Macroscopic observables detecting genuine multipartite entanglement and partial inseparability in many-body systems

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Abstract – We show a general approach for detecting genuine multipartite entanglement and partial inseparability in many-body systems by means of macroscopic observables (such as the energy) only. We show that the obtained criteria detect large areas of genuine multipartite entanglement and partial entanglement in typical mixed many-body states, which are not detected by other criteria. As genuine multipartite entanglement is a necessary property for several quantum information theoretic applications such as, e.g., secret sharing or certain kinds of quantum computation, our methods can be used to select or design appropriate condensed matter systems.

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Introduction. – Quantum entanglement (especially in multipartite settings [1]) is undoubtedly one of the most prominent and unique features of quantum mechanics. It is not only essential for technological applications such as quantum computation (see, e.g., [2]) or quantum cryptography (e.g., [3]) and quantum secret sharing (e.g., [4]), but also exists in a wide range of non-artificial systems. While the actual role of entanglement in nature is still widely unclear and attracts much attention and speculation (entanglement might, e.g., be responsible for the high efficiency of phenomena such as, photosynthesis [5,6], navigational orientation of animals [7], the imbalance of matter and antimatter in our universe [8] or evolution itself [9]), it is undoubtedly that entanglement at least exists in nature and appears to be of high importance in simple systems and processes, such as, e.g., in particle physics [10] or in crystal lattices and phase transitions [11].

Many-body systems have been studied particularly intensively in the context of entanglement in the past decade (see, e.g., refs. [12–20] or, for an overview, ref. [21]). Only few works [22–25] address the issue of partial separability or genuine multipartite entanglement (GME), however, only in the context of pure states. In fact, to the authors’ best knowledge the work in ref. [26] is the only one even mentioning the problem of partial separability in mixed states of condensed matter physics. However, while the approach presented in this work is, in principle, capable of detecting GME, this is neither done nor mentioned. Furthermore, since the method only yields non-optimal GME-witnesses (due to the estimations in the construction), it cannot offer a satisfactory detection power. Therefore, the role of GME and partial entanglement in many-body systems is still widely unknown (while especially the former is known to be of grave importance to applications like quantum secret sharing [27] or certain kinds of quantum computers [28], as well as to fundamental tests of quantum mechanics [29,30]).

In this letter, GME in mixed many-body systems consisting of lattices of interacting spin-\(\frac{1}{2}\) and spin-1 particles is investigated, using existing tools for detecting the different kinds of entanglement as well as approaches inspired by the studies of bipartite entanglement in many-body systems. The latter can be generalised, such that macroscopic thermodynamical observables, such as energy or entropy of the composite system, act as multipartite witnesses for different kinds of partial and genuine multipartite entanglement.

This work is organised as follows. First, a few basic definitions are reviewed, such that then methods for detecting partial entanglement and GME in many-body systems with macroscopic observables—the main result of this paper— can be formulated. Finally, the results will be discussed and illustrated in representative examples.
Partial separability and genuine multipartite entanglement. – A pure state \(|\Psi_k\rangle\) is called \(k\)-separable, iff it can be written as a tensor product of \(k\) factors \(|\psi_i\rangle\), each of which describes one or several subsystems:

\[
|\Psi\rangle = \bigotimes_{i=1}^{k} |\psi_i\rangle.
\]

A mixed state \(\rho\) is called \(k\)-separable, iff it can be decomposed into a mixture of \(k\)-separable pure states:

\[
\rho = \sum_i p_i |\Psi_i^k\rangle \langle \Psi_i^k|,
\]

where all \(|\Psi_i^k\rangle\) are \(k\)-separable (possibly with respect to different \(k\)-partitions) and the \(p_i\) form a probability distribution.

An \(n\)-partite state (pure or mixed) is called fully separable iff it is \(n\)-separable. It is called genuinely multipartite entangled (GME) iff it is not biseparable (2-separable). If neither of these is the case, the state is called partially entangled or partially separable.

Detection criteria. – The probably most important macroscopic observables of many-body systems are Hamiltonians, corresponding to energy measurements. Therefore, using Hamiltonians for entanglement detection is in principle a very promising approach, as used in the concept of the entanglement gap (as defined in ref. [14]), which we generalise with respect to GME and partial entanglement and will denote in similar fashion "the GME gap" and "the \(k\)-entanglement gap" respectively. It works as follows.

Consider a system whose dynamics are described by a Hamiltonian \(H\). As a consequence of the compactness of the set of \(k\)-separable states, there always has to be a unique and well-defined energy \(E_{k}\)-separ.

\[
E_{k\text{-sep}} = \min_{\psi \in S_k} \langle \psi | H | \psi \rangle,
\]

where \(S_k\) is the set of all \(k\)-separable states. Note that due to the convexity of \(S_k\), it suffices to optimise over pure states in order to obtain an optimum over the whole set, which is computationally feasible (and thus useful) for low particle numbers (as will be explicitly illustrated in examples later).

If now the ground state of \(H\) is not \(k\)-separable (or, in the case of a degenerate ground state, if there is no \(k\)-separable state in the ground-state manifold), this energy is bound to satisfy

\[
E_{k\text{-sep}} > E_0,
\]

where \(E_0\) is the ground-state energy of \(H\). Therefore, any state \(\rho\) satisfying

\[
E_\rho = \text{Tr}(\rho H) < E_{k\text{-sep}}
\]

is necessarily \(k\)-inseparable (or, in particular, GME if \(k = 2\)). For bipartite systems, the energy interval between \(E_0\) and \(E_{2\text{-sep}}\) is called the entanglement gap [14]. In analogy to this, we call the energy interval between \(E_0\) and \(E_{k\text{-sep}}\) the \(k\)-entanglement gap (or, for \(k = 2\), the GME gap). Note that since the sets of \(k\)-separable states for different \(k\) are convex subsets of the sets of \((k-1)\)-separable states, these energy gaps necessarily satisfy

\[
E_0 \leq E_{2\text{-sep}} \leq E_{3\text{-sep}} \leq \cdots \leq E_{n\text{-sep}},
\]

where \(n\) is the number of subsystems.

From the quantum informational point of view, this is nothing else than using \(H\) as an optimal entanglement witness. Any operator with an entangled eigenvector corresponding to the minimal (or maximal) eigenvalue can be used to detect entanglement effectively, namely by finding the minimal expectation value a separable state can attain and using this as the detection threshold. The same procedure can also be applied to the more sophisticated problem of GME or \(k\)-inseparability detection (by replacing separable states by biseparable or \(k\)-separable states, respectively). In addition, note that no actual knowledge of the ground state or the minimal-energy \(k\)-separable states is necessary, as only the corresponding energies are used to evaluate the criterion (and the ground state’s \(k\)-inseparability can also be inferred from them).

While the \(k\)-entanglement gap is probably the most straightforward and practical macroscopic entanglement witness for partial entanglement in many-body states, a similar approach can be applied to other observables as well. Also, in finite-dimensional systems, not only minima but also maxima can be used to construct entanglement witnesses (although these are of less interest, as the states investigated in many-body systems are usually ground states or thermal states, which typically are much closer to the ground state than to the highest excited state).

Furthermore, other methods of detecting entanglement by means of macroscopic observables can also often be generalised to detect \(k\)-inseparability and GME. As an example, consider the method in ref. [31]. The starting point is very similar to the one above: a function is minimised over all separable states, leaving all lower function values for states which can therefore be recognised to necessarily be entangled. However, in this case, the function is not a simple thermodynamical observable on a state, but the quantum relative entropy

\[
S(\rho|\sigma) = \text{Tr}(\rho \ln \rho - \rho \ln \sigma).
\]

By chosing \(\rho = |E_0\rangle \langle E_0|\) as the ground state of \(H\) and

\[
\sigma = \frac{1}{Z} \sum_i e^{-\frac{E_i}{T}} |E_i\rangle \langle E_i|
\]

as the thermal state with arbitrary temperature \(T\) (where \(k\) is Boltzmann’s constant, \(Z\) is the partition function, and the \(E_i\) are the eigenvalues corresponding to the eigenvectors \(|E_i\rangle\) of the Hamiltonian), this entropy becomes
equal to the von Neumann entropy of the thermal state $\sigma$. Now, if

$$S(\sigma) = S(|E_0\rangle\langle E_0|\sigma) < \min_{\omega\in\mathcal{S}} S(|E_0\rangle\langle E_0|\omega),$$

then $\sigma$ is detected to be entangled. Since the right hand side of the above inequality only depends on $|E_0\rangle$, knowledge of the ground state in principle suffices to use this criterion. By simply replacing separable states by $k$-separable states, one obtains a similar criterion for detecting $k$-inseparability in thermal states: If

$$S(\sigma) = S(|E_0\rangle\langle E_0|\sigma) < \min_{\omega\in\mathcal{S}_k} S(|E_0\rangle\langle E_0|\omega),$$

then $\sigma$ is detected not to be $k$-separable (or to be GME, in the case $k=2$).

However, as this criterion only works for thermal states and requires optimisation over all mixed separable or $k$-separable states (as the optimised function is not linear), it is much less useful for practical and computational reasons than the concept of the entanglement gap or the k-entanglement gap, respectively.

**Examples.** – **Example 1:** Consider a lattice of spin-$\frac{1}{2}$ particles with nearest-neighbor interaction, described by the commonly used Heisenberg model Hamiltonian [21]

$$\mathcal{H} = \frac{J}{2} \sum_{\langle i,j \rangle} \left[ (1+\gamma)\sigma^z_i \sigma^z_j + (1-\gamma)\sigma^y_i \sigma^y_j + 2\Delta \sigma^x_i \sigma^x_j \right] - h \sum_i \sigma^z_i,$$

where the sum over $\langle i,j \rangle$ runs over all pairs of nearest-neighboring particles. Note that this Hamiltonian can describe a one-, two- or three-dimensional lattice with arbitrary ordering structure, depending on the choice of index pairs $(i,j)$ in the sum (describing the elementary cell of the lattice).

For this example, let us choose the cubic antiferromagnetic case $J > 0$ with the parameter values $\gamma = [-1,1]$ and $\Delta = 1$. Without loss of generality we can even choose $J = 1$ and measure all energies in units of $J$. This Hamiltonian’s ground state is not only GME for large intervals of the external magnetic field $h$, but is also very strongly GME, as can be measured, e.g., by the GME concurrence $C_{\text{GME}}$ [32] (a quantity which is zero for biseparable states and one for maximally GME states and can be derived analytically for pure states), as shown in fig. 1. Thus, it is an optimal testing field for our criterion.

In order to test its detection power for mixed states as well, we compare it to the strongest criteria for GME known so far: A set of nonlinear inequalities of density matrix elements [33,34], which we denote by $Q_i$ ($0 \leq i \leq \frac{2}{3}$):

$$Q_0 = \langle 0| \otimes n \rho |1| \otimes n \rangle - \sum_{\gamma} \langle 0| \otimes n \rho \sigma_\gamma \otimes 2 \rho \sigma_\gamma |1| \otimes n \rangle,$$

for $1 \leq m \leq \frac{n}{2}$, where the first sum runs over all subsets $\alpha$ and $\beta$ of $\{1,2,3,\ldots,n\}$ which satisfy $|\alpha|=|\beta|=m$ and $|\alpha \cap \beta| = m-1$, the permutation operator $P_{\alpha,\beta}$ is the same as in the previous expression (swapping all subsystems contained in $\alpha$) and $|d_\alpha\rangle = \bigotimes_{\alpha \in \langle \alpha \rangle} |0\rangle_i \bigotimes_{\alpha \in \{\alpha\}} |1\rangle_i$.

If any $Q_i > 0$, the state under investigation is detected to be GME (while a value lower than or equal to zero does not imply any statement whatsoever about GME, i.e., the criteria are sufficient but not necessary for GME). While each $Q_i$ is sensitive to a specific kind of GME (and thus capable of revealing different kinds of information on investigated states), a combination of all these criteria yields a well-distributed detection power.

The mixed states of highest interest in many-body physics are thermal states, given by the Boltzmann distribution

$$\rho = \frac{1}{Z} \sum_i e^{-\frac{E_i}{kT}} |E_i\rangle \langle E_i|,$$

where $E_i$ is the i-th energy eigenvalue, corresponding to the eigenvector $|E_i\rangle$ of $\mathcal{H}$, $Z$ is a normalisation factor (called the partition function) and $kT$ is the temperature multiplied by Boltzmann’s constant. While it is clear from fig. 1, that this state is GME for values of $kT$ close to zero, the important questions are: How far can $kT$ rise without $\rho$ becoming biseparable? What regions of $k$-inseparability can be detected for $k > 2$?

In fig. 2, the detection power of our criterion is compared to the combined detection inequalities $Q_i$ for a two-by-two particle (i.e., two-dimensional quadratic) lattice for the choice $\gamma = 1$. 

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increasingly mixed states). Temperature in this case only comparatively slowly leads to \text{GME} for high magnetic field magnitudes (as an increasing big (see refs. [13]), which lead to particularly high temperature the ground state and the first excited state is usually rather detected to be so as well. Note, that the energy gap between As long as the ground state is \text{GME}, large intervals of weaker (by comparison) in weakly \text{GME} ground-state areas. highly \text{GME} ground states (i.e., \text{GME}).

detection via the \text{GME} gap is particularly strong in areas with highly \text{GME} ground states (i.e., near $h = 0$), while it is slightly weaker (by comparison) in weakly \text{GME} ground-state areas.

As long as the ground state is \text{GME}, large intervals of $kT$ are detected to be so as well. Note, that the energy gap between the ground state and the first excited state is usually rather big (see ref. [13]), which leads to particularly high temperature \text{GME} for high magnetic field magnitudes (as an increasing temperature in this case only comparatively slowly leads to increasingly mixed states).

**Example 2:** In order to illustrate that the concept of the $k$-entanglement and \text{GME} gap can also be applied to less common Hamiltonians and higher-spin systems, consider a chain of $n$ spin-1 particles with nearest-neighbor coupling, described by the Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{n} \left( \vec{S}_i \cdot \vec{S}_{i+1} + \beta (\vec{S}_i \cdot \vec{S}_{i+1})^2 \right) + h \sum_{i=1}^{n} S_i^z,$$  \hspace{1cm} (15)

where $\vec{S}_i = (S^x_i, S^y_i, S^z_i)$ is the vector of spin-1 operators. Let us choose $n = 3$ and $\beta = 1$ (the choice of $\beta$ only slightly influences the separability-behaviour of the Hamiltonian’s thermal states and thus does not play a significant qualitative role in our considerations). For these settings, the ground state is \text{GME} for $|h| < 3$. It can be seen from fig. 3 that in this case also significant areas of entanglement and \text{GME} are detected (again, in some areas better than with the previously known criteria $Q_1$, in other areas worse than that).

**Conclusion.** – The introduced concept of the $k$-entanglement gap —and, in particular, the \text{GME} (genuine multipartite entanglement) gap— i.e., the gap between the energy value minimised over all $k$-separable states and the ground-state energy, offers a simple detection criterion for partial entanglement and \text{GME} in a wide variety of pure- and mixed-state systems, the only requirement being that the ground states are not separable and the Hamiltonian is known (while explicit knowledge of the ground state is not required). Since its expectation values for $k$-separable states are bounded, any expectation value exceeding these bounds has to be due to a $k$-inseparable —or, for $k = 2$, \text{GME}— state. The detection power of this tool compares to some of the strongest developed criteria known so far for \text{GME} detection in mixed states. It can be measured simply by means of a single macroscopic observable, the energy. Since $k$-inseparability detection (like bipartite entanglement detection) is in general an NP-hard problem [36], no computable necessary and sufficient criteria exist, leaving sufficient-only criteria the only way to tackle this problem. \text{GME} detection in many-body systems is a crucial step not only in verifying experimental advances in this field, and also may eventually allow for these systems to be utilised in quantum informational technology. Since in experimental scenarios, the energy is often rather difficult to measure directly, related quantities —such as $e.g.$, the heat capacity [37]— can be measured instead (other approaches in this direction have already yielded fruitful results, as, $e.g.$, structure factors of crystal lattices can also be used to detect genuine multipartite entanglement [25], however, only for pure states). Using our introduced tool, we showed that genuine multipartite entanglement and partial entanglement are quite common phenomena even in mixed, finite-temperature many-body systems.

We also showed that the concept can be applied to other thermodynamical quantities as well, such as the relative entropy which is a powerful tool in analysing different quantum information theoretic issues. Furthermore, the concept can be generalised in order to improve its detection range further—for example, a similar quantity to
the $k$-entanglement gap could be defined by maximising (instead of minimising), thus detecting partial entanglement in the upper end of the energy spectrum—and to be sensitive to different types of multipartite entangled states.

As different kinds of multipartite entanglement (especially GME) are of grave importance not only to several quantum informational applications, but also to fundamental tests of quantum mechanics, our criterion can be used to experimentally verify the presence of such states and thus aid in investigating these foundational issues.

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