Detection of multipartite entanglement with two-body correlations

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Abstract We show how to detect entanglement with criteria built from simple two-body correlation terms. Since many natural Hamiltonians are sums of such correlation terms, our ideas can be used to detect entanglement by energy measurement. Our criteria can straightforwardly be applied for detecting different forms of multipartite entanglement in familiar spin models in thermal equilibrium.

1 Introduction

Entanglement is an important non-classical phenomenon in quantum mechanics which plays also a crucial role in the novel field of Quantum Information Theory. While for pure quantum states it is equivalent to correlations, for mixed states the two notions differ. In this general case, an $N$-qubit quantum state is entangled if its density matrix cannot be written as a convex sum of product states

$$
\rho = \sum_l p_l \rho_l^{(1)} \otimes \rho_l^{(2)} \otimes ... \otimes \rho_l^{(N)}. \quad (1)
$$

States of the form Eq. (1) are called separable. Based on this definition, several sufficient conditions for entanglement have been developed. In special cases, e.g. for $2 \times 2$ (two-qubit) and $2 \times 3$ (qubit-qudit) bipartite systems \cite{1} \cite{2}, and for bipartite multi-mode Gaussian states \cite{3}, even necessary and sufficient conditions are known.

However, in an experimental situation usually only limited information about the quantum state is available. In this case, only those approaches for entanglement detection can be applied which require the measurement of not too many observables. One of such approaches is using entanglement witnesses. They are entanglement conditions which are linear in expectation values of observables. The theory of entanglement witnesses has recently been rapidly developing \cite{2} \cite{4} \cite{5} \cite{6}. It has been shown how to generate entanglement witnesses that detect states close to a given one, even if it is mixed or a bound entangled state \cite{7} \cite{8}. It is also known how to optimize a witness operator in order to detect the most entangled states \cite{9}. Apart from constructing witnesses, it is also important to find a way to measure them. Optimal measurement of witnesses have been studied in Refs. \cite{10} \cite{11} \cite{12}. Recently, witnesses have been developed to detect entanglement in physical systems in the thermal-dynamical limit \cite{13} \cite{14} \cite{15}.

Entanglement witnesses can not only be used to detect entanglement experimentally, but can also be used to characterize the entanglement of a multipartite quantum state. As we will see later, in the multipartite setting several different classes of entanglement occur, and entanglement witnesses can be used to decide in which class a given state is \cite{17}.

In this paper we ask what we can do for systems of very many particles, e.g., for spin chains in thermal equilibrium. Entanglement in spin chains has already been extensively studied \cite{10}. In Section 2 we discuss how to detect entanglement in general in spin models based on the ideas presented in Ref. \cite{13}. In Section 3 we study the detection of different types of multipartite entanglement in these systems as discussed in Ref. \cite{15}. For this aim, we determine what the important questions are from this point of view in spin systems in the thermodynamical limit. Then we look for appropriate entanglement witnesses, which are easy to construct and study multipartite entanglement with them \cite{17}.

2 Bipartite entanglement

Let us consider first the two-qubit case. The simplest expression which can be used for entanglement detection must contain at least two correlation terms

$$
W := A^{(1)} A^{(2)} + B^{(1)} B^{(2)}, \quad (2)
$$

where $A_k$ and $B_k$ are operators acting on qubits $k = 1, 2$. For simplicity, let us consider $A_k$ and $B_k$ with eigenvalues $\pm 1$. Now, if we want to use $W$ for entanglement
detection, we have to make sure that
\[ \inf_{\psi} \langle W \rangle_{\psi} < \inf_{\phi \in \mathcal{P}} \langle W \rangle_{\phi}, \tag{3} \]
where the right hand side of the equation is minimized over the set of product states \( \mathcal{P} \). (Minimization over all mixed separable states would lead to the same value due to the convexity of the set of separable states.) Eq. 3 expresses the fact that the minimum of \( \langle W \rangle \) must be larger for separable states than for quantum states in general. For that it is necessary to have
\[ [A_k, B_k] \neq 0, \tag{4} \]
for \( k = 1, 2 \). Here \([\ldots]\) denotes the commutator. Eq. 4 expresses the fact that we have to measure two different observables at each party. For entanglement detection in an experiment, the ratio of the two minima in Eq. 3 must be the largest possible. It is straightforward to see that this is the case if we choose operators such that
\[ \{A_k, B_k\} = 0, \tag{5} \]
for \( k = 1, 2 \). Here \( \{\ldots\} \) denotes the anticommutator. An example for such an operator is then
\[ h_{XY} := X^{(1)} X^{(2)} + Y^{(1)} Y^{(2)}, \tag{6} \]
where \( X \) and \( Y \) denote Pauli spin matrices. For this operator the minimum of the expectation value is
\[ \inf_{\psi} \langle h_{XY} \rangle_{\psi} = -2. \tag{7} \]
The state giving the minimum is the two-qubit singlet
\[ |\psi_s\rangle := \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle). \tag{8} \]
For this state \( \langle X^{(1)} X^{(2)} \rangle = \langle Y^{(1)} Y^{(2)} \rangle = -1 \). The minimum for product states can be obtained as follows. For product states we have
\[ \langle h_{XY} \rangle = \langle X^{(1)}\rangle \langle X^{(2)} \rangle + \langle Y^{(1)}\rangle \langle Y^{(2)} \rangle \geq -1, \tag{9} \]
where the last inequality follows from the Cauchy-Schwarz inequality and knowing that \( \langle X^{(k)}\rangle^2 + \langle Y^{(k)}\rangle^2 \leq 1 \). Among operators with three correlation terms used for entanglement detection the following form is optimal
\[ h_H := X^{(1)} X^{(2)} + Y^{(1)} Y^{(2)} + Z^{(1)} Z^{(2)}. \tag{10} \]
The minimum of the expectation value of \( h_H \) is \(-3\). For separable states the minimum is \(-1\) which can be proved similarly as it has been done for \( h_{XY} \).

Now let us move to the \( N \)-qubit case. Consider the expression
\[ H_{XY} := J \sum_{k=1}^{N} X^{(k)} X^{(k+1)} + Y^{(k)} Y^{(k+1)}, \tag{11} \]
where \( J > 0 \) is the coupling constant and according to the usual assumption for a periodic boundary condition qubit \((N+1)\) is identical to qubit \((1)\). This is the Hamiltonian for the XY chain. The minimum for separable states is now
\[ \inf_{\phi \in \mathcal{P}} \langle H_{XY} \rangle_{\phi} = -JN. \tag{12} \]
This comes from knowing that for product states each term in the summation in Eq. 11 is bounded by \(-1\) as we have seen it before. The minimum for quantum states can be obtained from numerical calculations since the XY model is solvable \(18\). Similarly, we can define
\[ H_H := J \sum_{k=1}^{N} X^{(k)} X^{(k+1)} + Y^{(k)} Y^{(k+1)} + Z^{(k)} Z^{(k+1)}, \tag{13} \]
This is the Hamiltonian for the Heisenberg chain. The minimum for separable states is
\[ \inf_{\phi \in \mathcal{P}} \langle H_H \rangle_{\phi} = -JN. \tag{14} \]
The minimum for quantum states can be obtained for large \( N \) as
\[ \inf_{\psi} \langle H_H \rangle_{\psi} = -4 \left( \ln 2 - \frac{1}{4} \right)NJ \approx -1.77NJ. \tag{15} \]

For our spin chain Hamiltonians the ratio between the minimum for general quantum states and the minimum for separable states is smaller than for Eqs. (10) since there is not a quantum state saturating all two-body correlation terms. In fact, it is easy to see that there is not a Hamiltonian built from two-body correlations such that its unique ground state saturates all correlation terms and this ground state is true multipartite entangled \(20\).

What are the advantages of the expressions Eq. (11) and Eqs. (13) in detecting entanglement? They are easily measurable locally, since they are the sum of only a few two-body correlation terms. Moreover, in some physical systems Eq. (13) can directly be measured as the average nearest-neighbor correlation, or as the energy of the system if this system can be described by a Heisenberg Hamiltonian.

The previous ideas can straightforwardly be applied to spin chains in thermal equilibrium \(13\). Let us consider the Heisenberg Hamiltonian in an external magnetic field \( H_{HB} := H_H + B \sum_k Z^{(k)} \). For this Hamiltonian, it is easy to bound the minimum for separable states \(13\). Any time \( \langle H_H \rangle \) is below this value, we know that the thermal state is entangled. This is demonstrated in Fig. 1. It shows the nearest-neighbor entanglement vs. \( B \) and the temperature \( T \). The entanglement of formation was computed from the concurrence \(21\). Light color indicates the region where the thermal ground state is detected as entangled based on the ideas discussed before. As one can see, there are regions with \( E_F > 0 \) which are not detected. However, it can be seen in the Figure that when the system contains at least a small
amount of entanglement (∼ Tg) as a function of magnetic field Fig. 1

Heisenberg chain of 10 spins. Nearest-neighbor entanglement around 0.1

entanglement. Note that the sharp decrease of the nearest-neighbor entanglement around B_{crit} = 4 for T = 0 is due to a quantum phase transition.

3 Multipartite entanglement

In this section we will discuss how to detect multi-party entanglement by measuring the operators described before. Our motivation is that entanglement for many particles is qualitatively different from the two-party case, and many new phenomena arise. There are several possibilities to classify entanglement of many parties. We are now looking for the terminology which is appropriate for spin chains of many particles.

Let us first recall the notion of genuine multipartite entanglement. A pure state |ψ⟩ of a quantum system of N parties is called fully separable if it is a product state for all parties, |ψ⟩ = |φ₁⟩ ⊗ |φ₂⟩ ⊗ ... ⊗ |φₙ⟩. It is called biseparable, when a partition of the N parties into two groups A and B can be found, such that the state is a product state with respect to this partition, namely

|ψ⟩ = |φ_A⟩ ⊗ |φ_B⟩. \hspace{1cm} \text{(16)}

If this is not the case, the state is called genuine multipartite entangled. Note that the vectors |φ_A⟩ and |φ_B⟩ are allowed to contain entanglement within their partition. Thus, to prove genuine multipartite entanglement, it does not suffice to exclude full separability.

For mixed states, these definitions can, as usual, be extended via convex combinations. Indeed, the definition of full separability was already given in Eq. (1). A mixed state is biseparable, whenever we can write ρ = ∑_{i} p_i |ψ_i⟩⟨ψ_i| with biseparable |ψ_i⟩ and some probabilities p_i. Here, the states |ψ_i⟩ are allowed to be biseparable with respect to different partitions.

Another approach to classify multipartite entanglement asks whether multipartite entanglement is necessary to form a given state. In this approach, a state |ψ⟩ producible by k-party entanglement (or k-producible, in short) if we can write the state |ψ⟩ as a tensor product

|ψ⟩ = |φ₁⟩ ⊗ |φ₂⟩ ⊗ ... ⊗ |φₙ⟩, \hspace{1cm} \text{(17)}

where the states |φ_i⟩ are states on maximally k-qubits. In this definition, a two-producible state does not contain any multipartite entanglement, since it suffices to generate the two-qubit states |φ_i⟩ to arrive at the state |ψ⟩. In addition, we say that a state contains genuine k-party entanglement if it is not producible by (k - 1)-party entanglement. This definition can be extended to mixed states as before via convex combinations. Again, a mixed state which is k-producible requires only the generation of k-party pure entangled states and mixing for its production (see also Fig. 2). Consequently, a mixed state ρ contains k-party entanglement, iff the correlations cannot be explained by assuming the presence of (k - 1)-party entanglement only in the pure subensembles.

The notions of genuine multipartite entanglement and producibility are not completely independent. For example, the states containing N-party entanglement are just the genuine multipartite entangled states and the one-producible states are fully separable. If one can show that a reduced state of k + 1 qubits is genuine multipartite entangled, then this implies that the total state is not k-producible, while the converse is in general not true.

For spin chains of macroscopic size, it is in general very difficult to prove that the total state is genuine N-partite entangled via energy measurements. This is due to the fact that the notion of genuine N-partite entanglement is extremely sensitive to the properties of a single qubit. Indeed, in order to prove genuine multipartite entanglement, one has to exclude the possibility, that one single qubit can be separated from the remaining N - 1 qubits. However, multipartite entanglement in the reduced states of small numbers of qubits can easily be detected, as we will see. Moreover, if the reduced state is multipartite entangled then the state is not two-producible.

Now let us see our results for the XY model and the Heisenberg chain. The proofs for the following theorems are given in Ref. The always assume periodic boundary conditions and that the number of spins N is even.

**Theorem 1.** Let ρ be an N qubit state whose dynamics is governed by the XY-Hamiltonian in Eq. (11).
If \( \rho \) is one-producible (fully separable), then
\[
\langle H_{XY} \rangle \geq -JN \tag{18}
\]
holds. If \( \langle H_{XY} \rangle < -JN \) this implies that there are two neighboring qubits such that their reduced state is entangled. For two-producible states
\[
\langle H_{XY} \rangle \geq -\frac{9}{8}JN \tag{19}
\]
holds. If \( \langle H_{XY} \rangle < -9/8JN \) the state contains thus tripartite entanglement and if
\[
\langle H_{XY} \rangle < -\frac{1+\sqrt{2}}{2}JN \approx -1.207JN \tag{20}
\]
there exist three neighboring qubits \( i, i+1, i+2 \) such that the reduced state \( \rho_{i,i+1,i+2} \) of these qubits is genuine tripartite entangled.

For the Heisenberg model, we can state the following:

**Theorem 2.** Let \( \rho \) be an \( N \) qubit state with the Heisenberg Hamiltonian of Eq. (11). If \( \rho \) is one-producible (fully separable), then
\[
\langle H_H \rangle \geq -JN \tag{21}
\]
holds, while for two-producible states
\[
\langle H_H \rangle \geq -\frac{3}{2}JN \tag{22}
\]
holds. Thus, if \( \langle H_H \rangle < 3N/2 \) the state contains genuine tripartite entanglement. Furthermore, if
\[
\langle H_H \rangle < -\frac{1+\sqrt{2}}{2}JN \approx -1.618JN \tag{23}
\]
then there are three neighboring qubits such that their reduced state is genuine tripartite entangled.

Let us see an example. Consider the state shown in Figure 2(a)
\[
|\Phi_s\rangle = |\psi_s\rangle \otimes |\psi_s\rangle \otimes |\psi_s\rangle \otimes \ldots, \tag{24}
\]
where the two-qubit singlet is defined in Eq. (5). It is easy to see that state \( |\Phi_s\rangle \) saturates the inequality Eq. (22). It is not surprising, since it is a two-producible state. Let us now define operator \( S \) which shifts the qubits by one, i.e.,
\[
S|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes |\alpha_2\rangle \otimes \ldots \otimes |\alpha_N\rangle = |\alpha_N\rangle \otimes |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \ldots \otimes |\alpha_{N-1}\rangle. \tag{25}
\]
Consider the state
\[
\rho_m := \frac{1}{2}\left(|\Phi_s\rangle\langle\Phi_s| + S|\Phi_s\rangle\langle\Phi_s|S^\dagger\right). \tag{26}
\]
This state is the mixture of the singlet chains depicted in Figure 2(a) and (b). \( \rho_m \) is not fully separable and is not a product of single-qubit and two-qubit density matrices. Moreover, the state \( \rho_m \) has a negative partial transpose with respect to each partition. However, \( \rho_m \) also saturates the inequality Eq. (22) and it is also two-producible. That is, three-qubit entanglement is not needed to create it, and it contains no multipartite entanglement.

The previous results can straightforwardly be used for obtaining a limit temperature for the different forms of entanglement. We define thus the temperatures \( T_{R2}, T_{R3}, T_{C2} \) and \( T_{C3} \) below which either reduced states of two or three parties are entangled or the total state contains two or three-party entanglement. Obviously, \( T_{R2} = T_{C2} > T_{C3} > T_{R3} \) has to hold here. These temperature bounds are shown for a Heisenberg chains of a couple of spins in Table 1. As expected, the values for \( T_{C2} = T_{R2} \) coincide with the ones of Ref. [13]. The given values for \( T_{C3} \) and \( T_{R3} \) show that in the Heisenberg chain of ten spins at \( k_B T \approx J \) multipartite entanglement plays a role, namely at least one reduced state is genuine tripartite entangled and the total state contains tripartite entanglement.

| \( N \) | 2 | 4 | 6 | 8 | 10 |
|---|---|---|---|---|---|
| \( T_{C2} \) | 7.28 | 3.45 | 3.21 | 3.18 | 3.18 |
| \( T_{C3} \) | - | 2.10 | 1.75 | 1.65 | 1.62 |
| \( T_{R3} \) | - | 1.85 | 1.46 | 1.32 | 1.26 |

### 4 Conclusions

We discussed how to construct entanglement conditions using two-body correlations. This implies, that typical Hamiltonians as appearing in the XY model or the Heisenberg model can serve for entanglement detection in spin models. Also different forms of multipartite entanglement can be detected in this way.

A natural continuation of our work lies in the extension of our bounds to other systems. Here, spin systems in two or three dimensions as well as frustrated systems are of interest. Furthermore, it would be also desirable to derive energy bounds also for higher classes of multipartite entanglement, e.g. three-producible states.

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20. To be more specific, for H = ∑k=1,4,5,... X(k)X(k+1) + Z(k)Z(k+1) there is a ground state saturating all correlation terms: |ψs⟩ ⊗ |ψs⟩ ⊗ |ψs⟩ ⊗ ... However, this is the chain of two-particle siglets and it is not true multipartite entangled. For having a state with true multipartite entanglement, we would need that for a Hamiltonian like $H = Z(1)Z(2) + Q(2)Z(3)$ we have a ground state which saturates both correlation terms. (Here we assume that $Q(2)$ is different from $Z(2)$ and it has ±1 eigenvalues.) Simple calculation shows that there is not such a state. If we allow using many-body correlations then entanglement criteria with correlation terms can be constructed such that all correlation terms are saturated by a unique quantum state which is also true multipartite entangled as explained in Refs. [11,12]. The related problem of finding correlation operators for a quantum state such that the state is a simultaneous eigenstate of these operators is studied in stabilizer theory: See for example D. Gottesman, Phys. Rev. A 54, 1862 (1996); M.A. Nielsen and I.L. Chuang, Quantum Computation and Quantum Information, Cambridge University Press, Cambridge, United Kingdom (2000).

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