Energy as witness of multipartite entanglement in spin clusters

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We develop a general approach for deriving the energy minima of biseparable states in chains of arbitrary spins \(s\), and report numerical results for spin values \(s \leq 5/2\) (with \(N \leq 8\)). The minima provide a set of threshold values for exchange energy, that allow to detect different degrees of multipartite entanglement in one-dimensional spin systems. We finally demonstrate that the Heisenberg exchange Hamiltonian of \(N\) spins has a nondegenerate \(N\)-partite entangled ground state, and can thus witness such correlations in all finite spin chains.

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Entanglement is one of the most striking peculiarities of quantum systems and promises to play a crucial role in emerging quantum technologies [1]. This has fueled the development of theoretical and experimental means for its detection in diverse physical systems [2]. One of the most convenient such tools is represented by entanglement witnesses. These are observables whose expectation value can exceed given bounds only in the presence of specific forms of entanglement. Macroscopic observables such as magnetic susceptibility [3-5] and internal energy [6,7] allow for example to discriminate between fully separable and entangled spin states. In qubit systems, further inequalities for energy have been derived, whose violation implies multipartite entanglement [8,9]. Along the same lines, the measurement of collective observables [10] allows to detect multipartite entanglement in the vicinity of prototypical quantum states through the spin-squeezing inequalities [12,13]. The connection of these studies with quantum-information processing has however focused most of the attention on entanglement between qubits. Limited attention has instead been devoted to multipartite entanglement between composite systems of \(s > 1/2\) (pseudo)spins [14].

In the present paper, we address the problem of detecting multipartite entanglement in clusters of arbitrary spins \(s\) using exchange energy as a witness. We develop a general approach for deriving the energy minima \(E_{bs}^S\) of biseparable states \(|\psi_A\rangle \otimes |\psi_B\rangle\) in chains of \(N\) spins, that exploits the rotational symmetry of the system Hamiltonian. This allows to reduce the minimization problem to calculating the ground states of effective spin Hamiltonians within each subsystem \(A\) and \(B\). Minima derived for \(k\)-spin chains provide in turn a set of threshold values for energy, corresponding to \(k\)-partite entanglement in chains of \(n_k(k-1)+1\) or rings of \(n_k(k-1)\) spins. Analytical expressions of the minima are derived for the simplest cases, while numerical solutions are provided for \(s \leq 5/2\), that correspond to prototypical models of molecular nanomagnets [17-20]. As a general result, we finally demonstrate that the ground state of an \(N\)-spin chain with Heisenberg Hamiltonian is \(N\)-partite entangled. This implies an energy gap between biseparable and \(N\)-spin entangled states, and the possibility of detecting the latter ones by exchange energy, in finite spin chains with arbitrary \(N\) and \(s\).

Tripartite entanglement — Tripartite entangled states are detected by a three-spin Hamiltonian \(H_{123}\) if their energy exceeds the lower bound that applies to biseparable states [9]. Here, we seek such bound for \(H_{123} = s_1 \cdot s_2 + s_2 \cdot s_3 \equiv H_{12} + H_{23}\), and for a generic biseparable state \(|\psi_1\rangle \otimes |\psi_{23}\rangle\):

\[
E_{bs}^3 = \min_{|\psi_1\rangle,|\psi_{23}\rangle} \left\{ \langle \psi_1 | s_1 | \psi_1 \rangle \cdot \langle \psi_{23} | s_2 | \psi_{23} \rangle + \langle \psi_{23} | s_2 \cdot s_3 | \psi_{23} \rangle \right\}.
\]

(1)

If we identify the direction of \(\langle \psi_{23} | s_2 | \psi_{23} \rangle\) with the \(z\) axis, the first term in Eq. (1) simplifies to: \(\langle H_{12} \rangle = \langle \psi_1 | s_{1,2,3} | \psi_1 \rangle \langle \psi_{23} | s_{2,3} | \psi_{23} \rangle\), where \(\langle \psi_{23} | s_{2,3} | \psi_{23} \rangle \geq 0\) by definition. For any given \(|\psi_{23}\rangle\), the state of \(s_1\) that minimizes \(\langle H_{123} \rangle\) is thus given by \(|m_1=-s_1\rangle\), and the problem of deriving \(E_{bs}^3\) reduces to finding the state \(|\psi_{23}\rangle\) that minimizes:

\[
\langle \psi_{23} | H_{123} | \psi_{23} \rangle \equiv \langle \psi_{23} | -s_1 s_{2,3} + s_2 \cdot s_3 | \psi_{23} \rangle,
\]

(2)

i.e. the ground state of the two-spin Hamiltonian \(H_{12}\). In order to derive the energy minima, it is convenient to expand \(|\psi_{23}\rangle\) in the form:

\[
|\psi_{23}\rangle = \sum_{M=-s_2-s_3}^{s_2+s_3} \sqrt{P_M} \sum_{S=|M|} A_S^M |S,M\rangle \equiv \sum_{M=-s_2-s_3}^{s_2+s_3} \sqrt{P_M} |\psi_M^S\rangle,
\]

(3)

where \(S = s_2 + s_3\) and \(M\) is its projection along \(z\). Each real coefficient \(P_M\) gives the probability that \(S\) has a \(z\)-projection \(M\) (\(\sum P_M = 1\)). The normalization condition for the complex coefficients \(A_S^M = a_S^M e^{i\alpha_S^M}\) reads: \(\sum_S (a_S^M)^2 = 1\) (with \(a_S^M = |A_S^M|\)). Given that both the operators \(s_{2,3}\) and \(s_2 \cdot s_3\) commute with \(s_2\), the energy expectation value can be written as \(\langle H_{23} \rangle = \sum_M P_M E_{bs}^{3,M}\), where,

\[
E_{bs}^{3,M} = \langle \psi_M^S | H_{23} | \psi_M^S \rangle \equiv -s_1 f_M(a_M^M, a_M^\alpha) + g_M(a_M^M, a_M^\alpha),
\]

(4)

with \(a_M^M = (a_M^M, \ldots, a_{M+s_2}^M)\) and \(a_M^\alpha = (\alpha_M^M, \ldots, \alpha_{M+s_2}^M)\). The energy expectation value is thus given by an average, with probabilities \(P_M\), of functions \(E_{bs}^{3,M}\) that depend on disjoint groups of variables \(A_S^M\), each corresponding to a given \(M\). This allows to minimize the terms \(E_{bs}^{3,M}\) independently from one another, and to identify the overall minimum with the lowest \(E_{bs}^{3,M}\):

\[
E_{bs}^3 = \min_M \bar{E}_{bs}^{3,M}(\bar{a}_M, \bar{a}_M^\alpha).
\]

(5)
The dependence of $E_{\text{bs}}^{M}$ on the variables $A_{S}^{M}$ is derived as follows. The first contribution in Eq. [4] is proportional to: $f_{M} = \langle s_{2,2} | \sum_{S,S'} (A_{S}^{M})^{*} (A_{S}^{M}) | S, M \rangle s_{2,2} | S', M \rangle$. Here, the matrix element can be expressed in terms of the Clebsch-Gordan coefficients [21]: $\langle S, M | s_{2,2} | S', M \rangle = \sum_{m_{2}, m_{3}} \langle S, M | m_{2}, m_{3} \rangle \langle m_{2}, m_{3} | S', M \rangle m_{2}$ (with $m_{3} = M - m_{2}$). The second contribution in Eq. [4] is instead diagonal in the basis $|S, M\rangle$, and reads: $g_{M} = \langle s_{2} | s_{3} \rangle = \sum_{S} (a_{S}^{M})^{2} |S(S + 1) - s_{2}(s_{2} + 1) - s_{3}(s_{3} + 1)|/2$.

In order to analytically minimize - for $s \leq 3/2$ - the function $E_{\text{bs}}^{M}$ subject to the normalization constraints, we apply the method of Lagrange multipliers. The stationary points of the Lagrange function $\Lambda_{M}(A_{S}^{M}, \lambda) = E_{\text{bs}}^{M} + \lambda \sum_{S} (a_{S}^{M})^{2} - 1$, are identified by the equations $\partial \Lambda_{M}/\partial a_{S}^{M} = \partial \Lambda_{M}/\partial \alpha_{S}^{M} = \partial \Lambda_{M}/\partial \lambda = 0$, for $|M| \leq S \leq s_{2} + s_{3}$. In all the cases considered below, the lowest minima correspond to $M = 0$: $E_{\text{bs}}^{3} = E_{\text{bs}}^{M=0}$. We shall thus refer only to this subspace, and omit the apices $M$ from the notation. Besides, we focus on the case of identical spins.

In the $s = 1/2$ case, a lower bound for $\langle H_{123} \rangle$ in the absence of tripartite entanglement has already been derived by different means [6]. Here we show that such value actually corresponds to a minimum, and derive the corresponding biseparable state. The dependence of $E_{\text{bs}}^{M}$ on the parameters $\alpha_{S}$ and $\alpha_{S}$ is given by (see Eq. [4]): $f_{M} = -a_{0} a_{1} \cos(\alpha_{0} - \alpha_{1})$ and $g_{M} = -(3a_{0}^{2} + a_{1}^{2})/4$. As far as the phases $\alpha_{S}$ are concerned, $E_{\text{bs}}^{3}$ is minimized by $\alpha_{1} - \alpha_{0} = \pi$. The remaining conditions give rise to the energy minimum $E_{\text{bs}}^{3} = -(1 + \sqrt{5})/4$, that coincides with the lower bound derived in Ref. [6]. The corresponding biseparable state is given by:

$$
\alpha_{0} = \left(\frac{1}{2} + 1/\sqrt{5}\right)^{1/2}, \quad \alpha_{1} = \left(1/2 - 1/\sqrt{5}\right)^{1/2}. \tag{6}
$$

We proceed in the same way in the case $s = 1$, where the expression of energy is given by: $f_{M} = 2a_{1}(a_{0}\sqrt{2} + a_{2})/\sqrt{3}$ and $g_{M} = -2a_{0}^{2} - a_{1}^{2} + a_{2}^{2}$. Here, the conditions $\alpha_{S+1} - \alpha_{S} = \pi$, derived from $\partial \Lambda_{M}/\partial \alpha_{S} = 0$, have already been included. The analytic expression of the energy minimum is:

$$
E_{\text{bs}}^{3} = -2/3 \left\{1 + (\sqrt{2}/2) \cos(\varphi/3) + \sqrt{3} \sin(\varphi/3)\right\}, \tag{7}
$$

where $\varphi = \arccos[1/(10\sqrt{10})]$.

For the spin values $s = 3/2$, $s = 2$, and $s = 5/2$, we directly report the energy minima, and the corresponding biseparable states (Table I), that have been obtained through a conjugate gradient algorithm [22].

The comparison between the different spin values shows that the relative weight of the singlet state ($\bar{\alpha}_{0}$) decreases with increasing $s$, as well as the ratio between the energies of the entangled and unentangled spin pairs ($E_{22}/E_{12}$). In all cases, the inequality $H_{123} < E_{3}^{3}$ implies tripartite entanglement in the three-spin system. The criterion becomes $H < n_{3} E_{3}^{3}$ for any $H$ that can be written as the sum of $n_{3}$ three-spin Hamiltonians, such as chains of $2n_{3} + 1$ spins or rings with $2n_{3}$.

**Quadripartite entanglement** — We consider the expectation values of the four-spin Hamiltonian $H_{234} = s_{1} \cdot s_{2} + s_{2} \cdot s_{3} + s_{3} \cdot s_{4}$, corresponding to the biseparable states $|\psi_{22}^{4}\rangle = |\psi_{12}^{4}| \otimes |\psi_{34}^{4}\rangle$ and $|\psi_{13}^{4}\rangle = |\psi_{1}\rangle \otimes |\psi_{234}\rangle$. In the former case, we compute:

$$
E_{22}^{4} = \min_{|\psi_{1}^{4}\rangle,|\psi_{34}^{4}\rangle} \{ \langle\psi_{12}^{4}|s_{1} \cdot s_{2}|\psi_{12}^{4}\rangle + \langle\psi_{34}^{4}|s_{3} \cdot s_{4}|\psi_{34}^{4}\rangle
+ \langle\psi_{12}^{4}|s_{2} \cdot s_{1}|\psi_{234}^{4}\rangle \langle\psi_{34}^{4}|s_{3} \cdot s_{4}|\psi_{34}^{4}\rangle \}, \tag{8}
$$

where $z$ is defined as the direction of $|\psi_{34}^{4}\rangle$. The states $|\psi_{12}^{4}\rangle$ and $|\psi_{34}^{4}\rangle$ are expanded in the bases $|S = S_{12}, M = M_{12}\rangle$ and $|S' = S_{34}, M' = M_{34}\rangle$, respectively. For $|\psi_{12}^{4}\rangle$, we use the expression in Eq. [8] (and replace the indices 23 with 12). Similarly, $|\psi_{34}^{4}\rangle$ is expressed as: $|\psi_{34}^{4}\rangle = \sum_{M'} \sqrt{M'M} \sum_{S} B_{S}^{M'} |S', M'\rangle$, with $B_{S}^{M'} = b_{S}^{M'} e^{i\beta_{M}^{M'}}$, $\sum_{S} Q_{M'} = \sum_{S} (b_{S}^{M'})^{2} = 1$. Being both $M$ and $M'$ good quantum numbers, $E_{22}^{4} = \sum_{S} \sum_{M'} \sum_{M'} P_{S} Q_{M'} E_{22}^{4,MM'}$, where:

$$
E_{22}^{4,MM'} = g_{M}(A_{M}) + f_{M}(A_{M}) f_{M}(B_{M}) + g_{M}(B_{M}) \tag{9}
$$

and the functions $f_{M}$ and $g_{M}$ coincide with those reported in the previous section. The energy $E_{22}^{4,MM'}$ is minimized numerically by the conjugate gradient approach as a function of $a_{M}$ and $b_{M}$, while the minimization with respect to $\alpha_{M}$ and $\beta_{M}$ is straightforward. The minimum $E_{22}^{4}$ is then identified with the lowest $E_{22}^{4,MM'}$:

$$
E_{22}^{4} = \min_{M,M'} E_{22}^{4,MM'}(a_{M}, \alpha_{M}, b_{M}, \beta_{M}). \tag{10}
$$

For all values of $s$, the lowest minima belong to the subspace $M = M' = 0$. The minimum of $E_{22}^{4}$ is instead identified with the ground state energy of the three-spin Hamiltonian $H_{234} = -s_{1} s_{2} + s_{2} \cdot s_{3} + s_{3} \cdot s_{4}$, which belongs, in all the considered cases, to the subspace.
TABLE II: Left: Minima \( E_{12}^N \) and \( E_{13}^N \) for biseparable four-spin states \( \ket{\psi_{12}} \otimes \ket{\psi_{34}} \) and \( \ket{\psi_{1}} \otimes \ket{\psi_{234}} \), respectively. The states corresponding to the former partition are given by the displayed values of \( \bar{a}_S \), and by: \( B_S = A_S \), \( S_{S+1} = A_S = \pi \), and \( \beta_{S+1} = \beta_S = 0 \). Right: Energy minima \( E_{bs}^N \) of \( N \)-spin systems.

\[
\begin{array}{cccccccc}
 s & a_1 & a_2 & a_3 & a_4 & a_5 & E_1^4 & E_2^4 & E_3^4 \\
 1/2 & 1 & 0 & - & - & - & -1.500 & -1.190 & -1.780 \-2.366 \-2.697 \-3.244 \\
 1 & 0.921 & 0.387 & 0.0418 & - & - & -4.051 & -3.828 & -5.343 \-6.771 \-8.133 \-9.537 \\
 3/2 & 0.775 & 0.607 & 0.171 & 0.0281 & - & -8.131 & -7.957 & -10.90 \-13.75 \-16.56 \-19.39 \\
 2 & 0.687 & 0.669 & 0.278 & 0.0602 & 0.00649 & -13.74 & -13.59 & -18.46 \-23.24 \-27.99 \-32.75 \\
 5/2 & 0.627 & 0.669 & 0.359 & 0.134 & 0.110 & <10^{-4} & -21.18 \-20.71 & -28.03 \-35.23 \-42.42 \-49.62 \\
\end{array}
\]

with \( M = s \). The energy minima and the corresponding states are reported in the left part of Table II. We note that the bipartition \( \ket{\psi_{12}} \otimes \ket{\psi_{34}} \) always gives lower minima with respect to \( \ket{\psi_1} \otimes \ket{\psi_{234}} \): therefore, \( E_{bs}^a = \bar{E}_{bs}^2 \). For the four-qubit system, the expectation value of energy is minimized by the dimerized state \( \bar{0} \). This is not the case for \( s > 1/2 \), where the coupling between \( s_2 \) and \( s_3 \) induces a significant admixture with states of higher \( S \) and \( S' \). Besides, the energy is minimized by the state with \( \{s_2, s_3\} = -s_3 \) \( \{a_0 = B_0 \) and \( \beta_{S+1} = \beta_S = \pi \). We thus conclude that, for all the considered spin values, the inequality \( \langle H_{1234} \rangle < E_{bs}^k \) implies quadripartite entanglement in the four-spin system. The criterion generalizes to \( \langle H \rangle < n_k E_{bs}^k \) for any \( H \) that can be written as the sum of \( n_k \) four-spin Hamiltonians, such as chains of \( 3n_4 + 1 \) spins or rings with \( 3n_4 \).

\textbf{N-partite entanglement} — For larger spin numbers \( N \), the analytic derivations of the functions \( f_M \) and \( g_M \) becomes cumbersome, and a fully numerical approach is preferable. Given a partition of the spin chain in two subsystems, \( A \) and \( B \), consisting of \( N_A \) and \( N_B = N - N_A \) consecutive spins, the Hamiltonian can be written as \( H = H_A + H_B + H_{AB} \), where \( H_A = \sum_{i=1}^{N_A} s_i \cdot s_{i+1} \), \( H_B = \sum_{i=N_A+1}^{N} s_i \cdot s_{i+1} \), and \( H_{AB} = s_{N_A} \cdot s_{N_A+1} \). The energy minima for biseparable states \( \langle \psi \rangle = \langle \psi_A \rangle \otimes \langle \psi_B \rangle \) are:

\[
\begin{align*}
E_{N,A,B}^N &= \min_{\langle \psi_A \rangle, \langle \psi_B \rangle} \left\{ \langle \psi_A | H_A | \psi_A \rangle + \langle \psi_B | H_B | \psi_B \rangle \right\} \\
+ &\quad \langle \psi_A | s_{N_A} | \psi_A \rangle \cdot \langle \psi_B | s_{N_A+1} | \psi_B \rangle, \quad (11)
\end{align*}
\]

We identify the \( z \) direction with that of \( \langle \psi_A | s_{N_A} | \psi_A \rangle \) and define: \( z_A = \langle \psi_A | s_{N_A} | \psi_A \rangle \geq 0 \), \( z_B = \langle \psi_B | s_{N_A+1} | \psi_B \rangle \). Besides, the state \( | z_B \rangle \) that minimizes \( E_{bs}^{N,A,B} \) necessarily has an expectation value \( \langle s_{N_A+1} | z_B \rangle \) antiparallel to \( \bar{z} \) (and thus \( z_B \leq 0 \)): any rotation of the subsystem \( B \) with respect to such orientation would in fact increase \( \langle H_{AB} \rangle \), while leaving unaltered \( \langle H_A + H_B \rangle \). The minimization can now be split into two correlated eigenvalue problems, that consist in finding the ground states of \( H_A(z_B) = H_A + z_B s_{N_A} \) and \( H_B(z_A) = H_B + z_A s_{N_A+1} \). The self-consistent solution of the minimization problem Eq. (11) is thus represented by the state \( \bar{\psi} = | z_B \rangle \otimes | z_A \rangle \) with: \( \bar{z}_A = \langle \psi_A | s_{N_A} | \psi_A \rangle \otimes | z_B \rangle \) and \( \bar{z}_B = | z_B \rangle \otimes s_{N_A} \). The corresponding value of energy is given by

\[
\begin{align*}
\bar{H}_B(\bar{z}_A) = E_A^N(\bar{z}_B) + E_B^N(\bar{z}_A) - \bar{z}_A \bar{z}_B, \quad (12)
\end{align*}
\]

where the last term avoids the double counting of the contribution from \( s_{N_A} \cdot s_{N_A+1} \). The values of the overall minima for biseparable states, given by

\[
\begin{align*}
E_{bs}^N = \min_{N_A,N_B} E_{N,A,B}^N, \quad (13)
\end{align*}
\]

are reported in the right part of Table II for \( N \leq 8 \). For all the considered values of \( s \) and \( N \), the partition with lowest energy minimum is that with \( N_A = 2 \). We note that for even \( N_A \) and \( N_B \), the qubits only present a solution with \( \langle H_{AB} \rangle = 0 \); for \( s > 1/2 \), instead, the minimum corresponds to the additional solution, with finite \( \langle H_{AB} \rangle \). As in the cases of tri- and quadrupartite entanglement, these minima provide a criterion, namely \( \langle H \rangle < n_k E_{bs}^k \), for the detection of \( k \)-partite entanglement in chains and rings with \( n_k(k-1)+1 \) and \( n_k(k-1) \) spins, respectively.

We finally demonstrate the presence of \( N \)-partite entanglement in the ground state of all spin chains with even \( N \).

\textbf{Theorem.} — The ground state \( | \psi_0 \rangle \) of the spin Hamiltonian \( H = \sum_{i=1}^{N-1} s_i \cdot s_{i+1} \), with even \( N \), cannot be written in any biseparable form \( | \psi_{AB} \rangle = | \psi_A \rangle \otimes | \psi_B \rangle \), and is thus \( N \)-partite entangled.

\textbf{Proof.} — According to Marshall’s theorems [23], \( | \psi_0 \rangle \) is a nondegenerate singlet state.

A biseparable state \( | \psi_{AB} \rangle \) can only be a singlet if \( S_x = 0 \) (\( \chi \equiv A,B \)). In fact, one can write \( | \psi_A \rangle \) as a linear superposition of eigenstates of \( S_x^2 \)

\[
| \psi_A \rangle = \sum \langle \psi_A | s_{N_A} \rangle | \psi_A \rangle.
\]

The following inequality applies:

\[
\langle S_x^2 \rangle \geq \sum \langle \psi_A | s_{N_A} \rangle^2 (S_A - S_x)^2 + S_A + S_B \geq \sum \langle \psi_A | s_{N_A} \rangle^2 (S_A + S_B),
\]

where we make use of:

\[
\langle \psi_A | s_{N_A} \rangle \langle \psi_A | s_{N_A} \rangle^* \geq -S_A S_B.
\]

Therefore, \( S_x^2 \)

\[
| \psi_{AB} \rangle = \sum \langle \psi_A | s_{N_A} \rangle | \psi_A \rangle.
\]

The ground state \( | \psi_0 \rangle \) of the spin Hamiltonian \( H = \sum_{i=1}^{N-1} s_i \cdot s_{i+1} \), with even \( N \), cannot be written in any biseparable form \( | \psi_{AB} \rangle = | \psi_A \rangle \otimes | \psi_B \rangle \), and is thus \( N \)-partite entangled.

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corresponding to the partial spin sums $S_k = \sum_{i=1}^{k} s_i$, and $S_A = 0$ implies $S_{N_A-1} = s$. The operator $s_{N_A}$ commutes with all $S_k^2$ with $k \leq N_A - 1$. The matrix elements of the $N_A$-th spin can thus be reduced to those between the states of two spins $s$: $\langle \alpha', S_A', M_A' | s_{N_A} | \alpha, S_A, M_A \rangle = \delta_{\alpha,\alpha'} \langle S_A' | M_A' | S_A, M_A \rangle |0,0\rangle$. The latter matrix element is only finite, and equals $-\eta_s$, for $S_A' = 1$ and $M_A' = 0$; therefore, $s_{N_A} |\psi_A\rangle = -\eta_s \sum M_A |\alpha, 1, 0\rangle$, with $\eta_s = \left[\sum_{m=-s}^{s} m^2\right] / [2s + 1]^{1/2} > 0$. The same procedure can be applied to $B$, resulting in: $s_{N_B+1} |\psi_B\rangle = -\eta_s \sum B |\beta, 1, 0\rangle$. Here $|\psi_B\rangle = \sum B |\beta, S_B = 0, M_B = 0\rangle$, and $\beta$ denotes the quantum numbers $S_1, \ldots, S_{N_B-1}$ corresponding to $S_k = \sum_{i=1}^{k} s_{N+1-i}$. As a result, $|\psi_{AB}\rangle = \eta_s^2 \sum_{\alpha,\beta} D^A_{\alpha,0} D^B_{\beta,0} |\alpha, 1, 0\rangle \otimes |\beta, 1, 0\rangle$ has finite norm, belongs to the subspace $S_A/B = 1$ and $M_{A/B} = 0$, and is thus orthogonal to $|\psi_{AB}\rangle$.

We now show that $|\psi_{AB}\rangle$ coincides with the component of $H|\psi_{AB}\rangle$ with $S_{A/B} = 1$ and $M_{A/B} = 0$. In fact, $(H_A + H_B)|\psi_{AB}\rangle$ belongs to the $S_A/B = 0$ subspace, being $[H_A, S_k^2] = 0$ for $\chi, \chi' = A, B$. The states $s_{N_A+2} \sum \sum |\psi_{AB}\rangle$ belong instead to the subspaces $M_A = -M_B = \pm 1$. Therefore, $H|\psi_{AB}\rangle$ has a finite component $|\psi_{AB}\rangle$, and cannot be an eigenstate of $H$.

We finally consider the case where the spins of the subsystems are not consecutive. In the simplest case, the spins of $A$ are split into two sequences of $N_A$ and $N_A$, consecutive spins, separated by the $N_B$ spins of $B$. If $|\psi_A\rangle = |\psi_{A_1}\rangle \otimes |\psi_{A_2}\rangle$, then this case can be recast into the previous one, by redefining $A' = A_1$ and $B' = B \cup A_2$. If instead $A_1$ and $A_2$ are entangled, then $|\psi_{AB}\rangle$, is degenerate with any $|\psi'_{AB}\rangle$, where $|\psi_A\rangle$ is replaced by a state $|\psi'_{A}\rangle$ that gives the same reduced density matrices $\rho_{A_k}$ for $A_1$ and $A_2$; this is because correlations between uncoupled spins don’t affect $\langle H \rangle$. Therefore, the state of $|\psi_{AB}\rangle$ would be degenerate, which contradicts Marshall’s theorems. The same conclusion can be drawn for any bipartition where $A$ and $B$ don’t consist of consecutive spins, by recursively applying the above argument.

In conclusion, we have developed a simple approach for deriving the energy minima of biseparable states in chains of arbitrary spins $s$. These minima can be used for detecting $k$-partite entanglement in chains with $n_k(k - 1) + 1$ and rings with $n_k(n - 1)$ spins, respectively. This approach has been here applied to spin chains of up to 8 spins $s \leq 5/2$. Finally, we have demonstrated on general grounds that the Heisenberg interaction induces $N$-partite entanglement in the nondegenerate ground state of even-numbered chains with arbitrary $s$. Such entanglement can thus always be detected by using energy as a witness.

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