A Subsystem-Independent Generalization of Entanglement

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We present a generalization of entanglement based on the idea that entanglement is relative to a distinguished subspace of observables rather than a distinguished subsystem decomposition. A pure quantum state is entangled relative to such a subspace if its expectations are a proper mixture of those of other states. Many information-theoretic aspects of entanglement can be extended to this observable-based setting, suggesting new ways of measuring and classifying multipartite entanglement. By going beyond the distinguishable-subsystem framework, generalized entanglement also provides novel tools for probing quantum correlations in interacting many-body systems.

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Entanglement is a uniquely quantum phenomenon whereby a pure state of a composite quantum system may cease to be determined by the states of its constituent subsystems [1]. Entangled pure states are those that have *mixed* subsystem states. To determine an entangled state requires knowledge of the correlations between the subsystems. As no pure state of a classical system can be correlated, such correlations are intrinsically nonclassical, as strikingly manifested by the violation of local realism and Bell's inequalities [2]. In the science of quantum information processing (QIP), entanglement is regarded as the defining resource for quantum communication and an essential feature needed for unlocking the power of quantum computation. However, in spite of intensive investigation, a complete understanding of entanglement is far from being reached.

To unambiguously define entanglement requires a preferred partition of the overall system into subsystems. In conventional QIP scenarios, subsystems are associated with spatially separated "local" parties, which legitimates the *distinguishability* assumption implicit in standard entanglement theory. However, because quantum correlations are at the heart of many physical phenomena, it would be desirable for a notion of entanglement to be useful in contexts other than QIP. Strongly interacting quantum systems offer compelling examples of situations where the usual subsystem-based view is inadequate. Whenever indistinguishable particles are sufficiently close to each other, quantum statistics forces the accessible state space to be a proper subspace of the full tensor product space, and exchange correlations arise that are not a usable resource in the usual QIP sense. Thus, the natural identification of particles with preferred subsystems becomes problematic. Even if a distinguishable-subsystem structure may be associated with degrees of freedom different from the original particles (such as a set of modes [3]), inequivalent factorizations may occur on the same footing. Finally, the introduction of quasi-particles, or the purposeful transformation of the algebraic language used to analyze the system [4], may further complicate the choice of preferred subsystems. While efforts are under way to obtain entanglement-like notions for bosons and fermions [3,5] and to study entanglement in quantum critical phenomena [6–8], formulating a theory of entanglement applicable to the full variety of physical settings remains an important challenge.

In this Letter, we present a notion of *generalized entanglement* (GE), which incorporates the entanglement settings introduced to date in a unifying framework. This is achieved by realizing that entanglement is an *observer-dependent concept*, whose properties are determined by the expectations of a *distinguished subspace of observables* of the system of interest, without reference to a preferred subsystem decomposition. Distinguished observables may represent a limited means of manipulating and measuring the system. Standard entanglement is recovered when these means are limited to local observables acting on subsystems. The central idea is to generalize the observation that standard entangled pure states are those that look mixed to local observers. Each pure quantum state gives rise to a *reduced* state that provides only the expectations of the distinguished observables. The set of reduced states is convex and, similar to an ordinary quantum state space, it includes pure states (the extremal ones). We say that a pure state is *generalized unentangled* relative to the distinguished observables, if its reduced state is pure, and generalized entangled otherwise. The definition extends to mixed states in a standard way: A mixed state is unentangled if it can be written as a mixture (or convex combination) of unentangled pure states. Because our definition depends only on convex properties of the distinguished spaces of observables and states we consider, it provides a notion of entanglement within a general convex framework suitable for investigating the foundations of quantum mechanics and related physical theories (cf. [9] and references therein).

The mathematical foundation of GE is established in [10]. Here we highlight the significance of GE from a physics and information-physics perspective, by focusing on the case where the observable subspace is a Lie algebra.

A key result identifies pure generalized unentangled states with *generalized coherent states* (GCSs, a connection independently noted by Klyachko [11]), which are well known for their applications in physics [12]. We show how many information-theoretic notions previously thought to be specific to partitioning into subsystems extend to coherent state theory and beyond, define new measures of entanglement based on the general theory, and apply quantum information to condensed-matter problems. In particular, we discuss notions of *generalized local operations assisted by classical communication* (GLOCC) under which the ordinary measures of standard entanglement do not increase, as well as GE measures with the desired behavior under classes of GLOCC maps. New measures of standard entanglement can be constructed for the multipartite case. A simple GE measure obtained from the *purity relative to a Lie algebra* is a useful diagnostic tool for quantum many-body systems, playing the role of an *order* or *disorder parameter* for broken-symmetry quantum phase transitions.

Generalized entanglement.—We first revisit the standard setting for entanglement where we have two distinguishable subsystems forming a bipartite system. Let the mn-dimensional joint state space $\mathcal{H}$ factorize as $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$, with $\mathcal{H}_a$, $\mathcal{H}_b$ m-, n-dimensional, respectively. In this setting, physical considerations distinguish a preferred set of observables, spanned by traceless Hermitian operators of the form $A \otimes \mathbb{1}$ and $\mathbb{1} \otimes B$, which are the local observables acting on system a or b alone. For each pure state $|\psi\rangle \in \mathcal{H}_a \otimes \mathcal{H}_b$, one may consider the reduced state describing the expectations of measurements of local observables. The reduced state is determined by the pair of reduced density operators, $\rho_a := \mathrm{tr}_b|\psi\rangle\langle\psi|$ and $\rho_b := \mathrm{tr}_a|\psi\rangle\langle\psi|$. Because pure product states are exactly those for which subsystem states are pure, our definition of GE relative to the local observable subspace coincides with the standard definition of entanglement.

The extent to which our viewpoint extends the subsystem-based definition may be appreciated in situations where no physically natural subsystem partition exists and conventional entanglement is not directly applicable. Consider a single spin-1 system, whose three-dimensional state space $\mathcal{H}$ carries an irreducible representation of $\mathfrak{su}(2)$, with generators J_x, J_y, J_z satisfying $[J_\alpha, J_\beta] = i\varepsilon_{\alpha\beta\gamma}J_\gamma$ ($\varepsilon_{\alpha\beta\gamma}$ being the totally antisymmetric tensor). Suppose that operational access to the system is restricted to observables in the given representation of $\mathfrak{su}(2)$. The reduced states can be identified with vectors of expectation values of these three observables: They form a unit ball in $\mathbb{R}^3$, and the extremal points are those on the surface, having maximal spin component 1 for some linear combination of J_x, J_y, J_z. These are the "spin coherent states," or GCSs for SU(2) [12]. For any choice of spin direction, $\mathcal{H}$ is spanned by the $|1\rangle$, $|0\rangle$, $|-1\rangle$ eigenstates of that spin component; the first and last are GCSs, but $|0\rangle$ is *not*, characterizing $|0\rangle$ as a generalized entangled state relative to $\mathfrak{su}(2)$. All pure states appear unentangled if access to the full algebra $\mathfrak{g} = \mathfrak{su}(3)$ is available [that is, $\mathfrak{su}(3)$ is distinguished].

This example illustrates that, when the distinguished subspace forms an irreducibly represented Lie algebra, the set of unentangled states is the set of GCSs. Another, more physically motivated characterization is as the set of states that are unique ground states of a distinguished observable. To formally relate these characterizations of unentangled states, we review the needed Lie representation theory [13]. A *Cartan subalgebra* (CSA) $\mathfrak{c}$ of a semisimple Lie algebra $\mathfrak{h}$ is a maximal commutative subalgebra. A vector space carrying a representation of $\mathfrak{h}$ decomposes into orthogonal joint eigenspaces V_λ of the operators in $\mathfrak{c}$. That is, each V_λ consists of the set of states $|\psi\rangle$ such that for $x \in \mathfrak{c}$, $x|\psi\rangle = \lambda(x)|\psi\rangle$. The label λ is therefore a linear functional on $\mathfrak{c}$, called the *weight* of V_λ. In the above example, any spin component J_α spans a (one-dimensional) CSA $\mathfrak{c}_\alpha$. There are three weight spaces labeled by the angular momentum along α, and spanned by the states $|1\rangle$, $|0\rangle$, $|-1\rangle$ of the previous paragraph. The subspace of operators in $\mathfrak{h}$ orthogonal in the trace inner product to $\mathfrak{c}$ can be organized into orthogonal "raising and lowering" operators, which connect different weight spaces. In the example, choosing J_z as the basis of our CSA, these are $J_\pm := (J_x \pm iJ_y)/\sqrt{2}$. For a fixed CSA and irreducible representation, the weights generate a convex polytope; a lowest (or highest) weight is an extremal point of such a polytope, and the one-dimensional weight spaces having those weights are known as *lowest-weight states*. The set of lowest-weight states for all CSAs is the orbit of any one such state under the Lie group generated by $\mathfrak{h}$. These are the group-theoretic GCSs [12]. Notably, the GCSs attain minimum invariant uncertainty [14].

A natural way to relate a state $|\psi\rangle \in \mathcal{H}$ to a Lie algebra $\mathfrak{h}$ (or, more generally, any set) of operators acting on $\mathcal{H}$ is to project $|\psi\rangle\langle\psi|$ onto $\mathfrak{h}$. This projection determines the expectations of operators in $\mathfrak{h}$ for $|\psi\rangle$. The generalized unentangled states are the ones for which such a projection is extremal. This motivates the following definition. Let $\{x_i\}$ be a Hermitian ($x_i = x_i^\dagger$) orthogonal ($\mathrm{tr}\, x_i x_j \propto \delta_{ij}$) basis for $\mathfrak{h}$ [15]. The purity of $|\psi\rangle$ relative to $\mathfrak{h}$ (or $\mathfrak{h}$ purity) is $P_\mathfrak{h}(|\psi\rangle) := \sum_i |\langle\psi|x_i|\psi\rangle|^2$, where the x_i have a common, rescaled norm chosen to ensure that the maximal value is 1. $P_\mathfrak{h}(|\psi\rangle)$ is the square distance from 0 of the projection of $|\psi\rangle\langle\psi|$. For pure bipartite states, the $\mathfrak{su}(m) \oplus \mathfrak{su}(n)$ purity is (up to a constant) the conventional purity given by the trace of the square of either subsystem's reduced density operator.

Thus far, $\mathfrak{h}$ has been assumed to be a *real* Lie algebra of Hermitian operators. These may be thought of as a preferred family of Hamiltonians, which generate (via $h \mapsto e^{ih}$) a Lie group of unitary operators. More generally, we want Lie algebraically distinguished completely positive (CP) maps, $\rho \mapsto \sum_i A_i \rho A_i^\dagger$. A natural class is obtained by restricting the "Hellwig-Kraus" (HK) operators A_i to lie in the topological closure $\overline{e^{\mathfrak{h}_c \oplus \mathbb{1}}}$ of the Lie group generated by the *complex* Lie algebra $\mathfrak{h}_c \oplus \mathbb{1}$ [16]. Having HK operators in a group ensures closure under composition. Using $\mathfrak{h}_c \oplus \mathbb{1}$ allows nonunitary HK operators. Topological closure introduces singular operators such as projectors. The following characterizations of unentangled states (proven in [10]) demonstrate the power of the Lie algebraic setting.

Theorem.—The following are equivalent for an irreducible representation of $\mathfrak{h}$ on $\mathcal{H}$: (i) ρ is generalized unentangled relative to $\mathfrak{h}$. (ii) $\rho = |\psi\rangle\langle\psi|$ with $|\psi\rangle$ the unique ground state of some H in $\mathfrak{h}$. (iii) $\rho = |\psi\rangle\langle\psi|$ with $|\psi\rangle$ a lowest-weight vector of $\mathfrak{h}$. (iv) ρ has maximum $\mathfrak{h}$ purity. (v) ρ is a one-dimensional projector in $\overline{e^{\mathfrak{h}_c \oplus \mathbb{1}}}$.

Generalized LOCC.—The semigroup of LOCC maps [17] and the preordering it induces on states are at the core of entanglement theory. Given an HK representation $\{A_i\}$ of a CP map M, we can view each A_i as being associated with measurement outcome i, obtained with probability $\mathrm{tr}\, A_i^\dagger A_i \rho$, and leading to the state $A_i \rho A_i^\dagger$. The set $\{A_i\}$ and a list of maps M_i, with HK operators $\{B_{ij}\}$, specify a new map with representation $\{B_{ij} A_i\}$. This map can be implemented by first applying M and then, given measurement outcome i, applying M_i. We call this *conditional composition* of maps. Closing the set of one-party maps (for all parties) under conditional composition gives the LOCC maps. When the distinguished observables form a semisimple Lie algebra $\mathfrak{h}$, a natural multipartite structure can be exploited to generalize LOCC. $\mathfrak{h}$ can be uniquely expressed as a direct sum of simple Lie algebras, $\mathfrak{h} = \oplus_i \mathfrak{h}_i$. A Hilbert space irreducibly representing $\mathfrak{h}$ factorizes as $\mathcal{H} = \otimes_i \mathcal{H}_i$, with $\mathfrak{h}_i$ acting nontrivially on $\mathcal{H}_i$ only. This resembles ordinary entanglement, except that the local systems $\mathcal{H}_i$ may not be *physically* local, and actions on them are restricted to involve operators in the topological closure of a local Lie group representation which need not be $\mathrm{GL}(\dim(\mathcal{H}_i))$ as in standard entanglement. For each simple algebra $\mathfrak{h}_i$, a natural restriction is to CP maps with HK operators in $\overline{e^{(\mathfrak{h}_i)_c \oplus \mathbb{1}}}$. GLOCC, generalized LOCC, is the closure under conditional composition of the set of operations each of which is representable with HK operators in the topological closure of $e^{(\mathfrak{h}_i)_c \oplus \mathbb{1}}$ for some i.

Measures of generalized entanglement.—Because GE relative to $\mathfrak{h}$ reflects incoherence relative to $\mathfrak{h}$, which amounts to mixing from the point of view of $\mathfrak{h}$, a natural Lie algebraic GE measure is the *convex roof extension* of the pure-state measure $1 - P_{\mathfrak{h}}(\rho)$. This extension is defined as in standard entanglement theory: Given a pure-state measure σ, $\sigma(\rho)$ is the minimum, over pure-state ensembles for ρ, of the ensemble average of $\sigma(\rho)$; explicitly, $\sigma(\rho) = \min_{\pi_i, p_i \geq 0, \sum_i p_i = 1, \sum_i p_i \pi_i = \rho} \sum_i p_i \sigma(\pi_i)$. (This enforces the natural requirement of convexity.)

Another approach to pure-state GE measures is suggested by the convex structure of reduced states and uses natural *mixedness measures* σ on finite probability distributions $\mathbf{p} = (p_1, \ldots, p_k)$. Such measures are concave and permutation invariant. Examples are entropy, $\sigma_{\ln}(\mathbf{p}) := -\sum_i p_i \ln p_i$, and Renyi entropy, $\sigma_1(\mathbf{p}) := 1 - \sum_i p_i^2$. For a reduced state μ, define $\sigma(\mu)$ by minimizing $\sigma(\mathbf{p})$ over ways of writing $\mu = \sum_i p_i \mu_i$ with p_i probabilities and μ_i pure reduced states. For an (unreduced) pure state ρ with reduction ν, define $\sigma(\rho) := \sigma(\nu)$. Besides being convex, it is also desirable that measures be nonincreasing under GLOCC. We established in [10] that the convex roof extensions of these measures are nonincreasing under those GLOCC operations implementable via conditional composition of operations with *unitary* HK operators in the Lie group. As with standard entanglement, no single measure can capture the complexity of GE.

Generalized multipartite entanglement.—GE contributes to the study of conventional entanglement in multipartite systems. For N qubits, the relevant algebra for conventional entanglement is $\mathfrak{h} = \oplus_{i=1}^N \mathfrak{su}(2)_i$, generated by the Pauli matrices for each qubit; then $P_{\mathfrak{h}}(|\psi\rangle) = (2/N)\sum_i \mathrm{tr}\, \rho_i^2 - 1$, where ρ_i is qubit i's reduced density matrix. The pure product states have maximal purity $P_{\mathfrak{h}} = 1$ (unentangled), whereas the Greenberger-Horne-Zeilinger states $|\mathrm{GHZ}_N\rangle := 2^{-1/2}[|\uparrow\uparrow\cdots\uparrow\rangle + |\downarrow\downarrow\cdots\downarrow\rangle]$ (as well as products of $N/2$ Einstein-Podolsky-Rosen states $|\mathrm{EPR}\rangle^{\otimes N/2}$, for even N) have minimal purity 0 (are maximally entangled by this measure). States of the form $|\mathrm{W}_N\rangle := N^{-1/2} \sum_{i=1}^N |\uparrow\uparrow\cdots\uparrow\downarrow_i\uparrow\cdots\uparrow\rangle$ have an intermediate purity $(\frac{N-2}{N})^2$. In the $N \to \infty$ limit, $P_{\mathfrak{h}}(|\mathrm{W}_N\rangle) \to 1$, whereas $|\mathrm{GHZ}_N\rangle$ remains maximally entangled. Interestingly, for this special choice of $\mathfrak{h}$, we have proved that $1 - P_{\mathfrak{h}}$ coincides with the global entanglement measure introduced in [18]. Different observable algebras, or hierarchies of subalgebras, further characterize multipartite quantum correlations. Other measures such as $\sigma(\rho)$ give additional insight. Either approach can distinguish $|\mathrm{GHZ}_N\rangle$ from $|\mathrm{EPR}\rangle^{\otimes N/2}$.

Another example consists of two spin-1 particles in the *total spin* representation of $\mathfrak{su}(2)$. Suppose that the two spins can be accessed only collectively, e.g., using a global external field. Then the distinguished observable subspace is spanned by operators $J_\alpha := J_\alpha^{(1)} \otimes \mathbb{1} + \mathbb{1} \otimes J_\alpha^{(2)}$, $J_\alpha^{(1)}, J_\alpha^{(2)}$ being spin-1 generators for each $\mathfrak{su}(2)$. The (unentangled) GCSs here are states of maximal total spin projection in some direction α (states of the form $|1_\alpha\rangle|1_\alpha\rangle$), whereas product states, such as $|0_\alpha\rangle|0_\alpha\rangle$ with zero spin projection, are generalized entangled, with minimal purity relative to this algebra. This reflects the fact that no SU(2) spin rotation can connect $|0_\alpha\rangle|0_\alpha\rangle$ to the unentangled state $|1_\alpha\rangle|1_\alpha\rangle$.

Entanglement in condensed matter.—GE can be applied to the study of interacting quantum systems, where the characterization of quantum correlations is essential to a complete understanding of quantum phase transitions (QPTs). Consider the case of an anisotropic one-dimensional spin-1/2 XY model in a transverse

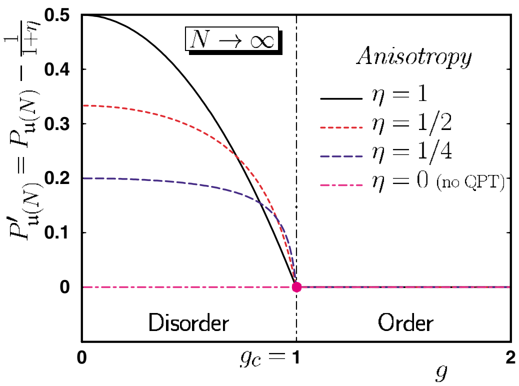

FIG. 1 (color online). Analytic behavior of the (shifted) purity, $\lim_{N\to\infty} P'_{\mathfrak{u}(N)}$, for the BCS state as a function of g. It scales with an exponent $\nu = 1$ near g_c [20]. Thus, the correlation length diverges as $(g_c - g)^{-\nu}$ (Ising universality class).

field, described by the Hamiltonian acting on the N-spin space:

$$H = -g \sum_{i=1}^{N} [(1+\eta) J_x^i J_x^{i+1} + (1-\eta) J_y^i J_y^{i+1}] + \sum_{i=1}^{N} J_z^i, \quad (1)$$

where $\eta \in [0, 1]$ is the anisotropy, $g \in [0, \infty)$ is a tunable parameter, and $J_\alpha^{N+1} = J_\alpha^1$. H can be diagonalized by performing a Jordan-Wigner mapping to spinless fermions. The resulting ground state is BCS-like. A transition between a paramagnetic state (disorder) and a ferromagnetic state (order) occurs for all $\eta > 0$ at the critical value $g_c = 1$, in the thermodynamic limit $N \to \infty$. Relevant algebras, generated by bilinear products of spinless-fermion operators [12], include $\mathfrak{u}(N) = \{c_i^\dagger c_i - \frac{1}{2}, (c_i^\dagger c_j + c_j^\dagger c_i)/\sqrt{2}, (c_i^\dagger c_j - c_j^\dagger c_i)/(i\sqrt{2})\}$, and $\mathfrak{so}(2N) = \mathfrak{u}(N) \oplus \{(c_i^\dagger c_j^\dagger + c_j c_i)/\sqrt{2}, (c_i^\dagger c_j^\dagger - c_j c_i)/(i\sqrt{2})\}$, $1 \le i < j \le N$. These are orthogonal, commonly normalized bases, facilitating the computation of purity. A BCS state is a GCS of $\mathfrak{so}(2N)$; thus it is generalized unentangled relative to $\mathfrak{so}(2N)$, capturing the fact that quasiparticles are *noninteracting* in this description. However, GE may be present relative to the smaller algebra $\mathfrak{u}(N)$ [19]. The thermodynamic limit of the purity relative to $\mathfrak{u}(N)$ as a function of g plays the role of a disorder parameter (Fig. 1), sharply detecting the QPT and characterizing its universality class. This appears to be a generic feature of broken-symmetry (here $\mathbb{Z}_2$) phase transitions. The purity, a sum of squared expectations of observables, is a *global measure of fluctuations*. Changes in the nature of the fluctuations identify QPTs. In some cases [6,7], nearest-neighbor lattice-site entanglement or other standard entanglement measures may suffice, but in general highly nonlocal correlations or fluctuations, depending on the physics and symmetries of the problem, may be required. An extended analysis will be presented elsewhere [20].

We presented a generalization of entanglement beyond the standard subsystem-based approach, as a feature of states relative to any physically relevant distinguished subspace of observables. Besides linking entanglement with the theory of coherent states, our results carry the potential for a number of conceptual and practical advances. From a condensed-matter perspective, GE might naturally provide measures of correlation strength useful for establishing, for example, whether interactions within a given quasiparticle description are sufficiently weak for a mean-field theory to be meaningful. Conversely, one might use a typology of GE to better understand situations where mean-field theory is not easily applied. For QIP, our formalism can give additional insight into standard entanglement theory and suggest novel measures for multipartite correlations. By scaling system sizes, asymptotic measures can be obtained for investigating information-theoretic or thermodynamic limits, with possible uses in renormalization group analyses.

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