Entanglement Measure for Composite Systems

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A general description of entanglement is suggested as an action realized by an arbitrary operator over given disentangled states. The related entanglement measure is defined. Because of its generality, this definition can be employed for any physical systems, pure or mixed, equilibrium or nonequilibrium, and characterized by any type of operators, whether these are statistical operators, field operators, spin operators, or anything else. Entanglement of any number of parts from their total ensemble forming a multiparticle composite system can be determined. Interplay between entanglement and ordering, occurring under phase transitions, is analyzed by invoking the concept of operator order indices.

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Entanglement is the term Schrödinger coined for characterizing superposition of multipartite quantum states [1], which results in the appearance of specific quantum correlations between parts of a composite system. Nowadays there is a growing interest in studying entanglement due to its potential applications in quantum computing and quantum information processing [2,3]. In order to be a well-defined characteristic, entanglement has to be quantifiable. One usually considers pairwise entanglement, for which several measures have been suggested, based on some kinds of reduced or relative entropies [2–8]. In the frame of a brief communication, it is impossible to present a detailed description of these measures, whose exhaustive account can be found in books [2,3], reviews [4–8], and references therein. But it is important to stress that the known entanglement measures are defined for quantifying only two-partite entanglement, and there is presently no definitive measure for entanglement between three or more subsystems. Also, there is no well-defined entanglement measure for mixed multipartite systems.

The aim of this paper is to introduce a general entanglement measure that would be valid for any system. Aiming at reaching a high level of generality, it is necessary, for a while, to leave aside all physical applications and to focus our attention on the mathematical structure of the considered concept.

Since entanglement deals with composite systems, we need, first of all, to concretize the meaning of the latter. In the present case, a system implies an object characterized by its space of states. Naming a space composite means that it is composed of some parts. Let the parts be labeled by an index $i \in \mathbb{I}$. The *label manifold* $\mathbb{I}$ can be discrete or continuous. In the simplest case, $i = 1, 2, \ldots$. Let each part be characterized by a *single-partite space* $\mathcal{H}_i$, which is a Hilbert space $\mathcal{H}_i \equiv \bar{\mathcal{L}}\{|n_i\rangle\}$, being a closed linear envelope of a single-partite basis $\{|n_i\rangle\}$. Any vector $\varphi_i \in \mathcal{H}_i$ is presentable as an expansion $\varphi_i = \sum_{n_i} a_{n_i}|n_i\rangle$. The *composite space* $\mathcal{H} \equiv \otimes_i \mathcal{H}_i$ is the tensor product, which is a closed linear envelope $\mathcal{H} = \bar{\mathcal{L}}\{|\{n_i\}\rangle\}$ of a multipartite basis $\{|\{n_i\}\rangle\}$ whose vectors can be written as $|\{n_i\}\rangle = \otimes_i |n_i\rangle$. For any $\varphi \in \mathcal{H}$, one has an expansion $\varphi = \sum_{\{n_i\}} c_{\{n_i\}} |\{n_i\}\rangle$.

Two remarks are in order. If the label manifold $\mathbb{I}$ is discrete, then $\otimes_i \mathcal{H}_i$ is the standard tensor product with $i = 1, 2, \ldots$. When $\mathbb{I}$ is continuous, then $\otimes_i \mathcal{H}_i$ is the continuous tensor product, introduced by von Neumann [9] and employed for particular cases in Refs. [10,11]. Second, $\mathcal{H}$ is not compulsory a complete tensor product. It may happen that some selection rules are imposed on the latter, such as some symmetry requirements. Then $\mathcal{H}$ is a subspace of the complete tensor product and it is called [9] an incomplete tensor product.

Among all admissible vectors of $\mathcal{H}$, one may separate out those of two types. One type forms the *disentangled set*

$$\mathcal{D} = \{\otimes_i \varphi_i \mid \varphi_i \in \mathcal{H}_i\} \tag{1}$$

whose vectors $f \in \mathcal{D} \subset \mathcal{H}$ have the structure of the tensor product $f = \otimes_i \sum_{n_i} a_{n_i} |n_i\rangle$ and are termed disentangled states. All other possible vectors of $\mathcal{H}$ constitute the complement $\mathcal{H} \setminus \mathcal{D}$ whose elements cannot be presented as products of $\varphi_i \in \mathcal{H}_i$ and which are named entangled states. For instance, in the case of a bipartite system with two-dimensional single-partite spaces $\mathcal{H}_i$, the examples of entangled states would be $c_{12}|12\rangle + c_{21}|21\rangle$ and $c_{11}|11\rangle + c_{22}|22\rangle$, which, clearly, do not pertain to $\mathcal{D}$.

Entanglement, by its philological meaning, implies an action or a process by which disentangled states are transformed into entangled ones. A transforming action can always be described by an operator. Hence, one may consider entanglement produced by different operators. Let an operator A be given on $\mathcal{H}$. Acting on $\mathcal{D}$, this operator will, generally, transform disentangled into entangled states. We shall say that A is an *entangling operator*, provided that $A\mathcal{D} = \mathcal{H} \setminus \mathcal{D}$. Of course, not each operator is entangling. And we shall call A a *nonentangling operator* when $A\mathcal{D} = \mathcal{D}$.

For each operator A on $\mathcal{H}$, we may put into correspondence a nonentangling operator $A^{\otimes}$ having the

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structure of a tensor product $\otimes_i A_1^i$ of *single-partite operators*

$$A_1^i \equiv \text{const} \times \text{Tr}_{\{\mathcal{H}_j \neq i\}} A. \tag{2}$$

In order that the choice of a constant in Eq. (2) would preserve a scale-invariant form of $A^{\otimes}$, we require the validity of the normalization condition

$$\text{Tr}_{\mathcal{H}} A = \text{Tr}_{\mathcal{D}} A^{\otimes}. \tag{3}$$

As a result, we obtain the *nonentangling operator*

$$A^{\otimes} \equiv \frac{\text{Tr}_{\mathcal{H}} A}{\text{Tr}_{\mathcal{D}} \otimes_i A_1^i} \otimes_i A_1^i \tag{4}$$

associated with A. Note that the trace over the set $\mathcal{D}$, which is a restricted subset of the Hilbert space $\mathcal{H}$, is called the restricted trace. Such traces are widely used in statistical mechanics [10] and quantum information theory [2–7]. Their rigorous mathematical definition can be done by employing the corresponding projecting operators or, more generally, by invoking weighted Hilbert spaces [10]. In the present case, however, we do not need a general definition, since here the trace over $\mathcal{D}$ is applied only to the factor operators $\otimes_i A_1^i$, for which this reduces just to the shorthand notation $\text{Tr}_{\mathcal{D}} \otimes_i A_1^i \equiv \prod_i \text{Tr}_{\mathcal{H}_i} A_1^i$.

Now we come to the central problem of quantifying entanglement produced by an operator A on $\mathcal{D}$. The principal idea suggesting the way of constructing this measure stems from the following arguments. Entanglement, generally speaking, has to do with correlations between parts of a composite system. Interparticle correlations in physics are often connected with a kind of order classifying different thermodynamic phases and characterizing phase transitions. The level of ordering in physical systems can be described by *order indices* [12] advanced for reduced density matrices. This concept has been generalized by introducing *operator order indices* [13] defined for arbitrary operators. The definition of these order indices involves the norms of the corresponding operators. It is the operator norm that contains an essential information on the amount of order hidden in the action of this operator. Following this way of thinking, the amount of entanglement should also be related to operator norms. More precisely, we should correlate the actions on $\mathcal{D}$ of a given operator A and of its nonentangling counterpart (4) by comparing the related norms $\|A\|_{\mathcal{D}}$ and $\|A^{\otimes}\|_{\mathcal{D}}$. Thus we finally arrive at the definition of the *entanglement measure*

$$\varepsilon(A) \equiv \log \frac{\|A\|_{\mathcal{D}}}{\|A^{\otimes}\|_{\mathcal{D}}} \tag{5}$$

for the entanglement produced by an arbitrary operator A on the disentangled set $\mathcal{D}$. As is evident, the measure $\varepsilon(A) = \varepsilon(A, \mathcal{D})$ is defined with respect to A as well as $\mathcal{D}$. But, for short, we may write $\varepsilon(A)$ when $\mathcal{D}$ is fixed. The operator norms can be understood as those associated with the vector norms, so that $\|A\|_{\mathcal{D}} \equiv \sup_{f \in \mathcal{D}} \|Af\|_{\mathcal{D}}$, where $\|f\|_{\mathcal{D}} = 1$. The norm over a set $\mathcal{D} \subset \mathcal{H}$ is well defined [12], since it is straightforwardly reformulated to the norm $\|A\|_{\mathcal{D}} \equiv \|\mathcal{P}_{\mathcal{D}} A \mathcal{P}_{\mathcal{D}}\|_{\mathcal{H}}$ over the Hilbert space $\mathcal{H}$ by means of the projector $\mathcal{P}_{\mathcal{D}}$, such that $\mathcal{P}_{\mathcal{D}} \mathcal{H} = \mathcal{D}$. It is easy to show that the entanglement measure (5) possesses the following natural properties.

1. Semipositivity: For any bounded operator A,

$$\varepsilon(A) \geq 0. \tag{6}$$

2. Nullification: Measure is zero for nonentangling operators having the structure of a tensor product $A = A^{\otimes}$,

$$\varepsilon(A^{\otimes}) = 0. \tag{7}$$

In particular, there is no self-entanglement of a single part, when $A = A_1 = A^{\otimes}$, and $\varepsilon(A_1) = 0$. The property (7) can be generalized to the case when $A = \oplus_\nu p_\nu A_\nu^{\otimes}$, where $\|A_\nu^{\otimes}\|_{\mathcal{D}} = \|A^{\otimes}\|_{\mathcal{D}}$ and $\sum_\nu |p_\nu| = 1$, that is, $\varepsilon(\oplus_\nu p_\nu A_\nu^{\otimes}) = 0$.

3. Additivity: For an operator $A = \otimes_\nu A_\nu$,

$$\varepsilon(\otimes_\nu A_\nu) = \sum_\nu \varepsilon(A_\nu). \tag{8}$$

4. Invariance: Measure is invariant under local unitary operations U_i,

$$\varepsilon(\otimes_i U_i^{+} A \otimes_i U_i) = \varepsilon(A). \tag{9}$$

5. Continuity: If any considered operator A, being parametrized as $A(t)$, with $t \in \mathbb{R}$, is continuous by norm, such that $\|A(t)\|_{\mathcal{D}} \to \|A(0)\|_{\mathcal{D}}$ as $t \to 0$, then measure (5) is also continuous,

$$\varepsilon(A(t)) \to \varepsilon(A(0)) \qquad (t \to 0). \tag{10}$$

In this way, we may quantify entanglement produced by an arbitrary operator. Turning to physical systems, we could consider entanglement caused by any physical operator, for example, due to a Hamiltonian, number-of-particle operator, momentum, spin, and so on. It is, however, customary to examine entanglement only with respect to the von Neumann density operator $\hat{\rho}$. The entanglement measure (5) can be easily calculated for this operator too, as we demonstrate below by several examples. For brevity, we shall write $|i\rangle$ instead of $|n_i\rangle$.

(i) Einstein-Podolsky-Rosen states: The density operator for this famous example of a pure state is $\hat{\rho}_{\text{EPR}} = |\text{EPR}\rangle\langle\text{EPR}|$, where $|\text{EPR}\rangle \equiv (1/\sqrt{2})(|12\rangle \pm |21\rangle)$. For measure (5), we immediately get $\varepsilon(\hat{\rho}_{\text{EPR}}) = \log 2$, which is unity if the logarithm is to the base 2.

(ii) Bell states: For the density operator $\hat{\rho}_B = |B\rangle\langle B|$, where $|B\rangle \equiv (1/\sqrt{2})(|11\rangle \pm |22\rangle)$, we again have $\varepsilon(\hat{\rho}_B) = \log 2$.

(iii) Greenberger-Horne-Zeilinger states: This is a three-partite state with $\hat{\rho}_{\text{GHZ}} = |\text{GHZ}\rangle\langle\text{GHZ}|$, where

$|\mathrm{GHZ}\rangle \equiv (1/\sqrt{2})(|111\rangle \pm |222\rangle)$. The corresponding measure is $\varepsilon(\hat{\rho}_{\mathrm{GHZ}}) = 2\log 2$.

(iv) Multicat states: These states are a generalization of the previous cases, the density operator being $\hat{\rho}_{\mathrm{MC}} = |\mathrm{MC}\rangle\langle\mathrm{MC}|$, with $|\mathrm{MC}\rangle \equiv c_1|11\cdots1\rangle + c_2|22\cdots2\rangle$, where $|c_1|^2 + |c_2|^2 = 1$ and N parts are assumed. The entanglement measure (5) is

$$\varepsilon(\hat{\rho}_{\mathrm{MC}}) = (1 - N)\,\mathrm{logsup}\{|c_1|^2, |c_2|^2\}.$$

The maximum is reached for $|c_1|^2 = |c_2|^2 = \frac{1}{2}$, when $\varepsilon(\hat{\rho}_{\mathrm{MC}}) = (N - 1)\log 2$.

(v) Multimode states: Such states, that are a generalization of the multicat states, can be created in coherent systems of N parts, each of which can accept m different modes [14,15]. For the density operator $\hat{\rho}_{\mathrm{MM}} = |\mathrm{MM}\rangle\langle\mathrm{MM}|$, with $|\mathrm{MM}\rangle \equiv \sum_n c_n|n\cdots n\rangle$, where $\sum_n |c_n|^2 = 1$ and $\sum_n 1 = m$, measure (5) becomes

$$\varepsilon(\hat{\rho}_{\mathrm{MM}}) = (1 - N)\,\mathrm{logsup}_n |c_n|^2.$$

Its maximal value happens for $|c_n|^2 = 1/m$, when $\varepsilon(\hat{\rho}_{\mathrm{MM}}) = (N - 1)\log m$.

(vi) Hartree-Fock states: These describe N parts in different quantum states. The density operator is $\hat{\rho}_{\mathrm{HF}} = |\mathrm{HF}\rangle\langle\mathrm{HF}|$, with $|\mathrm{HF}\rangle \equiv (1/\sqrt{N!})\sum_{\mathrm{sym}}|12\cdots N\rangle$, where a symmetrized sum is implied, symmetric or antisymmetric, depending on the type of statistics, Bose or Fermi, respectively. Measure (5) takes the form

$$\varepsilon(\hat{\rho}_{\mathrm{HF}}) = \log\frac{N^N}{N!}.$$

(vii) Mixed states: The von Neumann density operator can be of any type, but not only being related to pure states, as in the examples above. In general, it can be any nonequilibrium operator $\hat{\rho}(t)$, which leads to the evolutional entanglement, varying with time [15]. In the case of an equilibrium system, the von Neumann operator is $\hat{\rho} = Z^{-1}e^{-\beta H}$, where Z is a partition function, β is inverse temperature, and H is a Hamiltonian. Measure (5) provides the opportunity of quantifying entanglement for any p parts of an N-partite system. To illustrate this, let us treat the case when a mixed p-partite state is obtained by tracing out $N - p + 1$ variables from the Hartree-Fock state of N parts, that is, $\hat{\rho}^p_{\mathrm{HF}} \equiv \mathrm{Tr}_{\mathcal{H}_{p+1}}\cdots\mathrm{Tr}_{\mathcal{H}_N}\hat{\rho}_{\mathrm{HF}}$. The entanglement of this p-partite mixed state is measured as

$$\varepsilon(\hat{\rho}^p_{\mathrm{HF}}) = \log\frac{(N - p)!N^p}{N!}.$$

(viii) Statistical states: Mixed states in statistical mechanics, as is mentioned above, can be characterized by entanglement produced by the von Neumann statistical operator. However, this is not the sole possibility. Another way is to measure entanglement realized by reduced density matrices. This way in many cases may be much simpler, since the properties of the reduced density matrices have been thoroughly studied [12]. This method also provides a direct opportunity of quantifying entanglement for any p parts of a given statistical system. The procedure is as follows. Let $x^p \equiv \{x_1, x_2, \ldots, x_p\}$ be a set of variables characterizing the annihilation, $\psi(x)$, and creation, $\psi^\dagger(x)$, field operators. A p-partite density matrix $\rho_p = [\rho_p(x^p, \bar{x}^p)]$ is defined as a matrix with respect to x^p and $\bar{x}^p$, with the elements

$$\rho_p(x^p, \bar{x}^p) \equiv \mathrm{Tr}_{\mathcal{F}}\psi(x_1)\cdots\psi(x_p)\hat{\rho}\psi^\dagger(\bar{x}_p)\cdots\psi^\dagger(\bar{x}_1), \tag{11}$$

where the trace is over the Fock space and $\hat{\rho}$ is a statistical operator. Under the variables x, one may mean, e.g., spatial coordinates, or momentum variables, or multiindices in any convenient representation. The studied statistical system has N parts. These can be indistinguishable particles, with the field operators satisfying the boson or fermion commutation relations. Then a p-partite density matrix ρ_p describes correlations between any p particles from the ensemble of N identical particles. It is reasonable to associate the single-partite space $\mathcal{H}_i$ with a span of the natural orbitals [12] that are the eigenvectors of the single-partite density matrix $\rho^i_1 = [\rho_1(x_i, \bar{x}_i)]$. In the considered case, for the nonentangling operator (4), we have

$$\rho^{\otimes}_p = \frac{N!}{(N - p)!N^p}\otimes_{i=1}^p \rho^i_1. \tag{12}$$

Keeping in mind identical particles, for which $\|\rho^i_1\|_{\mathcal{H}i} = \|\rho_1\|_{\mathcal{H}1}$, we obtain the entanglement measure (5) as

$$\varepsilon(\rho_p) = \log\frac{(N - p)!N^p\|\rho_p\|_{\mathcal{D}}}{N!\|\rho_1\|^p_{\mathcal{H}1}}. \tag{13}$$

What now is left is to find the norms of ρ_p and ρ_1 for a given statistical system, which can be done following the known prescriptions [12].

(ix) Spin states: Density matrices can be constructed not only of the field operators, as in Eq. (11), but of any other operators [13]. For instance, investigating spin systems, one may introduce *spin density matrices* [13] as follows. Let $\mathbf{S}_i = \{S^\alpha_i\}$ be a spin operator associated with a lattice site $i = 1, 2, \ldots, N$. We may define a p-partite spin density matrix $R_p = [R^{\{\alpha,\beta\}}_{\{ij\}}]$ as a matrix with respect to all indices, the matrix elements being

$$R^{\{\alpha\beta\}}_{\{ij\}} \equiv \mathrm{Tr}S^{\alpha_1}_{i_1}\cdots S^{\alpha_p}_{i_p}\hat{\rho}S^{\beta_p}_{j_p}\cdots S^{\beta_1}_{j_1}, \tag{14}$$

with the trace over all spin states. The single-partite space $\mathcal{H}_1$ is defined as a span of the eigenvectors of the single-partite matrix $R_1 = [R^{\alpha\beta}_{ij}]$. The nonentangling matrix (4) is a p-fold tensor product $R^{\otimes}_p = R_1 \otimes R_1 \otimes \cdots \otimes R_1$. The entanglement measure (5) becomes

$$\varepsilon(R_p) = \log\frac{\|R_p\|_{\mathcal{D}}}{\|R^{\otimes}_p\|_{\mathcal{D}}}. \tag{15}$$

(x) Phase transitions: Since entanglement is related to correlations existing in a composite system, it would not be surprising if entanglement would be sensitive to a physical order arising under phase transitions. Hence the latter can be accompanied by *entanglement transitions*. To prove this, let us consider some examples of phase transitions.

A. Bose-Einstein condensation: The changes in the reduced density matrices happening under this transition are well known [12,13]. Essentially above the condensation point, one has $\|\rho_p\|_{\mathcal{D}} \simeq \|\rho_1\|^p_{\mathcal{H}_1}$, because of which the entanglement measure (13) takes the form $\varepsilon(\rho_p) = \log(N-p)!N^p/N!$ typical of the mixed Hartree-Fock states. But below the condensation point, we have $\|\rho_p\|_{\mathcal{D}} = N!/(N-p)!$. Consequently, entanglement vanishes, $\varepsilon(\rho_p) = 0$.

B. Superconducting transition: Employing the properties of fermion density matrices, covered in great detail in [12], we find the following. Above the critical point, entanglement measure $\varepsilon(\rho_p)$ is again of the Hartree-Fock form. But below the critical point, one has $\|\rho_p\|_{\mathcal{D}} \simeq c_p N^{(p-1)/2}$, when p is odd, and $\|\rho_p\|_{\mathcal{D}} \simeq c_p N^{p/2}$, if p is even [12], where c_p is a constant of the order of 1. Thus, for measure (13), we obtain

$$\varepsilon(\rho_p) \simeq \begin{cases} \frac{p-1}{2}\log N & (p = 1, 3, \ldots), \\ \frac{p}{2}\log N & (p = 2, 4, \ldots), \end{cases}$$

where the large number of particles $N \gg 1$ is assumed. Consequently, entanglement increases, which is opposite to the case of Bose-Einstein condensation.

C. Ferromagnetic transition: We shall study measure (15), based on spin density matrices [13]. For concreteness, let us keep in mind a Heisenberg model with long-range interactions, when the mean-field treatment becomes asymptotically exact in the thermodynamic limit. Then, using the properties of spin density matrices [13], we can derive measure (15). In the paramagnetic phase, we have

$$\varepsilon(R_p) = \log\frac{(2p)!}{2^p p!},$$

but for the ferromagnetic phase we find $\varepsilon(R_p) = 0$. Here the situation is analogous to Bose-Einstein condensation, where the arising long-range order leads to vanishing entanglement. Such a similarity can be understood if one remembers that, under ferromagnetic phase transition, there occurs condensation of magnons [13].

As we see, phase transitions are really accompanied by entanglement transitions. However entanglement behaves differently under different phase transitions, sometimes vanishing but sometimes increasing, In order to fully understand the intimate relation between entanglement and ordering, occurring in physical systems, it is advantageous to resort to the notion of order indices that have been introduced for density matrices [12] and generalized to the case of arbitrary operators [13]. The *operator order index* for an operator A is

$$\omega(A) \equiv \frac{\log\|A\|}{\log|\mathrm{Tr}A|}.$$

For characterizing ordering in physical systems, the role of A is played by the appropriate density matrices, such as ρ_p or R_p. It is important that there may develop two types of long-range order, total and even [12,13]. When there is no order, then $\|A\| \ll |\mathrm{Tr}A|$ and $\omega(A) \ll 1$. If, under a phase transition, there develops *total order*, then $\|A\| \sim |\mathrm{Tr}A|$, so that the order index increases, $\omega(A) \to 1$, but at the same time, because of the normalization condition (3), entanglement vanishes, $\varepsilon(A) \to 0$. This is the situation taking place at Bose-Einstein condensation or ferromagnetic transitions. Another case happens under the appearing *even order*, when $\|\rho_p\| \sim \sqrt{\mathrm{Tr}\rho_p/N}$, if p is odd, while $\|\rho_p\| \sim \sqrt{\mathrm{Tr}\rho_p}$, if p is even. Then the order index increases to $\omega(\rho_p) = (p-1)/2p$, when p is odd, and to $\omega(\rho_p) = 1/2$, if p is even. This results in the increase of the entanglement measure $\varepsilon(\rho_p)$, as it is shown above for superconducting transition.

Concluding, a general entanglement measure is introduced, which describes entanglement realized by an arbitrary operator. For physical systems, it is convenient to consider entanglement caused by reduced density matrices. The relation between entanglement measure and order indices is investigated.

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