Identifying quantum phase transitions via geometric measures of nonclassicality

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It is shown that divergences in the susceptibility of any geometric measure of nonclassicality are sufficient conditions to identify phase transitions at arbitrary temperature. This establishes that geometric measures of nonclassicality, in any quantum resource theory, are generic tools to investigate phase transitions in quantum systems. For the zero-temperature case, we show that geometric measures of quantum coherence are especially useful for identifying first-order quantum phase transitions and can be a particularly robust alternative to other approaches employing measures of quantum correlations.

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I. INTRODUCTION

The development of various characterizations and notions of nonclassicality in recent years have led to several proposals to apply such notions in order to probe a system undergoing a phase transition. Examples include entanglement [1–3], quantum discord [4,5], and, more recently, quantum coherence [6–9]. Because these methods study the intrinsic nonclassical properties of quantum states, they do not require any prior knowledge about the order parameters associated with the phase transition. Notions of quantum nonclassicality are also often accompanied by novel operational interpretations. For instance, entanglement has operational interpretations in terms of quantum teleportation [10], quantum cryptography [11], and superdense coding [12]. Quantum discord has been shown to be a useful resource for entanglement distribution [13] and remote state preparation [14]. Quantum coherence has been applied to quantum state merging [15], quantum computation [16,17], and nonclassical light [18]. Probing phase transitions using such notions of nonclassicality therefore opens up the use of powerful mathematical machinery that was developed in order to study and interpret nonclassicality in the quantum information sciences [19–23].

In this article, we provide geometric justifications for the use of geometric measures of nonclassicality [24–26] to identify quantum phase transitions [8,9,27–29] under very general conditions. Specifically, we argue that, for arbitrary quantum resource theories, divergences in the geometric nonclassical susceptibility or its first derivative are sufficient for identifying phase transitions. This opens up the use of any geometric measure of nonclassicality, including but not limited to entanglement, quantum discord, or quantum coherence, to probe the phase transitions of a quantum system.

In particular, for quantum phase transitions at zero temperature, we show that first-order phase transitions can always be identified by a diverging geometric coherence susceptibility. This is true even when entanglement or quantum discord may potentially fail to identify the phase transition. We also present arguments showing how the geometric coherence susceptibility approach may be more general than several other methods employing Berry phases [30,31] or order parameters. This suggests that out of all the possible measures of nonclassicality, measures of quantum coherence may be particularly relevant to the study of phase transitions in quantum systems.

II. PRELIMINARIES

A phase transition is characterized by dramatic changes in the system of interest when there is a small variation in some physical control parameter λ. A critical parameter is then some value $\lambda = \lambda_c$ where a phase transition occurs.

A quantum phase transition (QPT) [32] is defined as a phase transition that occurs at zero temperature. At zero temperature, contributions from thermal fluctuations are completely removed from consideration and since thermal fluctuations are typically considered to be classical contributions, any critical phenomena that remains can be thought of as purely quantum in nature. In this scenario, a system in thermal equilibrium occupies the ground state of the Hamiltonian, $H(\lambda)$, which depends on the control parameter λ.

In this article, we adopt a geometric approach to the study of phase transitions. Suppose the control parameter λ is a real number which labels the points along some curve in state space, $\rho(\lambda)$. We consider some distance measure D, also called a metric, within this state space. Recall that D is a proper distance measure when it satisfies the following properties: for any quantum states ρ, σ, and τ, (i) $D(\rho,\sigma) \geqslant 0$, (ii) $D(\rho,\sigma) = 0$ if and only if $\rho = \sigma$, (iii) $D(\rho,\sigma) = D(\sigma,\rho)$, and (iv) $D(\rho,\sigma) \leqslant D(\rho,\tau) + D(\sigma,\tau)$. The last property is particularly noteworthy and is called the triangle inequality.

For a given distance measure D, we consider the distance between two infinitesimally close states along the curve $\rho(\lambda)$ and $\rho(\lambda+\delta\lambda)$. This is called a line element and is denoted ds. Its derivative with respect to λ is denoted $ds/d\lambda := \lim_{\delta\lambda\to 0^+} D[\rho(\lambda+\delta\lambda),\ \rho(\lambda)]/\delta\lambda$. Note that this is defined as a limit over positive $\delta\lambda$ so $ds/d\lambda$ is a non-negative quantity that directly quantifies the rate of change of state for an infinitesimal variation in the control parameter. When a system undergoes a phase transition, it is expected that $ds/d\lambda$ becomes nonanalytic because that signals structural changes

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in the system when λ is varied. This viewpoint is in line with the differential geometric approach, which identifies quantum phase transitions via nonanalyticities in the quantum geometric tensor [33]. We note that given a (Riemannian) metric tensor, a proper distance measure may be defined, while the converse may not be true in general. In this sense, the derivative $ds/d\lambda$ can be considered a generalization of the quantum geometric tensor approach.

A quantum coherence measure is a basis-dependent measure of the amount of quantum superposition among orthogonal quantum states. Let us consider a complete basis $\{|e_i\rangle\}$. We say that a quantum state ρ is incoherent if its density matrix has no nonzero off-diagonal elements, i.e., $\rho_{ij} := \langle e_i|\rho|e_j\rangle = 0$ for every $i \neq j$. Otherwise, we say that the state has coherence. Since the diagonal elements of the density matrix and hence the coherence is always defined with respect to some given basis $\{|e_i\rangle\}$, this is called the incoherent basis, and a state ρ is incoherent if and only if its density matrix is diagonal with respect to this basis.

An important class of coherence measures are the so-called geometric coherence measures. They are coherence measures of the form

$$\mathcal{C}_D(\rho) := \min_{\sigma\in\mathcal{I}} D(\rho,\sigma),$$

where D is some distance measure and the minimization is over the set of all incoherent states $\mathcal{I}$. For instance, one can choose the distance measure $D(\rho,\sigma)$ to be $\|\rho-\sigma\|_{l1}$, where $\|\cdot\|_{l1}$ is the $l1$ norm. This then gives rise to the so-called $l1$ norm of coherence [26] which turns out to be the absolute sum of all off-diagonal elements $\mathcal{C}_{l1}(\rho) = \sum_{i\neq j}|\rho_{ij}|$.

Based on the above definition of the geometric coherence, we can also define the geometric coherence susceptibility (GCS), which quantifies the rate of change of the geometric coherence of a state $\rho(\lambda)$ with respect to a change in the parameter λ. It is defined as

$$\begin{aligned}\mathcal{X}_D[\rho(\lambda)] &:= \frac{d\mathcal{C}_D[\rho(\lambda)]}{d\lambda}\\ &= \lim_{\delta\lambda\to 0}\{\mathcal{C}_D[\rho(\lambda+\delta\lambda)] - \mathcal{C}_D[\rho(\lambda)]\}/\delta\lambda.\end{aligned}$$

More generally, for arbitrary quantum resource theories, one may further define a geometric nonclassicality quantifier $\mathcal{N}_D(\rho) := \min_{\sigma\in\mathcal{S}} D(\rho,\sigma)$, where $\mathcal{S}$ is any set of classical states. The corresponding geometric nonclassical susceptibility (GNS) is denoted $\mathcal{X}_{\mathcal{N},\mathcal{D}}[\rho(\lambda)]$. Such measures play a significant role in the study of quantum resources such as entanglement [24] and quantum discord [25].

In the following sections, we consider the role of GNS and GCS in identifying QPTs.

III. GEOMETRIC NONCLASSICAL SUSCEPTIBILITY AND PHASE TRANSITIONS AT ARBITRARY TEMPERATURE

We first consider the GNS for arbitrary quantum resource theories. It may be expected that a diverging GNS implies a sudden structural change in the system and therefore indicates a phase transition. The following theorem provides a general geometric argument that this is true for any quantum resource theory under consideration.

Theorem 1. If the nonclassical susceptibility $\mathcal{X}_{\mathcal{N},\mathcal{D}}[\rho(\lambda)]$ diverges at some critical parameter $\lambda = \lambda_c$, then $ds/d\lambda$ also diverges and λ_c is a critical parameter indicating a phase transition.

Proof. Suppose $\rho(\lambda)$ is the ground-state density matrix of some Hamiltonian $H(\lambda)$ which depends on some external parameter λ. The coherence susceptibility of the geometric coherence with respect to some external parameter λ is then defined as the quantity

$$\begin{aligned}\mathcal{X}_{\mathcal{N},D}[\rho(\lambda)] &:= d\mathcal{N}_D[\rho(\lambda)]/d\lambda\\ &= \lim_{\delta\lambda\to 0}\{\mathcal{N}_D[\rho(\lambda+\delta\lambda)] - \mathcal{N}_D[\rho(\lambda)]\}/\delta\lambda.\end{aligned}$$

Let us consider $\mathcal{N}_D[\rho(\lambda+\delta\lambda)] - \mathcal{N}_D[\rho(\lambda)]$. Without any loss in generality, we can assume that $\mathcal{N}_D[\rho(\lambda+\delta\lambda)] - \mathcal{N}_D[\rho(\lambda)] \geqslant 0$ because otherwise we can always reparametrize λ to go in the other direction such that the assumption will always be true. Suppose $\sigma(\lambda)$ is the optimal state that achieves $\mathcal{N}_D[\rho(\lambda)] = D[\rho(\lambda),\sigma(\lambda)]$. We have the following series of inequalities:

$$\mathcal{N}_D[\rho(\lambda+\delta\lambda)] - \mathcal{N}_D[\rho(\lambda)] = \min_{\sigma\in\mathcal{I}} D[\rho(\lambda+\delta\lambda),\sigma] - \min_{\sigma\in\mathcal{I}} D[\rho(\lambda),\sigma] \quad (1)$$

$$\leqslant D[\rho(\lambda+\delta\lambda),\sigma(\lambda)] - D[\rho(\lambda),\sigma(\lambda)] \quad (2)$$

$$\leqslant D[\rho(\lambda+\delta\lambda),\rho(\lambda)]. \quad (3)$$

Equation (1) comes from the definition of geometric nonclassicality. The inequality (2) comes from fact that $\sigma(\lambda)$ is the optimal state that minimizes the distance to $\rho(\lambda)$, but in general may be suboptimal for the state $\rho(\lambda+\delta\lambda)$. The inequality (3) comes from the reverse triangle inequality $|D(A,C) - D(B,C)| \leqslant D(A,B)$.

Now suppose that $\mathcal{X}_{\mathcal{N},D}$ diverges at point λ_c such that $\mathcal{X}_{\mathcal{N},D}[\rho(\lambda_c)] = \infty$, then from inequality (3), we must also have $D[\rho(\lambda+\delta\lambda),\rho(\lambda)]/\delta\lambda \to \infty$ as $\delta\lambda \to 0$. This implies that $ds/d\lambda$ diverges at $\lambda = \lambda_c$, so there must be a phase transition at that point. ∎

Phase transitions can also be accompanied by a cusp or a kink in the GNS, i.e., the first derivative of the GNS diverges instead of the GNS itself. The following theorem provides a geometric argument that such features in the GNS can also be used to identify phase transitions under general conditions.

Theorem 2. If the first derivative of the nonclassical susceptibility $d\mathcal{X}_{\mathcal{N},\mathcal{D}}[\rho(\lambda)]/d\lambda$ diverges at some critical parameter $\lambda = \lambda_c$, then $d^2s/d\lambda^2$ diverges and $ds/d\lambda$ is nonanalytic at $\lambda = \lambda_c$.

Proof. The derivative $d\mathcal{X}_{\mathcal{N},D}[\rho(\lambda)]/d\lambda$ is just the second-order derivative of the nonclassicality quantifier $\mathcal{N}_D[\rho(\lambda)]$. This can be written as the limit

$$d\mathcal{N}_D[\rho(\lambda)]\lambda := \lim_{\delta\lambda\to 0}\frac{\mathcal{N}_D[\rho(\lambda+\delta\lambda)] - 2\mathcal{N}_D[\rho(\lambda)] + \mathcal{N}_D[\rho(\lambda-\delta\lambda)]}{\delta\lambda^2}.$$

As in the proof of Theorem 1, let $\sigma(\lambda)$ is the optimal state that achieves $\mathcal{N}_D[\rho(\lambda)] = D[\rho(\lambda), \sigma(\lambda)]$. We again assume without any loss in generality that $d\mathcal{X}_{\mathcal{N},D}[\rho(\lambda)]/d\lambda \geqslant 0$ because otherwise we can just appropriately reparametrize λ. We then consider the numerator, which can be shown to obey the following series of inequalities:

$$\begin{aligned} &\mathcal{N}_D[\rho(\lambda+\delta\lambda)] - 2\mathcal{N}_D[\rho(\lambda)] + \mathcal{N}_D[\rho(\lambda-\delta\lambda)] \\ &\quad \leqslant D[\rho(\lambda+\delta\lambda), \sigma(\lambda)] - 2D[\rho(\lambda), \sigma(\lambda)] \\ &\quad\quad + D[\rho(\lambda-\delta\lambda), \sigma(\lambda)] \quad (4) \\ &\quad \leqslant D[\rho(\lambda+\delta\lambda), \rho(\lambda)] + D[\rho(\lambda-\delta\lambda), \rho(\lambda)] \quad (5) \\ &\quad = D[\rho(\lambda+\delta\lambda), \rho(\lambda)] - 2D[\rho(\lambda), \rho(\lambda)] \\ &\quad\quad + D[\rho(\lambda-\delta\lambda), \rho(\lambda)]. \quad (6) \end{aligned}$$

In Eq. (4), we used the fact that $\sigma(\lambda)$ is the optimal state that minimizes the distance to $\rho(\lambda)$, but is suboptimal in general for $\rho(\lambda \pm \delta\lambda)$. In Eq. (5), we applied the reverse triangle inequality $|D(A, C) - D(B, C)| \leqslant D(A, B)$. Equation (6) then follows from the fact that $D[\rho(\lambda), \rho(\lambda)] = 0$, which is a fundamental property of any distance measure D.

We then observe that

$$\begin{aligned} \frac{d^2 s}{d\lambda^2} = \lim_{\delta\lambda\to 0} \{&D[\rho(\lambda+\delta\lambda), \rho(\lambda)] - 2D[\rho(\lambda), \rho(\lambda)] \\ &+ D[\rho(\lambda-\delta\lambda), \rho(\lambda)]\}/\delta\lambda^2. \quad (7) \end{aligned}$$

Therefore, if $d\mathcal{X}_{\mathcal{N},D}[\rho(\lambda)]/d\lambda = \infty$ at some $\lambda = \lambda_c$, then from Eqs. (6) and (7), we must also have $d^2s/d\lambda^2 = \infty$. Since the derivative of $ds/d\lambda$ diverges, it is nonanalytic at $\lambda = \lambda_c$. ■

Theorems 1 and 2 provide geometric justification for the use of geometric measures of any nonclassical quantum resource for identifying quantum phase transitions. We note that, in these arguments, no prior assumptions are made about the nature of the state $\rho(\lambda)$, so the results apply to quantum systems at arbitrary temperature.

IV. GEOMETRIC COHERENCE SUSCEPTIBILITY AND QUANTUM PHASE TRANSITIONS

In this section, we consider the special case of QPTs at zero temperature. We are therefore interested in probing phase transitions that occur in the ground state $|\psi_0(\lambda)\rangle$ of some Hamiltonian $H(\lambda)$. A sudden change in the ground state represented by a discontinuity in $|\psi_0(\lambda)\rangle$ across the critical parameter is typical of a first-order QPT. The following theorem demonstrates that any such change in the ground state is equivalent to the existence of some incoherent basis where the GCS diverges.

Theorem 3. At zero temperature, a first-order quantum phase transition occurs and $ds/d\lambda$ diverges at some critical parameter $\lambda = \lambda_c$ if and only if there exists an incoherent basis where the coherence measure $\mathcal{C}_D[\rho(\lambda)]$ is discontinuous at $\lambda = \lambda_c$, and $\mathcal{X}_D[\rho(\lambda)]$ diverges at $\lambda = \lambda_c$.

Proof. Let the Hamiltonian describing the system be $H(\lambda)$, and the ground state be $|\psi_0(\lambda)\rangle$. The corresponding density matrix is denoted $\rho_0(\lambda)$.

Suppose for a given distance measure D, $ds/d\lambda$ diverges at $\lambda = \lambda_c$ and there is a discontinuity in the quantum state along the curve parametrized by λ. This means that the states as you approach $\lambda = \lambda_c$ from above and below are different, i.e., $\lim_{\delta\to 0^+} \rho_0(\lambda_c - \delta) \neq \lim_{\delta\to 0^+} \rho_0(\lambda_c + \delta)$.

Let us choose an incoherent basis $\{|e_i\rangle\}$ such that $|e_0\rangle = |\psi_0(\lambda_c - \delta)\rangle$, where $\delta > 0$. We observe that, in the basis $\{|e_i\rangle\}$, $\mathcal{C}_D[\rho_0(\lambda_c - \delta)] = 0$.

Consider $|\psi_0(\lambda_c + \delta)\rangle$ where $\delta > 0$. Since $|\psi_0(\lambda_c + \delta)\rangle \neq |\psi_0(\lambda_c - \delta)\rangle$ as we take the limit $\delta \to 0$, there are only two special cases we need to consider. $|\psi_0(\lambda_c + \delta)\rangle$ is either orthogonal to $|\psi_0(\lambda_c - \delta)\rangle$, or it has partial overlap with $|\psi_0(\lambda_c - \delta)\rangle$.

If it is orthogonal, we can just choose a basis where $|e_i\rangle \neq |\psi_0(\lambda_c + \delta)\rangle$ for every $i \geqslant 1$. Since $|\psi_0(\lambda_c + \delta)\rangle$ is not an element of the incoherent basis, this means that $\mathcal{C}_D[\rho_0(\lambda_c + \delta)] > 0$ even in the limit $\delta \to 0$.

If there is partial overlap, then we can write $|\psi_0(\lambda_c + \delta)\rangle = a|\psi_0(\lambda_c - \delta)\rangle + b|\psi^\perp\rangle$, where $|\psi^\perp\rangle$ is some normalized vector orthogonal to $|\psi_0(\lambda_c - \delta)\rangle$. Since there is a discontinuity in the ground state, we are guaranteed that b will not go to zero as $\delta \to 0$. We can therefore choose $|e_1\rangle = |\psi^\perp\rangle$. Since $|e_0\rangle = |\psi_0(\lambda_c - \delta)\rangle$ and $|\psi_0(\lambda_c + \delta)\rangle = a|e_0\rangle + b|e_1\rangle$, this means that we have $\mathcal{C}_D[\rho_0(\lambda_c + \delta)] > 0$ even in the limit $\delta \to 0$.

In either case, it suggests that we can always find a basis $\{|e_i\rangle\}$ where $\lim_{\delta\to 0^+} \mathcal{C}_D[\rho_0(\lambda_c - \delta)] = 0$ and $\lim_{\delta\to 0^+} \mathcal{C}_D[\rho_0(\lambda_c + \delta)] > 0$, so $\mathcal{C}_D[\rho_0(\lambda)]$ is a step function in the immediate vicinity of $\lambda = \lambda_c$. This implies that $\mathcal{X}_D[\rho(\lambda)]$ diverges at $\lambda = \lambda_c$. This proves the theorem in the forward direction.

For the converse direction, suppose the coherence measure $\mathcal{C}_D$ is discontinuous and $\lim_{\delta\lambda\to 0^+} |\mathcal{C}_D[\rho(\lambda_c - \delta\lambda)] - \mathcal{C}_D[\rho(\lambda_c + \delta\lambda)]| = \Delta$, for some $\Delta > 0$. Without any loss in generality, we assume that the coherence decreases as we increase λ such that $\mathcal{C}_D[\rho(\lambda_c - \delta\lambda)] > \mathcal{C}_D[\rho(\lambda_c + \delta\lambda)]$, as otherwise we can reparametrize λ to go in the other direction. Let σ be the optimal state achieving $\mathcal{C}_D[\rho(\lambda_c + \delta\lambda)] = D[\rho(\lambda_c + \delta\lambda), \sigma]$. We then have the following series of inequalities:

$$\begin{aligned} &\mathcal{C}_D[\rho(\lambda_c - \delta\lambda)] - \mathcal{C}_D[\rho(\lambda_c + \delta\lambda)] \\ &\quad \leqslant D[\rho(\lambda_c - \delta\lambda), \sigma] - D[\rho(\lambda_c + \delta\lambda), \sigma] \quad (8) \\ &\quad \leqslant D[\rho(\lambda_c - \delta\lambda), \rho(\lambda_c + \delta\lambda)]. \quad (9) \end{aligned}$$

In Eq. (8), we used the definition $\mathcal{C}_D(\rho) = \min_{\sigma\in\mathcal{I}} D[\rho, \sigma]$ and the fact that σ is optimal for the state $\rho(\lambda_c + \delta\lambda)$, but is in general suboptimal for $\rho(\lambda_c - \delta\lambda)$. In Eq. (9), we used the inverse triangle inequality $|D(A, C) - D(B, C)| \leqslant D(A, B)$.

Finally, combining Eq. (9) and the fact that $\lim_{\delta\lambda\to 0^+} |\mathcal{C}_D[\rho(\lambda_c - \delta\lambda)] - \mathcal{C}_D[\rho(\lambda_c + \delta\lambda)]| = \Delta$ implies $\lim_{\delta\lambda\to 0^+} D[\rho(\lambda_c - \delta\lambda), \rho(\lambda_c + \delta\lambda)] > \Delta$, which shows that there is a discontinuity in the ground state, so there is a first order QPT. ■

Theorem 3 therefore singles out geometric measures of quantum coherence as a useful tool to probe first-order QPTs where other nonclassical measures may potentially fail. We illustrate this with an example in a subsequent section.

V. GEOMETRIC COHERENCE SUSCEPTIBILITY, BERRY PHASES, AND ORDER PARAMETERS

For many systems, the Berry phase is a useful tool for studying QPTs. Here, we consider the relationship between GCS and the Berry phase at the critical parameter.

Suppose the ground state of the Hamiltonian $H(\lambda)$ is $|\psi_0(\lambda)\rangle$ and that the system is adiabatically evolved through some close looped trajectory in state space. The evolution of the ground state at any point along this closed loop can be described by $U(\mu)|\psi_0(\lambda)\rangle$, where $U(\mu) := e^{-iG(\mu)}$ and $G(\mu)$ is a Hermitian operator that depends on the parameter $\mu \in [0, 2\pi]$. Since the trajectory follows a closed loop, the unitary $U(\mu)$ and the Hermitian operator $G(\mu)$ must satisfy the cyclic property $U(0)|\psi_0(\lambda)\rangle = |\psi_0(\lambda)\rangle = U(2\pi)|\psi_0(\lambda)\rangle$.

We now consider the Berry phase generated by an evolution described by $G(\mu) = \mu O$, where O is some Hermitian operator.

Corollary 3.1. Consider a Berry phase generated by a cyclic unitary of the type $U(\mu) := e^{-i\mu O}$, $\mu \in [0, 2\pi]$ acting on a ground state $|\psi_0(\lambda)\rangle$ of the system Hamiltonian $H(\lambda)$.

Suppose at some critical parameter $\lambda = \lambda_c$ that the Berry phases just before and after the critical parameter is given by $\phi^B(\lambda_c^-) = \phi^-$ and $\phi^B(\lambda_c^+) = \phi^+$, respectively, where $\lambda_c^- < \lambda_c < \lambda_c^+$.

Then the Berry phase is discontinuous such that $\phi^- \neq \phi^+$ only if $\mathcal{X}_D(|\psi_0(\lambda)\rangle)$ is divergent at $\lambda = \lambda_c$ for some incoherent basis.

Proof. We first compute the Berry phase generated by the unitary $U(\mu)$. It can be verified that it is given by

$$\phi^B = i\int_0^{2\pi} \langle\psi_0(\lambda)|U(\mu)^\dagger d\mu U(\mu)|\psi_0(\lambda)\rangle \quad (10)$$

$$= -i^2\int_0^{2\pi} \langle\psi_0(\lambda)|U(\mu)^\dagger U(\mu)O|\psi_0(\lambda)\rangle \quad (11)$$

$$= 2\pi\langle\psi_0(\lambda)|O|\psi_0(\lambda)\rangle, \quad (12)$$

where $|\psi_0(\lambda)\rangle$ is the ground state of the Hamiltonian $H(\lambda)$. The density matrix of $|\psi_0(\lambda)\rangle$ is denoted $\rho_0(\lambda) = |\psi_0(\lambda)\rangle\langle\psi_0(\lambda)|$.

Suppose the Berry phase is discontinuous and $\phi^- \neq \phi^+$. This implies that $\phi^-/2\pi = \langle\psi_0(\lambda_c^-)|O|\psi_0(\lambda_c^-)\rangle \neq \langle\psi_0(\lambda_c^+)|O|\psi_0(\lambda_c^+)\rangle = \phi^+/2\pi$ for $\lambda_c^- < \lambda_c < \lambda_c^+$. This also implies $\lim_{\delta\to 0^+}\rho_0(\lambda_c + \delta/2) \neq \lim_{\delta\to 0^+}\rho_0(\lambda_c - \delta/2)$, so there is a first-order QPT at $\lambda = \lambda_c$. Theorem 3 then shows that the coherence susceptibility $\mathcal{X}_D(|\psi_0(\lambda)\rangle)$ is divergent for some incoherent basis at the critical parameter. ■

A similar argument also shows that if some order parameter is discontinuous at a critical parameter, then it must also be identifiable by a diverging GCS.

Corollary 3.2. Let O be a Hermitian observable representing some order parameter for a system described by a Hamiltonian $H(\lambda)$. Let $|\psi_0(\lambda)\rangle$ be the ground state of the system.

Suppose at some critical parameter $\lambda = \lambda_c$, the mean value of the order parameter as we approach the critical parameter from below and above are $\langle\psi_0(\lambda_c^-)|O|\psi_0(\lambda_c^-)\rangle$ and $\langle\psi_0(\lambda_c^+)|O|\psi_0(\lambda_c^+)\rangle$, respectively, where $\lambda_c^- < \lambda_c < \lambda_c^+$.

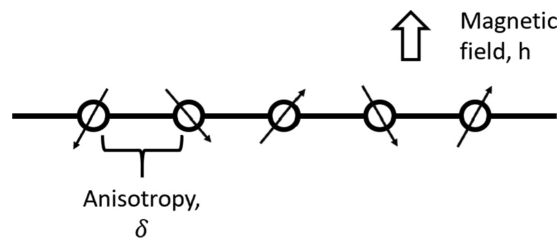

FIG. 1. XY model for the spin-$\frac{1}{2}$ chain. The total Hamiltonian $H(\delta, h)$ is parametrized by δ, which represents the anisotropy in the nearest neighbor interaction, and h, which represents the strength of the local magnetic field along the z axis.

Then the mean value of the order parameter is discontinuous and $\langle\psi_0(\lambda_c^-)|O|\psi_0(\lambda_c^-)\rangle \neq \langle\psi_0(\lambda_c^+)|O|\psi_0(\lambda_c^+)\rangle$ only if $\mathcal{X}_D(|\psi_0(\lambda)\rangle)$ is divergent at $\lambda = \lambda_c$ for some incoherent basis.

Proof. Let the density matrix of the ground state $|\psi_0(\lambda)\rangle$ be denoted by $\rho_0(\lambda) = |\psi_0(\lambda)\rangle\langle\psi_0(\lambda)|$.

Since $\langle\psi_0(\lambda_c^-)|O|\psi_0(\lambda_c^-)\rangle \neq \langle\psi_0(\lambda_c^+)|O|\psi_0(\lambda_c^+)\rangle$ for $\lambda_c^- < \lambda_c < \lambda_c^+$, and this remains true even as λ_c^- and λ_c^+ approaches λ_c, we must have that $\lim_{\delta\to 0}\rho_0(\lambda_c + \delta/2) \neq \lim_{\delta\to 0}\rho_0(\lambda_c - \delta/2)$. The rest of the argument follows identically as for Corollary 3.1. ■

Corollaries 3.1 and 3.2 demonstrate how the GCS approach is more general than many types of Berry phases or order parameters that are used to identify first-order phase transitions. This supports the view that GCS can be a useful alternative for probing QPTs.

VI. EXAMPLE

To illustrate the results, we consider a one-dimensional spin-$\frac{1}{2}$ chain with XY interaction (see Fig. 1). The simplest nontrivial example of this is a two-spin system. As we shall see, this example is particularly instructive and describes many of the salient features of the results that were discussed in the previous sections.

The Hamiltonian of a two-site system is given by

$$H(\delta, h) = -\frac{1+\delta}{2}\sigma_1^x\sigma_2^x - \frac{1-\delta}{2}\sigma_1^y\sigma_2^y - \frac{h}{2}(\sigma_1^z + \sigma_2^z).$$

The parameter δ describes the anisotropy between the X and the Y interactions, while h describes the strength of the local magnetic field pointing in the $+z$ direction. For any given δ and h, we let $|\psi_0(\delta, h)\rangle$ denote the ground state of the Hamiltonian $H(\delta, h)$.

The above system is described by a 4×4 matrix, so we can directly compute the eigenvalues and eigenvectors of the Hamiltonian. The ground state at zero temperature then corresponds to the eigenvector with the lowest eigenvalue. One may verify that the Hamiltonian has the eigenvalues ± 1 and $\pm r$, where $r = (\delta^2 + h^2)^{1/2}$. As such, there are only two possible ground states, corresponding to the two negative eigenvalues (see Table I).

We observe that $|g_-\rangle$, the eigenvector corresponding to the eigenvalue -1, is an odd-parity state. The eigenvector $|g_+(\delta, h)\rangle$ corresponding to the eigenvalue $-r$ is an even-parity state whose amplitude depends on $\tan\theta := \delta/h$.

TABLE I. The two lowest-energy eigenstates for two spins with XY interaction.

Eigenvector	Eigenvalue
$\vert g_-\rangle := (\vert 01\rangle_{1,2} + \vert 10\rangle_{1,2})/\sqrt{2}$	-1
$\vert g_+(\delta, h)\rangle := \cos\frac{\theta}{2}\vert 00\rangle_{1,2} + \sin\frac{\theta}{2}\vert 11\rangle_{1,2}$	$-r$

Depending on the value of r, $|g_-\rangle$ and $|g_+(\delta, h)\rangle$ competes to be the ground state of the system. When $r > 1$, the ground state is $|\psi_0(\delta, h)\rangle = |g_+(\delta, h)\rangle$. When $r < 1$, the ground state is $|\psi_0(\delta, h)\rangle = |g_-\rangle$. The point $r = 1$ therefore identifies a critical parameter, since there is discontinuity in the ground state around this point.

For comparison, let us consider the Berry phase generated by the cyclic unitary $U(\mu) = \exp[-i\mu(\sigma_1^z + \sigma_2^z)/2]$. Such Berry phases have been experimentally observed [34]. One may verify that this will transform the two possible ground states in the following way:

$$U(\mu)\,|g_-\rangle = |g_-\rangle = \frac{1}{\sqrt{2}}(|01\rangle_{1,2} + |10\rangle_{1,2}),$$
$$U(\mu)\,|g_+(\delta, h)\rangle = \cos\frac{\theta}{2}|00\rangle_{1,2} + e^{-2i\mu}\sin\frac{\theta}{2}|11\rangle_{1,2}.$$

Integrating over $\mu \in [0, 2\pi]$, we see that, when $r < 1$, the accumulated Berry phase is $\phi^- = 0$, and, when $r > 1$, the accumulated Berry phase is $\phi^+ = -4\pi\cos\theta$. The Berry phase is therefore discontinuous at $r = 1$, pointing to a first-order phase transition at that point.

Let us also consider the order-parameter approach. First, we choose the total magnetization $O = \sigma_1^z + \sigma_2^z$ to be our order parameter. We see that, when $r < 1$, $\langle g_-|O|g_-\rangle = 0$, and when $r > 1$, we have $\langle g_+(\delta, h)|O|g_+(\delta, h)\rangle = \sin^2\frac{\theta}{2} - \cos^2\frac{\theta}{2} = -\cos\theta$. The discontinuity in the order parameter also indicates a first-order phase transition.

In summary, we see that there is a discontinuity in the ground state at the point $r = 1$, and that this discontinuity is accompanied by a sudden accumulation of the Berry phase and the total magnetization at the critical parameter when $0 < |\cos\theta| < 1$. This in turn suggests that the QPT at the critical point may also be detected by observing the divergences in the GCS (see Theorem 1 and Corollaries-3.1 and 3.2).

We now proceed to verify this. Let us choose the distance measure D to be the $l1$-norm-induced distance. The corresponding geometric coherence measure is then $\mathcal{C}_{l1}$, which is commonly referred to as the $l1$ norm of coherence. The $l1$ norm of coherence is chosen because it is particularly easy to compute. For any given state ρ and basis $\{|e_i\rangle\}$, the $l1$ norm of coherence is given by the absolute sum of all the off-diagonal elements, i.e., $\mathcal{C}_{l1}(\rho) = \sum_{i\neq j}|\langle e_i|\rho|e_j\rangle|$.

We then calculate the $l1$ norm of coherence in the computational basis $\{|00\rangle_{1,2}, |01\rangle_{1,2}, |10\rangle_{1,2}, |11\rangle_{1,2}\}$. One may verify that $\mathcal{C}_{l1}(|g_-\rangle) = 1$, while $\mathcal{C}_{l1}[|g_+(\delta, h)\rangle] = |\sin\theta| < 1$ when $0 < |\cos\theta| < 1$. The coherence is therefore a step function in the vicinity of $r = 1$, which means the coherence susceptibility $\mathcal{X}_{l1}[|\psi_0(\delta, h)\rangle]$ diverges at $r = 1$. This means that the coherence susceptibility is able to correctly identify the critical parameter. This example demonstrates how the coherence susceptibility can be at least as robust as the Berry-phase or order-parameter approaches.

We now compare this to the entanglement approach. For this purpose, we focus on the special case where $h = 0$, i.e., there is no local magnetic field along the z direction. When the local magnetic field is absent, the system no longer has a preferred direction along the z axis. To verify this, we see that, at $h = 0$, $\theta = \pi/2$. Substituting $\theta = \pi/2$ into the expression for $|g_+(\delta, h = 0)\rangle$ we get the maximally entangled ground state

$$|g_+(\delta, h = 0)\rangle = \frac{1}{\sqrt{2}}(|00\rangle_{1,2} + |11\rangle_{1,2})$$

when $r > 1$. We compare this with the ground state at $r < 1$, which is

$$|g_-\rangle = \frac{1}{\sqrt{2}}(|01\rangle_{1,2} + |10\rangle_{1,2}),$$

so we see that neither of the possible ground states identifies a preferred direction along the z axis. Importantly, we see that both $|g_-\rangle$ and $|g_+(\delta, h = 0)\rangle$ are maximally entangled states, so $E(|g_-\rangle) = E(|g_+(\delta, h = 0)\rangle)$ for any entanglement measure E. The total entanglement in the system does not change at the critical parameter $r = 1$. This quantum phase transition is therefore not supported by any change in the observed entanglement and so cannot be detected by divergences in the entanglement susceptibility, regardless of the entanglement measure being employed. Note that since quantum discord and entanglement are equivalent over the set of pure states, and that ground states of a Hamiltonian are pure states by definition, measures of quantum discord will also not be able to detect this energy-level crossing.

Nonetheless, Theorem 1 suggests that we should still be able to find an incoherent basis where the GCS diverges, regardless of whether the entanglement approach fails. To verify this, one can compute $\mathcal{C}_{l1}$ in the incoherent basis $\{\frac{1}{\sqrt{2}}(|01\rangle_{1,2} + |10\rangle_{1,2}), \frac{1}{\sqrt{2}}(|01\rangle_{1,2} - |10\rangle_{1,2}), |00\rangle_{1,2}, |11\rangle_{1,2}\}$. In this basis, we see that $\mathcal{C}_{l1}(|g_-\rangle) = 0$ and $\mathcal{C}_{l1}[|g_+(\delta, h)\rangle] = 1$. Again, we see that the coherence is a step function in the vicinity of the critical parameter, and that $\mathcal{X}_{l1}[|\psi_0(\delta, h)\rangle]$ diverges at $r = 1$. This demonstrates how coherence-based approaches may be a robust method of identifying quantum phase transitions as compared with correlation-based methods.

We now consider the more general case of N spins with the XY interaction (see Fig. 1). For general N, the Hamiltonian has the form

$$H(\delta, h) = -\sum_{j=1}^{N}\left(\frac{1+\delta}{4}\sigma_j^x\sigma_{j+1}^x + \frac{1-\delta}{4}\sigma_j^y\sigma_{j+1}^y + \frac{h}{2}\sigma_j^z\right),$$

where N is the total number of spins, and σ_j^a, $a = x, y, z$ are the canonical Pauli operators acting on the jth spin.

In Ref. [27], the derivative of the entanglement density was investigated in the thermodynamic limit $N \to \infty$. It was observed that the phase transition at $h = 0$, $\delta = 1$ was not identified by the entanglement susceptibility. This is similar to the two-spin example which was previously discussed.

It is known that, for $N > 1$, the ground state belongs to either one of the parity sectors. At $h = \pm(1 - \delta^2)^{1/2}$, i.e., $r =$

$(\delta^2 + h^2)^{1/2} = 1$, a phase transition occurs where the parity of the ground state flips [35]. We already see this from the two-spin case, where at $r = 1$, there is an energy-level crossing and the ground state flips from the odd-parity state $|g_-\rangle$ to the even-parity state $|g_+(\delta, h)\rangle$.

We now show that, unlike the entanglement susceptibility, one can always find incoherent bases where the coherence susceptibility will diverge at $r = 1$. This argument applies for any number of spins N. To do this, we first introduce some notation. Let $p = \pm$ denote the parity of the ground state when $r < 1$. For $r < 1$, we denote the ground state as $|g_p(\delta, h)\rangle$, and for $r > 1$, the ground state is denoted $|g_{-p}(\delta, h)\rangle$.

Suppose the subspace with parity $-p$ is spanned by some orthonormal set $\{|e_m\rangle\}_{m=0}^{M_p-1}$ and the subspace with parity p is spanned by another orthonormal set $\{|e_m\rangle\}_{m=M_p}^{2^N}$. Just before the critical parameter $r = 1$, the parity is p, so the ground state belongs to the subspace spanned by $\{|e_m\rangle\}_{m=M_p}^{2^N}$. We are therefore allowed us to choose a basis where $|e_{M_p}\rangle = |g_p(\delta^-, h^-)\rangle$ at some δ^-, h^- close to criticality such that $r < 1$.

Similarly, we observe that just after the critical parameter $r = 1$, the parity is $-p$, so the ground state belongs to the subspace spanned by $\{|e_m\rangle\}_{m=0}^{M_p-1}$ instead. For the subspace with parity $-p$, we are allowed to choose a basis where $|e_0\rangle = |g_{-p}(\delta^+, h^+)\rangle$ at some δ^+, h^+ close to criticality such that $r > 1$. We then perform a discrete Fourier transform

$$|e'_{m'}\rangle := \sum_{m=0}^{M_p-1} \exp\left[-\frac{2\pi i}{M_p} mm'\right] \Big/ \sqrt{M_p} |e_m\rangle.$$

Since the Fourier transform is unitary, it maps one orthonormal set $\{|e_m\rangle\}_{m=0}^{M_p-1}$ into another orthonormal set $\{|e'_m\rangle\}_{m=0}^{M_p-1}$.

To calculate the coherence, we choose the incoherent basis to be $\{|e'_m\rangle\}_{m=0}^{M_p-1} \bigcup \{|e_m\rangle\}_{m=M_p}^{2^N}$.

The purpose of the exercise above is twofold. First, it ensures that the ground state at $r < 1$ always has zero coherence, i.e., $\mathcal{C}_D(|g_p(\delta^-, h^-)\rangle) = 0$. This is because $|g_p(\delta^-, h^-)\rangle$ is an element of the set $\{|e_m\rangle\}_{m=M_p}^{2^N}$, so it is also an element of the incoherent basis $\{|e'_m\rangle\}_{m=0}^{M_p-1} \bigcup \{|e_m\rangle\}_{m=M_p}^{2^N}$. Every element of the coherent basis has no off-diagonal matrix elements, so it must have zero coherence.

Second, it ensures that immediately after the critical parameter at $r > 1$, the ground state has a finite, nonzero coherence $\mathcal{C}_D(|g_p(\delta^+, h^+)\rangle) > 0$. This is because $|g_p(\delta^+, h^+)\rangle$ is spanned by, but is not an element of, the orthonormal set $\{|e'_m\rangle\}_{m=0}^{M_p-1}$. This means that at least some of the off-diagonal elements of $\mathcal{C}_D(|g_p(\delta^+, h^+)\rangle)$ must be nonzero in the incoherent basis, i.e., $\mathcal{C}_D(|g_p(\delta^+, h^+)\rangle) > 0$. There is therefore a discontinuous jump in the coherence measure $\mathcal{C}_D$ as we cross the point $r = 1$, so we are guaranteed that the coherence susceptibility $\mathcal{X}_D(|\psi_0(\delta, h)\rangle)$ diverges at the critical parameter for arbitrary N. This generalizes the observations that were already made for the case $N = 2$.

Coherence measures are also useful for identifying quantum phase transitions for models beyond the XY interaction. See Refs. [8,9,29] for other examples where geometric measures of coherence were also used to identify QPTs. A more in-depth discussion of quantum correlation measures in the XY model can also be found in Ref. [36].

VII. CONCLUSION

In this article, we considered the role that geometric measures of nonclassicality play in the identification of phase transitions. Theorems 1 and 2 show that geometry-based measures of nonclassicality are generic tools that can be used to probe phase transitions at arbitrary temperature. These results apply to any quantum resource theory, which include notions such as entanglement, quantum discord and quantum coherence. While we have only considered geometric measures of nonclassicality, one may also expect that many nongeometric measures will exhibit similar behavior during phase transitions, although this still needs to be verified on a case-by-case basis. This is because both geometric and nongeometric measures are ultimately trying to capture the same underlying notion of nonclassicality.

Stronger statements can be made for QPTs at zero temperature. In this regime, Theorem 3 shows that a discontinuity in the ground state at the point of criticality can always be picked up by a diverging GCS, measured with respect to some incoherent basis. In addition, Corollaries 3.1 and 3.2 show that large classes of QPTs that can be detected via Berry phases, or order parameters can also be detected by a diverging GCS.

We illustrate the case by considering a one-dimensional spin-$\frac{1}{2}$ chain with an XY interaction. For a simple two-site case, we demonstrate that the energy-level crossing in this model is not detected when using entanglement or quantum correlation measures, since the total quantum correlation remains unchanged across the critical parameter. Nonetheless, by appropriately defining the incoherent basis, one may demonstrate that a diverging GCS occurs at the point of phase transition. Such observations can also be extended for an arbitrary number N of particles. This shows how quantum coherence measures can be a useful alternative for probing certain types of QPTs where other quantum-correlation-based methods may fail. We can intuitively understand this to be because quantum correlations such as entanglement and discord may be viewed as special kinds of quantum coherence [37,38].

We hope that this work will spur continued research on the relationship between nonclassicality and quantum phase transitions.

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