Distribution of Quantum Coherence in Multipartite Systems

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The distribution of coherence in multipartite systems is examined. We use a new coherence measure with entropic nature and metric properties, based on the quantum Jensen-Shannon divergence. The metric property allows for the coherence to be decomposed into various contributions, which arise from local and intrinsic coherences. We find that there are trade-off relations between the various contributions of coherence, as a function of parameters of the quantum state. In bipartite systems the coherence resides on individual sites or is distributed among the sites, which contribute in a complementary way. In more complex systems, the characteristics of the coherence can display more subtle changes with respect to the parameters of the quantum state. In the case of the *XXZ* Heisenberg model, the coherence changes from a monogamous to a polygamous nature. This allows us to define the shareability of coherence, leading to monogamy relations for coherence.

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The concept of wave particle duality introduced the importance of quantum coherence in physical phenomena such as low temperature thermodynamics [1], quantum thermodynamics [2–4], nanoscale physics [5], and biological systems [6,7], and is one of the most basic aspects of quantum information science [8]. For this reason, understanding quantum coherence has a long history and is of fundamental importance to many fields. In quantum optics [9,10], the approach has been typically to examine quantities such as phase space distributions and higher order correlation functions [11]. While this method distinguishes between quantum and classical coherence, it does not quantify coherence in a rigorous sense. More recently, a procedure to quantify coherence using methods of quantum information science was developed [12–15]. In the seminal work of Ref. [12], basic quantities such as incoherent states, incoherent operations, and maximally coherent states were defined and the set of properties a functional should satisfy to be considered as a coherence measure were listed.

One fundamental task that is desirable is to pinpoint what part of a quantum system is responsible for any coherence that is present. To understand the possibilities, let us consider a two qubit system as an example. Coherence is a basis-dependent quantity [15,16], and the reference incoherent states are chosen as $|0\rangle, |1\rangle$. We can consider then two types of states that possess coherence, $(|0\rangle - |1\rangle)(|0\rangle - |1\rangle)$ and $|0\rangle|0\rangle - |1\rangle|1\rangle$. In the former, the coherence lies on each qubit, while the latter has a kind of collective coherence, i.e., entanglement. An interesting aspect of this is that the types of coherence are complementary to each other—an increase in one type leads to a corresponding decrease in the other. In order to have maximum coherence on a particular qubit, it is optimal to create a superposition on each one, which excludes entanglement. On the other hand, for the Bell state, tracing out one of the qubits leaves a completely mixed (incoherent) state on the other qubit.

This complementary behavior is reminiscent of another quantum feature, monogamy of entanglement, which has attracted a lot of attention recently [17–21]. Monogamy is a concept related to the shareability of entanglement between different constituents in a multipartite system. For example, in a tripartite system, if Alice and Bob have a maximally entangled state, then this rules out entanglement to Charlie. The monogamy relation for three qubits was introduced in Ref. [17], and has also been generalized to multipartite systems [19]. Both of these examples illustrate the trade-off nature of quantum mechanical features, where increasing one imposes restrictions on the other. Another fundamental question that this raises is the relationship between coherence and entanglement [15,16]. The framework outlined in Ref. [12] closely followed the format of entanglement quantification developed in Refs. [22–24]. While entanglement is clearly a form of coherence, the converse is not necessarily true. In this Letter we explore the question of how we can quantify various types of coherence and examine their trade-off relations within a multipartite system. By understanding the distribution of coherence in a multipartite system, this leads us to find the relation between concepts such as coherence, entanglement, and monogamy.

One of the tools that we will use in this study is a coherence measure which has both entropic and geometric properties. In Ref. [12], two different functionals, one based on the relative entropy and the other based on the ℓ_1 norm, were found to satisfy the necessary properties as a coherence measure. Of these, the former is an entropic measure while the other is a geometric measure that can be used as a formal distance measure. Any measure $\mathcal{D}$ is considered as a formal distance over the set X if $\forall\, \rho, \sigma \in X$ it satisfies the following properties: (i) $\mathcal{D}(\rho,\sigma) > 0$ for $\rho \neq \sigma$ and $\mathcal{D}(\rho,\rho) = 0$, and (ii) $\mathcal{D}(\rho,\sigma) = \mathcal{D}(\sigma,\rho)$ (symmetry). If $\mathcal{D}$ satisfies (iii) $\mathcal{D}(\rho,\sigma) + \mathcal{D}(\sigma,\tau) \geq \mathcal{D}(\rho,\tau)$ (the triangle inequality) in addition to the properties given above, then $\mathcal{D}$ is a metric for the space X. The relative entropy $S(\rho\|\sigma) \equiv \mathrm{Tr}\rho\log(\rho/\sigma)$ is not a distance since it is asymmetric and further it is well defined only when the support of σ is equal to or larger than that of ρ. Towards this end, we introduce here an alternative, the quantum version of the Jensen-Shannon divergence (QJSD):

$$\mathcal{J}(\rho,\sigma) = \frac{1}{2}[S(\rho\|(\rho+\sigma)/2) + S(\sigma\|(\rho+\sigma)/2)]. \quad (1)$$

The QJSD is known to be a distance measure, to be bounded $0 \leq \mathcal{J} \leq 1$, and is well defined irrespective of the nature of the support of ρ and σ [25–27]. The QJSD does not obey the triangle inequality, but its square root obeys it for all pure states. In the case of mixed states there is no general proof of the triangle inequality, but numerical studies up to five qubits [27] strongly indicate its validity.

Quantum coherence trade-offs.—The quantum coherence is defined as [12]

$$\mathcal{C}(\rho) \equiv \min_{\sigma\in\mathcal{I}^{(b)}} \mathcal{D}(\rho,\sigma), \quad (2)$$

where $\mathcal{D}$ is a distance measure and $\mathcal{I}^{(b)}$ are the set of incoherent states in a particular basis b. The functional $\mathcal{C}$ is a quantum coherence measure if it obeys the properties [12] (i) $\mathcal{C}(\rho) \geq 0$ and $\mathcal{C}(\rho) = 0$ iff $\rho \in \mathcal{I}^{(b)}$, (ii) $\mathcal{C}(\rho)$ is invariant under unitary transformations, (iii) $\mathcal{C}(\rho)$ is monotonic under an incoherent completely positive and trace preserving map, (iv) $\mathcal{C}(\rho)$ is monotonic under selective incoherent measurements on average, and (v) $\mathcal{C}(\rho)$ is nonincreasing under mixing of quantum states (convexity).

Equation (2) states that the amount of coherence in a given state is the distance to the closest incoherent state. This definition clearly depends on what we deem to be an incoherent state, and is responsible for the basis-dependent nature of $\mathcal{C}$. Most generally, one may assume a form for an incoherent state $\sigma = \sum_k p_k |b_k\rangle\langle b_k|$, where the $\{|b_k\rangle\}$ are a fixed particular basis choice b and p_k are probabilities. Without the constraint of the fixed basis, it is always possible to write $\sigma = \rho$ by taking $|b_k\rangle$ to be eigenvectors of ρ, which immediately gives $\mathcal{C} = 0$. In this Letter we are interested in how the overall coherence is distributed in a multipartite system. For this reason it will be most interesting to choose a local basis choice,

$$\sigma = \sum_k p_k \tau_{k,1}^{(b)} \otimes \cdots \otimes \tau_{k,N}^{(b)}, \quad (3)$$

where $\tau_{k,n}^{(b)}$ is the incoherent state on the subsystem n; i.e., $\tau_{k,n}^{(b)} = \sum_k p_{k,n} |b_{k,n}\rangle\langle b_{k,n}|$. The set of states that are separable and in a basis b are called $\mathcal{I}_S^{(b)}$.

This gives a natural way to study various coherence contributions within a multipartite system. As discussed above, we can distinguish between coherence that is localized on the subsystems n and collective coherence, which cannot be attributed to particular subsystems [see Fig. 1(a)]. To remove the contribution from the subsystems, we may relax the basis constraint b and minimize over the set of states Eq. (3). This contribution is independent of the basis choice, and is the coherence that is intrinsic within the system. We thus define the intrinsic coherence,

$$\mathcal{C}_I(\rho) \equiv \min_{\sigma_S\in\mathcal{I}_S} \mathcal{D}(\rho,\sigma_S), \quad (4)$$

where $\mathcal{I}_S$ is the set of states of the form as given in Eq. (3), but is not necessarily in the basis b. Thus the only constraint here is the general form of the basis, that it is separable, but the particular basis is not specified. Equation (4) is in fact equal to the entanglement, which is reasonable from the point of view that entanglement must contribute to coherence [15]. The remaining contribution then originates from coherence that exists on the subsystems, and we can write the local coherence as

$$\mathcal{C}_L(\rho) \equiv \mathcal{D}(\sigma_S^{\min}, \rho^d), \quad (5)$$

where $\sigma_S^{\min}$ and ρ^d are the minimum solutions of Eqs. (4) and (2), respectively, and are implicit functions of ρ.

We may visualize the two different contributions according to Fig. 1(b). According to the metric properties of $\mathcal{D}$, and the triangle inequality, we immediately see that

$$\mathcal{C} \leq \mathcal{C}_L + \mathcal{C}_I. \quad (6)$$

For a product state $\sigma_S^{\min}$, the coherence measure is subadditive, which leads to $\mathcal{C}_L \leq \sum_n \mathcal{C}_{L,n}$. We thus have

$$\mathcal{C} \leq \sum_{n=1}^{N} \mathcal{C}_{L,n} + \mathcal{C}_I, \quad (7)$$

where $\mathcal{C}_{L,n}$ is the coherence on each subsystem n separately.

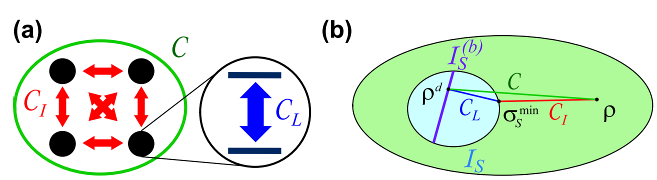

FIG. 1. Quantum coherence in multipartite systems. (a) The total coherence $\mathcal{C}$ has contributions from local coherence $\mathcal{C}_L$ on subsystems and collective coherence $\mathcal{C}_I$. (b) Definitions of various coherences according to the distance between states. $\mathcal{I}_S$ is the set of separable states, while $\mathcal{I}_S^{(b)}$ is the set of separable states in a fixed basis b. ρ_d is the solution of Eq. (2) and $\sigma_S^{\min}$ is the solution of Eq. (4).

An illustrative example of the coherence decomposition is given by the ground state of the $N = 2$ Ising model described by the Hamiltonian

$$H = \lambda\sigma_1^x\sigma_2^x + J(\sigma_1^x + \sigma_2^x) + \epsilon\lambda(\sigma_1^z + \sigma_2^z), \tag{8}$$

where J, λ are coupling parameters and ϵ is a small symmetry-breaking term. The numerically estimated values of $\mathcal{C}_L$, $\mathcal{C}_I$, and $\mathcal{C}$ are given in Fig. 2(a), where we use the square root of the Jensen-Shannon divergence as our distance measure,

$$\mathcal{D}(\rho,\sigma) = \sqrt{\mathcal{J}(\rho,\sigma)} = \sqrt{S\left(\frac{\rho+\sigma}{2}\right) - \frac{S(\rho)}{2} - \frac{S(\sigma)}{2}},$$

where $S(\rho) = -\mathrm{Tr}\rho\log\rho$ is the von Neumann entropy. Taking the $\{|0\rangle_n, |1\rangle_n\}$ basis as the reference state (this will be the case throughout this Letter), we see that there is a crossover between coherence contributions from intrinsic when $J \ll \lambda$ to local as $J \gg \lambda$. This is due to the fact that for $J = 0, \epsilon \to 0$ the ground state approaches a Bell state $|00\rangle - |11\rangle$, and for $\lambda = 0$ the ground state is $(|0\rangle - |1\rangle)(|0\rangle - |1\rangle)$, with intermediate J/λ giving an interpolation to these limits. The total coherence is less than the sum of the local and intrinsic contributions, following Eq. (6).

Multipartite coherence.—The bipartite case studied above is the simplest case of more general trade-off relations in multipartite systems. One of the fundamental properties we investigate is the shareability of coherence between subsystems. For example, in a tripartite system ρ_{123} we may decompose the coherence using Eq. (6) according to

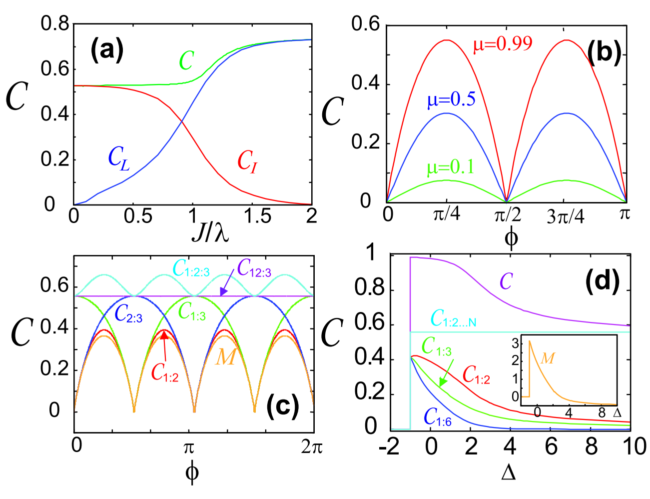

FIG. 2. Coherence as measured by the quantum Jensen-Shannon divergence for various states. Coherence of (a) the $N = 2$ site Ising model with $\epsilon = 0.2$, (b) the Werner GHZ state, (c) the W state with $\theta = \pi/4$, and (d) the $N = 10$ site XXZ Heisenberg model ground state with $J = 1$. Inset: Monogamy for the XXZ Heisenberg model as defined in Eq. (14).

$$\mathcal{C}_{123} \le \mathcal{C}_1 + \mathcal{C}_2 + \mathcal{C}_3 + \mathcal{C}_{1:2:3}, \tag{9}$$

where we have introduced a shorthand for the local coherence on subsystem n as $\mathcal{C}_n = \mathcal{C}_{L,n}(\rho_n)$, and ρ_n is the reduced density matrix. For the product states $\sigma_S^{\min}$ Eq. (9) holds exactly. The intrinsic coherence $\mathcal{C}_{1:2:3} = \mathcal{C}_I(\rho_{123})$ is minimized over the set of separable states on the tripartite system. We note that as $\mathcal{C}_{1:2:3}$ is an intrinsic coherence, it does not contain any coherence located *on* the sites, but contains all coherences *between* the sites.

We can decompose a tripartite system in a bipartite fashion, leading to the relation

$$\mathcal{C}_{123} \le \mathcal{C}_1 + \mathcal{C}_2 + \mathcal{C}_3 + \mathcal{C}_{2:3} + \mathcal{C}_{1:23}, \tag{10}$$

where we first find the intrinsic coherence between 2 and 3, then we estimate the intrinsic coherence between 1 and the bipartite subsystem 23. Similar decompositions can be carried out with respect to the bipartitions 2 : 13 and 3 : 12 as well. From Eqs. (9) and (10) and the other possible bipartitions suggested above, we may deduce that

$$\mathcal{C}_{1:2:3} \simeq \mathcal{C}_{2:3} + \mathcal{C}_{1:23} \simeq \mathcal{C}_{1:2} + \mathcal{C}_{12:3} \simeq \mathcal{C}_{1:3} + \mathcal{C}_{13:2}. \tag{11}$$

To illustrate the various contributions, first let us consider the mixed Greenberger-Horne-Zeilinger (GHZ) states defined as $\rho_{\mathrm{GHZ}} = (1-\mu/8)\hat{\mathbb{1}} + \mu|\mathrm{GHZ}\rangle\langle\mathrm{GHZ}|$, with $|\mathrm{GHZ}\rangle = \cos\phi|000\rangle + \sin\phi|111\rangle$, $\phi \in [0, 2\pi)$, and $0 \le \mu \le 1$. The coherence is plotted in Fig. 2(b). For this class of states we find that the various contributions due to one and two sites are always zero: $\mathcal{C}_n = \mathcal{C}_{m:n} = 0$. This means that the only coherence contributions originate from the intrinsic coherence where all three sites are involved. The total coherence is thus identical to the tripartite coherence $\mathcal{C} = \mathcal{C}_{1:2:3}$, which is verified numerically. It is also equal to the bipartitioned intrinsic coherence $\mathcal{C} = \mathcal{C}_{l:mn}$, where l, m, n are all permutations of the sites. This verifies the relation Eq. (11) for this class of states.

In contrast to the GHZ state where there is only one coherence contribution, the W states have a trade-off relation similar to that seen in the transverse Ising model. These are defined as $|W\rangle = \sin\theta\cos\phi|100\rangle + \sin\theta\sin\phi|010\rangle + \cos\theta|001\rangle$, with $0 \le \phi < 2\pi$ and $0 \le \theta \le \pi$. The GHZ and W states are two classes of states that are unrelated under local operations and classical communications. From Fig. 2(c) we see that the calculated coherence can be attributed to several contributions. First, the coherence $\mathcal{C}_{12:3}$ is always constant as the state for the choice $\theta = \pi/4$ can be written as $|W\rangle = [(\cos\phi|10\rangle + \sin\phi|01\rangle)|0\rangle + |00\rangle|1\rangle]/\sqrt{2}$; thus, there is always intrinsic coherence between the bipartition of sites 12 and 3. The coherences $\mathcal{C}_{1:3}$ and $\mathcal{C}_{2:3}$ show complementary behavior as the system oscillates between a Bell state between sites 13 ($\phi = n\pi$) and 23 [$\phi = (n + 1/2)\pi$], with the remaining site being decoupled. The coherence between the sites 12 ($\mathcal{C}_{1:2}$) has twice the oscillatory frequency of $\mathcal{C}_{1:3}$ and $\mathcal{C}_{2:3}$.

The same ideas can be equally applied to more complex multipartite systems. The various coherence contributions can be used to understand the nature of the quantum states in quantum many-body systems. We illustrate this by analyzing the one-dimensional Heisenberg XXZ model, one of the fundamental models in magnetism. The Hamiltonian of this model is

$$H = J\sum_n (\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y + \Delta\sigma_n^z\sigma_{n+1}^z), \qquad (12)$$

where J is the nearest neighbor spin coupling and Δ is the anisotropy parameter. For an antiferromagnetic coupling $J > 0$, the system has a phase transition from the ferromagnetic axial regime to the antiferromagnetic planar regime at $\Delta = -1$. Using exact diagonalization techniques we estimate various types of coherence as shown in Fig. 2(d). In the ferromagnetic phase with $\Delta < -1$, all coherences vanish due to spontaneous symmetry breaking selecting a unique ferromagnetic ground state with all spins aligned in the σ^z basis. In the opposite limit $\Delta \gg 1$, the state is a superposition of Néel states, due to the twofold degeneracy of these states: $(|0101\ldots01\rangle + |1010\ldots10\rangle)/\sqrt{2}$. The coherence thus approaches the Bell state value $\mathcal{C} = \mathcal{C}_{1:2,\ldots,N} \approx 0.56$, with all other coherence contributions vanishing. Because of the spin-flip symmetry, coherence on each site is always zero, $\mathcal{C}_n = 0$, and $\mathcal{C}_{1:2,\ldots,N}$ can always be written in a Bell state form, resulting in a constant value. The coherence contributions between two sites decrease with distance as expected $\mathcal{C}_{1:n}$, due to the reduced correlations between these sites. Interestingly, at $\Delta = -1$ the two-site correlations all converge to the same value, which we attribute to the fact that this is close to the antiferromagnetic-ferromagnetic phase transition, which has the effect of increasing the overall coherence in the system.

Monogamy of coherence.—From our coherence decompositions, we arrive naturally at the notion of monogamy of coherence. In a tripartite system, if subsystems 2 and 3 are maximally coherent with respect each other, this limits the amount of coherence that subsystem 1 has with 2 and 3. This is immediately evident from Eq. (10), where the coherence is decomposed into these two contributions. If subsystem 3 is coherently connected to 1 and 2, then the tripartite system is described to be polygamous, and otherwise is monogamous. The coherence monogamy relations may be identified from Eq. (11), where we observe that the tripartite coherence $\mathcal{C}_{1:2:3}$ can be decomposed into several bipartite coherences. The genuine tripartite coherence can be estimated by subtracting pairwise bipartite terms, giving

$$\mathcal{C}_{1:2:3} - \mathcal{C}_{1:2} - \mathcal{C}_{2:3} - \mathcal{C}_{1:3} \simeq \mathcal{C}_{1:23} - \mathcal{C}_{1:2} - \mathcal{C}_{1:3}. \qquad (13)$$

For a multipartite system the monogamy inequality reads $\mathcal{C}_{1:2,\ldots,N} \geq \sum_{n=2}^{N} \mathcal{C}_{1:n}$. Thus, we define the multipartite monogamy of coherence with respect to a measure as

$$M = \sum_{n=2}^{N} \mathcal{C}_{1:n} - \mathcal{C}_{1:2,\ldots,N}, \qquad (14)$$

which is monogamous for $M \leq 0$ due to the multipartite coherence that is present. For $M > 0$, it is polygamous since the dominant coherence is distributed in a pairwise fashion.

In Fig. 2(c) we calculate Eq. (14) for the W states. We find that $M \geq 0$ for all θ, ϕ; hence, the state is strictly polygamous. For the GHZ states as shown in Fig. 2(b) there is only one coherence contribution with $\mathcal{C}_{1:n} = 0$, which results in $M = -\mathcal{C}$, meaning that it is strictly monogamous. This is as expected since the GHZ states are tripartite entangled, whereas the W state has a bipartite nature [28]. For the Heisenberg spin chain we find both monogamous ($\Delta > 2.9$) and polygamous behavior ($-1 < \Delta < 2.9$) [see Fig. 2(d) inset]. For $\Delta \gg 1$ region when the ground state is a Néel state, the two-site coherences vanish $\mathcal{C}_{1:n} \to 0$. Then the coherence is entirely due to the $1:2,\ldots,N$ bipartition, resulting in a monogamous state. This can be understood to be due to the fact that the Néel state superposition is essentially the same as a GHZ state up to a redefinition of state labels. For small Δ, there is a larger effect from the off-diagonal terms, $\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y = 2(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+)$. This term tends to create coherence on nearby sites, which is more characteristic of a polygamous behavior. In this way the parameter Δ switches the nature of the coherence between monogamy and polygamy by redistributing it between relatively local sites to a genuinely multipartite form.

Conclusions.—Multipartite coherence is decomposed into local and intrinsic parts and quantified using an entropic measure with metric nature. This decomposition into various contributions can be used not only to characterize a given state but also to locate the origin of the coherence. In many cases there is a crossover behavior between the coherences of different origins, which depends upon the type of the state examined. In the transverse Ising model, the coherence transitions between local coherence on the sites to a GHZ-type multipartite nature. The coherence decompositions lead to a multipartite monogamy inequality for coherence measures, giving another way of characterizing the nature of coherence in these systems. In the Heisenberg XXZ model the coherence displays a crossover between monogamous and polygamous behavior when the anisotropy parameter is varied. The framework provided in this Letter allows for a simple way to understand the nature of an arbitrary quantum state, by characterizing the various coherence contributions, even for relatively complicated states in quantum many-body problems.

In addition to providing a framework for decomposing coherence, we believe that the general method is potentially applicable in several contexts. In the field of quantum simulation and quantum computing, it is often of interest to understand what kind of quantum state is generated, either to understand the nature of a many-body system [29] or for the purposes of benchmarking [30,31]. Finding the distribution of coherence provides a more illuminating way of understanding the nature of a quantum state. One of the contributions that quantum information made to condensed matter physics is the introduction of entanglement as a quantity that can be used to characterize the state of a system [32]. It is an interesting question of whether particular types of coherence could be used to analyze similarly quantum phase transitions. Furthermore, quantum limits to shareability (i.e., monogamy) of entanglement is known to be related to frustration in many-body systems [33–37], and affects the coherence and entanglement structure in the system. This has a direct effect on approaches to efficiently capture the wave function of interacting quantum many-body systems, such as matrix product states and their variants [38,39]. In quantum metrology, a recent development has been the use of local rather than global strategies to gain interferometric advantages [40–42], which highlights the resource nature of coherence. An interesting future possibility for the QJSD is that, due to its distance and metric properties and entropic nature, it could contribute to differential-geometry-based approaches to quantum information theory and to the understanding of geometry of quantum states [43].

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