventional inverse Fourier transform does not work because we are now dealing with linear maps in the \( \mathfrak{sl}(\mathfrak{u}(n)) \) space. To efficiently establish a set of equations governing the CHER of pure dephasing, we inevitably encounter increasingly many mathematical terminologies, especially those specifying the intrinsic algebraic structures within the CHER. To make our procedure transparent, we instead demonstrate several examples, each of which reveals the central concepts of our procedure, rather than elaborate the mathematical tutorial. Our approach can be easily generalized to higher dimensional pure dephasing.

**Procedure towards the CHER of pure dephasing.** We begin with the case of qubit pure dephasing. Although this problem has been discussed\(^{14}\), it relies on the conventional Fourier transform and Bochner’s theorem\(^{41}\) and cannot be generalized to higher dimensional systems. Here we recast it into Eq. (4). This helps us to establish a systematic procedure for higher dimensional problems.
Within a properly chosen basis, a qubit pure dephasing, reduced from a system-environment arrangement, can be expressed in the same form as Eq. (2). Unlike the one resulting from ensemble average, the dephasing factor \( \phi(t) = \exp[-i\theta(t) - \Phi(t)] \) is determined by the system-environment interaction, where \( \theta(t) (\Phi(t)) \) is a real odd (even) function on time \( t \), respectively, such that \( \phi(0) = 1 \), \( |\phi(t)| \leq 1 \), and \( \phi(-t) = \phi^*(t) \). The dynamical linear map \( \mathcal{E}_t^{(\tilde{\sigma})} \) can be constructed by applying 
\[ \mathcal{E}_t^{(\tilde{\sigma})} = \sum_{l=0}^{3} \hat{\sigma}_l [\mathcal{E}_t^{(\tilde{\sigma})}]_{lm} \]
on each generator, where \( \hat{\sigma}_0 = \mathcal{T} \) is the identity and \( \hat{\sigma}_{1,2,3} \) denotes the three Pauli matrices.

To find the CHER, we mean to find a (quasi-)distribution \( \wp(\omega) \) encapsulated within the simulating HE \( \{(\wp(\omega), \hat{H}_\omega = \omega \hat{\sigma}_z / 2)\}_\omega \) satisfying
\[
\mathcal{E}_t^{(\tilde{\sigma})} = \int_{\mathbb{R}} \wp(\omega) e^{-i(\omega \hat{\sigma}_z / 2)t} d\omega. \quad (6)
\]
The same conclusion \( \exp[-i\theta(t) - \Phi(t)] = \int_{\mathbb{R}} \wp(\omega) e^{-i\omega t} d\omega \) is easily seen after diagonalizing Eq. (6) (see Supplementary Note 4 for more details). Finally, performing the conventional inverse Fourier transform leads to the desired result \( \wp(\omega) \).

To understand the deeper insight behind the diagonalization, we observe that the diagonalization changes the basis from the three pauli matrices into raising and lowering operators and leaves \( \hat{\sigma}_z \) invariant; namely, \( \{\hat{\sigma}_+, \hat{\sigma}_-, \hat{\sigma}_z\} \), which are the generators of \( \mathfrak{sl}(2) \). In other words, they are the common “eigenvectors” of \( \hat{H}_\omega \) with “eigenvalues” \( \pm 1 \) in the sense of the adjoint representation, 
\[
\tilde{H}_\omega(\hat{\sigma}_\pm) = [\omega \hat{\sigma}_z / 2, \hat{\sigma}_\pm] = \pm 1 \cdot \omega \hat{\sigma}_\pm \]
(see Supplementary Note 5 for more details). The eigenvalues \( \pm 1 \) are therefore referred to as the roots (denoted by \( \alpha_{1,2} \)) associated to the root spaces \( \text{span}\{\hat{\sigma}_\pm\} \), spanned by the operators \( \hat{\sigma}_\pm \), respectively. However, for higher dimensional systems, the roots are
no longer real scalars but vectors in an Euclidean space. This can be better seen as follow.

A qutrit pure dephasing can be written as

$$\rho(t) = \mathcal{E}_t(\rho_0) = \begin{bmatrix} \rho_{11} & \rho_{12} \phi_1(t) & \rho_{13} \phi_4(t) \\ \rho_{21} \phi_2(t) & \rho_{22} & \rho_{23} \phi_6(t) \\ \rho_{31} \phi_5(t) & \rho_{32} \phi_7(t) & \rho_{33} \end{bmatrix}.$$ \hspace{1cm} (7)

To guarantee the Hermicity of $\rho(t)$, the dephasing factors must further satisfy $\phi_1(t) = \phi_2^*(t)$, and so on.

To expand $\rho$ as a nine-dimensional column vector, it is natural to use the Gell-Mann matrices (denoted by $\hat{\sigma}_m$, $m = 1, \ldots, 8$) as the generators of $su(3)$. However, after the diagonalization, the basis is changed into that of $\mathfrak{gl}(3)$ (e.g., $\hat{L}_0 = \hat{I}$, $\hat{L}_1 = \hat{L}_2 = (\hat{\sigma}_1 + i\hat{\sigma}_2)/2$, and $\hat{L}_3 = \hat{\sigma}_3$). Within this basis, the dynamical linear map $\mathcal{E}_t(\hat{L})$ is diagonalized, i.e., $\mathcal{E}_t(\hat{L}_m) = \hat{L}_m \phi_m(t)$.

In this case, we consider the member Hamiltonian $\hat{H}(\lambda_3, \lambda_8) = (\lambda_3 \hat{L}_3 + \lambda_8 \hat{L}_8)/2 \in \mathfrak{h}$ and $\vec{\lambda} = (\lambda_3, \lambda_8) \in \mathbb{R}^2$. After estimating all the commutators $[\hat{H}(\lambda_3, \lambda_8), \hat{L}_m] = (\hat{\alpha}_m \cdot \vec{\lambda})\hat{L}_m$, we obtain its adjoint representation $\tilde{H}(\lambda_3, \lambda_8) = (\lambda_3 \hat{L}_3 + \lambda_8 \hat{L}_8)/2$, which is diagonal in the $\mathfrak{gl}(3)$ basis.

Finally, according to Eq. (7) $\mathcal{E}_t^{(\tilde{L})} = \int_{\mathbb{R}^2} \varphi(\lambda_3, \lambda_8) e^{-i \tilde{H}(\lambda_3, \lambda_8)t} d\lambda_3 d\lambda_8$, we conclude that the (quasi-)distribution $\varphi(\lambda_3, \lambda_8)$ is governed by the following simultaneous Fourier transforms:

$$\begin{align*}
\phi_1(t) &= \int_{\mathbb{R}^2} \varphi(\lambda_3, \lambda_8) e^{-i (\hat{\alpha}_1 \cdot \vec{\lambda})t} d\lambda_3 d\lambda_8 \\
\phi_4(t) &= \int_{\mathbb{R}^2} \varphi(\lambda_3, \lambda_8) e^{-i (\hat{\alpha}_4 \cdot \vec{\lambda})t} d\lambda_3 d\lambda_8 \\
\phi_6(t) &= \int_{\mathbb{R}^2} \varphi(\lambda_3, \lambda_8) e^{-i (\hat{\alpha}_6 \cdot \vec{\lambda})t} d\lambda_3 d\lambda_8 .
\end{align*}$$ \hspace{1cm} (8)
On the other hand, we can collect the six non-zero root vectors $\vec{\alpha}_m$. They are two-dimensional vectors of equal length in the $\lambda_3$-$\lambda_8$ plane forming the root system $R$ of $su(3)$. We plot them in Fig. Further details are given in Supplementary Note 6.

Similarly, for $n$-dimensional pure dephasing, each member Hamiltonian $\hat{H}_\vec{\lambda}$, taken from the $su(n)$, possesses $n - 1$ free parameters $\vec{\lambda} = \{\lambda_{k^2-1}\}_{k=2,3,...,n}$; meanwhile, the (quasi-)distribution $\varphi(\vec{\lambda})$ in the simulating HE is a distribution function over the $(n - 1)$-dimensional Euclidean space. Moreover, the action of $\hat{H}_\vec{\lambda}$ on the $n^2 - n$ root spaces $\text{span}\{\hat{L}_m\}$ is described by the root system $R = \{\vec{\alpha}_m\}_m$, consisting of $n^2 - n$ real vectors of $(n - 1)$-dimension. Further properties of $R$ reduce the complexity of our procedure (see Methods).

Consequently, combining the techniques, i.e., the adjoint representation, the Fourier transform on groups, and the root space decomposition, we can concisely formulate our procedure to find the CHER $\varphi(\vec{\lambda})$ for the $n$-dimensional pure dephasing. We restrict ourselves to the diagonal member Hamiltonians (in $\mathfrak{su}(n)$) and establish its root system $R$. The (quasi-)distribution $\varphi(\vec{\lambda})$ is characterized by the $(n^2 - n)/2$ Fourier transforms with respect to positive roots and its corresponding dephasing factor $\phi_m(t)$ associated to the root space $\text{span}\{\hat{L}_m\}$:

$$\phi_m(t) = \int_{\mathbb{R}^{n-1}} \varphi(\vec{\lambda}) e^{-i(\vec{\alpha}_m \cdot \vec{\lambda})t} d^{n-1}\vec{\lambda}, \text{ for positive roots } \vec{\alpha}_m.$$ (9)

Furthermore, the simple roots define a new set of random variables $x_m = \vec{\alpha}_m \cdot \vec{\lambda}$, for simple roots $\vec{\alpha}_m$, and their corresponding equations define the marginals of $\varphi(\vec{\lambda})$ along $x_m$. The other equations describe the correlations among $x_m$. 

Example: qubit pair pure dephasing. As an instructive paradigm demonstrating our procedure to find the CHER of pure dephasing, we consider the extended spin-boson model consisting of a non-interacting qubit pair coupled to a common boson bath (see Fig. a) with total Hamiltonian

\[
\hat{H}_T = \sum_{j=1,2} \omega_j \hat{\sigma}_{z,j}/2 + \sum_{k} \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_{j,k} \hat{\sigma}_{z,j} \otimes (g_{j,k} \hat{b}_k^\dagger + g_{j,k}^* \hat{b}_k).
\]

We now focus on the pure dephasing of the qubit pair as a $4 \times 4$ system. The full dynamics has been given in Ref. [13].

To simulate the qubit pair pure dephasing, the diagonal member Hamiltonian is taken from the $\mathfrak{su}(4)$ Hamiltonian $\hat{H}_x = (\lambda_3 \hat{L}_3 + \lambda_8 \hat{L}_8 + \lambda_{15} \hat{L}_{15})/2$ and $\varphi(\vec{\lambda})$ is a (quasi-)distribution over $\mathbb{R}^3$ space with $\lambda_3$, $\lambda_8$, and $\lambda_{15}$ being its axes. Note that the $\mathfrak{su}(4)$ has six positive root vectors and three among them are simple, and all positive root vectors can be obtained by combining simple ones (see Fig. b). We perform the change of variables $x_m = \vec{\alpha}_m \cdot \vec{\lambda}$, $m = 1, 6, 13$. Then, the (quasi-)distribution changes as $\varphi(\vec{\lambda}) \mapsto \varphi'(x_1, x_6, x_{13})$. The three axes of $\varphi'(\vec{x})$ are defined by the three simple root vectors.

Additionally, since $\phi_6(t) = 1$, by observing the special correspondences between root vectors and dephasing factors, we can assume that

\[
\varphi'(\vec{x}) = \varphi_6(x_6)\varphi_{1,13}(x_1, x_{13})
\]

is separable into two parties. The Fourier equation for $\phi_6(t)$ leads to the result that $\phi_6(x_6) = \delta(x_6)$ and those for $\phi_1(t)$ and $\phi_{13}(t)$ specify the marginals of $\varphi_{1,13}(x_1, x_{13})$ along the direction $\vec{\alpha}_1$ and $\vec{\alpha}_{13}$, respectively; meanwhile the one for $\phi_9(t)$

\[
\phi_9(t) = \int_{\mathbb{R}^2} \varphi_{1,13}(x_1, x_{13})e^{-ix_1t}e^{-ix_{13}t}dx_1dx_{13}
\]

(11) describes the correlation between $x_1$ and $x_{13}$. 

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For the case of Ohmic spectral density $J(\omega) = \omega \exp(-\omega/\omega_c)$ in the zero-temperature limit, Eq. (11) can be recast into a conventional two-dimensional Fourier transform by a simple ansatz. Then, $\varphi_{1,13}(x_1, x_{13})$ can be easily obtained by conventional inverse transform and the numerical result is shown in Fig. c. It exhibits manifest negative regions and illustrates the nonclassical nature of the qubit pair pure dephasing. Detailed calculations are given in Supplementary Note 7.

Finally, having introducing our procedure to find the CHER, we combine it with the investigation on the intrinsic algebraic structure. Then the uniqueness of the CHER for pure dephasing is intelligible and the detailed proof is given in Supplementary Note 8.

It is worthwhile to recall that similar models, in which several qubits were coupled identically to a common bath, had been considered\cite{42,43}, wherein the suppression of decoherence within certain Hilbert subspace had been discovered. These studies spurred the development of the theory of decoherence-free-subspace\cite{45,46}, which is conceived as a promising solution to circumvent the obstacle of decoherence in quantum information science. The phenomenon of coherence-preserving can be observed in our paradigm as well and is related to the delta component $\varphi_6(x_6) = \delta(x_6)$ on $x_6$. Consequently, our procedure provides a potential application in the detection of decoherence-free-subspace in terms of delta components in the (quasi-)distribution.

**Discussion**

The studies on unveiling genuine quantum properties are very important since these discover the fundamental principle of nature and spur the growth of different branches in physics and technolo-
gies. Particularly, in the field of quantum information science, highly quantum-correlated systems are critical resources for prominent quantum information tasks which can hardly be accomplished efficiently by classical computers.

By genuine quantum properties, we refer to those that can never be resembled by classical strategies. For example, Bell’s inequality is derived based on the the assumption of realism and locality, while the Wigner function explain a boson field in terms of classical phase space. Inspired by these works, our characterization of process nonclassicality stems from the correspondence between the averaged dynamics of an HE and the dynamics reduced from a system-environment arrangement.

By introducing the CHER, the role of classical strategy played by the simulating HE for a dynamics is even more apparent. The (quasi-)distribution is endowed with an explanation in terms of a random phase model. This also implies that the nonclassical properties of a dynamics can be well-characterized by a (quasi-)distribution.

In particular, given a pure dephasing dynamics of any dimension, one can always construct a unique simulating HE consisting of diagonal member Hamiltonians. Therefore, the CHER of pure dephasing is faithful. Accordingly, based on our studies, we propose a measure of nonclassicality of pure dephasing by comparing the (quasi-)distributions in terms of variational distance. We also show that our measure is reasonable due to its convexity.

In order to make our measure viable, we also systematically establish a procedure to find
the CHER for pure dephasing dynamics. Our approach combines several techniques including Lie algebra representations, Fourier transforms on groups, and root space decompositions. We finally derive a set of equations from which the (quasi-)distribution can be retrieved. Finally, we remark that our approach may have potential application in the theory of decoherence-free-subspace.

Methods

Adjoint representation. The adjoint representation is a particularly important tool in the theory of Lie algebra. It assigns each element in a Lie algebra \( \mathfrak{L} \) an endomorphism in \( \mathfrak{gl}(\mathfrak{L}) \) (i.e., a homomorphism from \( \mathfrak{L} \) to itself) in terms of Lie bracket. Therefore, \( \mathfrak{gl}(\mathfrak{L}) \) is a Lie algebra consisting of linear maps acting on \( \mathfrak{L} \), wherein \( \mathfrak{L} \) plays the role of a vector space with the generators being its basis. The adjoint representation of each generator is constructed in terms of structure constants \( c_{klm} \). See Supplementary Note 1 for more details.

Cartan subalgebra. The structure of a Lie algebra \( \mathfrak{L} \) is largely determined by its Lie bracket, i.e., the commutator acting on \( \mathfrak{L} \). A Lie algebra is said to be abelian if all its elements are mutually commutative. Let \( \mathfrak{H} \) be a Lie subalgebra of \( \mathfrak{L} \). \( \mathfrak{H} \) is said to be the CSA of \( \mathfrak{L} \) if \( \mathfrak{H} \) is the maximal abelian (and semisimple) subalgebra. A very important property is that, for a Lie algebra consists of matrices, the elements in its CSA are all simultaneously diagonalizable for a suitably chosen basis.

In our case, to simulate pure dephasing dynamics, we deal with traceless and diagonal member Hamiltonians, taken from \( \mathfrak{H} \) of \( \mathfrak{su}(n) \). To be noted, since the adjoint representation preserves
the Lie bracket, the adjoint representation of $\mathfrak{h}$ is also a CSA of $\mathfrak{sl}(u(n))$. However, even if $\mathfrak{h}$ is diagonal, its adjoint representation may not necessarily be diagonal as well since the generators of $u(n)$ are not the suitable basis for diagonalizing it.

**Root system.** For $n$-dimensional systems, there are $n - 1$ generators in the $\mathfrak{h}$ of $\mathfrak{su}(n)$. Therefore, each member Hamiltonian possesses $n - 1$ parameters $\hat{H}_\lambda = \sum_{k=2}^{n} \lambda_k \hat{L}_k$, with $\{\hat{L}_k\}_{k=2,3,\ldots,n}$ being the generators of $\mathfrak{h}$. Additionally, the $n^2 - n$ roots $\vec{\alpha}_m$, associated to each root space $\text{span}\{\hat{L}_m\}$, are $(n - 1)$-dimensional vectors, forming the root system $R = \{\vec{\alpha}_m\}_m$ of $\mathfrak{su}(n)$. Besides, according to the theory of root space decomposition, the root system possesses the following critical properties: (1) the roots come in pairs in the sense that, if $\vec{\alpha}_m$ is a root, then $-\vec{\alpha}_m$ is a root as well. This reduces the number of equations half since we are sufficient to consider the positive roots alone. (2) Among the $(n^2 - n)/2$ positive roots, $n - 1$ simple roots provide the marginal of $\varphi$ along different directions and the others provide the information on the correlations between them. (3) For $\mathfrak{su}(n)$, the angle between any two non-pairing roots must be either $\pi/3$, $\pi/2$, or $2\pi/3$. Furthermore, with the Fourier transform on groups, an $n$-dimensional pure dephasing is characterized by $(n^2 - n)/2$ complex functions $\phi_m(t)$, which are the dephasing factors associated to each root space $\text{span}\{\hat{L}_m\}$.

**Data availability.** Data sharing not applicable to this article as no datasets were generated or analysed during the current study.
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Author contributions

H.-B.C. conceived the research and carried out the calculations, with the help from P.-Y.L. and C.G., under the supervision of Y.-N.C. J.B. proposed the idea of variational distance. Y.-N.C. and F.N. were responsible for the integration among different research units. All authors contributed to the discussion of the central ideas and to the manuscript.

Additional information

Competing financial interests: The authors declare no competing financial interests.
**Figure 1** The nonclassicality in Eq. (5). Here we consider the qubit pure dephasing reduced from the extended spin-boson model as a function of $\varphi$ for Ohmic spectral density in the zero-temperature limit at $\omega_c = 1$.

**Figure 2** The root system $R$ of $su(3)$. It consists of six non-zero root vectors on the $\lambda_3 - \lambda_8$ plane. Among them, $\vec{\alpha}_1$ (blue), $\vec{\alpha}_4$ (green), and $\vec{\alpha}_6$ (blue) are positive and the other three (red) are negative. Also, $\vec{\alpha}_1$ and $\vec{\alpha}_6$ are simple because $\vec{\alpha}_4 = \vec{\alpha}_1 + \vec{\alpha}_6$.

**Figure 3** Nonclassicality of the qubit pair pure dephasing. **a** A schematic illustration of our extended spin-boson model, describing a pair of non-interacting qubits coupled to a common boson environment. **b** To simulate the qubit pair pure dephasing, $\wp(\vec{\lambda})$ is a (quasi-)distribution over $\mathbb{R}^3$ space spanned by $\lambda_3$, $\lambda_8$, and $\lambda_{15}$. Here we show the six positive root vectors of $su(4)$. Three simple root vectors (blue) define a new set of random variables. The other three non-simple root vectors (green) can be expressed as a combination of simple ones, e.g., $\vec{\alpha}_9 = \vec{\alpha}_1 + \vec{\alpha}_6 + \vec{\alpha}_{13}$. **c** The function $\wp_{1,13}(x_1, x_{13})$ distributes over the plane spanned by $x_1$ and $x_{13}$. For the case of Ohmic spectral density in the zero-temperature limit and $\omega_c = 1$, it shows manifest negative regions and therefore indicates the nonclassicality of the qubit pair pure dephasing.