Energy as a witness of multipartite entanglement in chains of arbitrary spins

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We develop a general approach for deriving the energy minima of biseparable states in chains of arbitrary spins s, and we report numerical results for spin values $s \leqslant 5/2$ (with $N \leqslant 8$). The minima provide a set of threshold values for exchange energy that allow us 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 it 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 of 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 [6–8], 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 [9,10]. Along the same lines, the measurement of collective observables [11] 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 [15,16] using exchange energy as a witness. We develop a general approach for deriving the energy minima $\bar{E}_{\rm bs}^N$ 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 us 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 $n_k(k-1)+1$ spins or rings with $n_k(k-1)$. Analytical expressions of the minima are derived for the simplest cases, while numerical solutions are provided for $s \leqslant 5/2$, 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 a 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.

I. 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 a bound for $H_{123} = \mathbf{s}_1 \cdot \mathbf{s}_2 + \mathbf{s}_2 \cdot \mathbf{s}_3 \equiv H_{12} + H_{23}$, and for a generic biseparable state $|\psi_1\rangle \otimes |\psi_{23}\rangle$:

$$\bar{E}_{\rm bs}^3 = \min_{|\psi_1\rangle,|\psi_{23}\rangle} \{\langle\psi_1|\mathbf{s}_1|\psi_1\rangle \cdot \langle\psi_{23}|\mathbf{s}_2|\psi_{23}\rangle + \langle\psi_{23}|\mathbf{s}_2\cdot\mathbf{s}_3|\psi_{23}\rangle\}. \tag{1}$$

If we identify the direction of $\langle\psi_{23}|\mathbf{s}_2|\psi_{23}\rangle$ with the z axis, the first term in Eq. (1) simplifies to $\langle H_{12}\rangle = \langle\psi_1|s_{1,z}|\psi_1\rangle\langle\psi_{23}|s_{2,z}|\psi_{23}\rangle$, where $\langle\psi_{23}|s_{2,z}|\psi_{23}\rangle \geqslant 0$ 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 $\bar{E}_{\rm bs}^3$ reduces to finding the state $|\psi_{23}\rangle$ that minimizes

$$\langle\psi_{23}|\tilde{H}_{23}|\psi_{23}\rangle \equiv \langle\psi_{23}| - s_1 s_{2,z} + \mathbf{s}_2\cdot\mathbf{s}_3|\psi_{23}\rangle, \tag{2}$$

i.e., the ground state of the two-spin Hamiltonian $\tilde{H}_{23}$. To derive the energy minima, it is convenient to expand $|\psi_{23}\rangle$ in the form

$$|\psi_{23}\rangle = \sum_{M=-s_2-s_3}^{s_2+s_3} \sqrt{P_M} \sum_{S=|M|}^{s_2+s_3} A_S^M |S,M\rangle \equiv \sum_{M=-s_2-s_3}^{s_2+s_3} \sqrt{P_M}\,|\psi_{23}^M\rangle, \tag{3}$$

where $\mathbf{S} = \mathbf{s}_2 + \mathbf{s}_3$ and M is its projection along z. Each real coefficient P_M gives the probability that $\mathbf{S}$ has a z projection M ($\sum_M P_M = 1$). The normalization condition for the complex coefficients $A_S^M = a_S^M e^{i\alpha_M^S}$ reads $\sum_S (a_S^M)^2 = 1$ (with $a_S^M = |A_S^M|$). Given that both the operators $s_{2,z}$ and $\mathbf{s}_2\cdot\mathbf{s}_3$ commute with S_z, the energy expectation value can be written as $\langle\tilde{H}_{23}\rangle = \sum_M P_M E_{\rm bs}^{3,M}$, where

$$E_{\rm bs}^{3,M} = \langle\psi_{23}^M|\tilde{H}_{23}|\psi_{23}^M\rangle \equiv -s_1 f_M(\mathbf{a}^M,\alpha^M) + g_M(\mathbf{a}^M,\alpha^M), \tag{4}$$

with $\mathbf{a}^M = (a_{|M|}^M,\ldots,a_{s_i+s_j}^M)$ and $\alpha^M = (\alpha_{|M|}^M,\ldots,\alpha_{s_i+s_j}^M)$. The energy expectation value is thus given by an average, with probabilities P_M, of functions $E_{\rm bs}^{3,M}$ that depend on disjoint groups of variables $\mathbf{A}^M$, each corresponding to a given M.

TABLE I. Minima $\bar{E}^3_{\rm bs}$ of H_{123} for biseparable states $|\psi_1\rangle \otimes |\psi_{23}\rangle$ and corresponding coefficients $\bar{a}_S$ and $\bar{\alpha}_S$. The ground state energies E_0 of H_{123} are also reported, as well as $\bar{E}_{12} = -sf(\bar{\mathbf{a}},\bar{\alpha})$ and $\bar{E}_{23} = g(\bar{\mathbf{a}},\bar{\alpha})$.

s	$\bar{a}_0$	$\bar{a}_1$	$\bar{a}_2$	$\bar{a}_3$	$\bar{a}_4$	$\bar{a}_5$	$\bar{\alpha}_{S+1} - \bar{\alpha}_S$	$\bar{E}^3_{\rm bs}$	$\bar{E}_{12}$	$\bar{E}_{23}$	E_0
1/2	0.973	0.230					0	−0.8090	−0.1118	−0.6972	−1.0
1	0.858	0.506	0.0839				0	−2.481	−0.7583	−1.722	−3.0
3/2	0.749	0.631	0.198	0.0269			0	−5.162	−1.933	−3.230	−6.0
2	0.671	0.676	0.298	0.0696	0.00819		0	−8.849	−3.601	−5.248	−10.0
5/2	0.612	0.687	0.373	0.120	0.0232	0.00244	0	−13.74	−5.768	−7.771	−15.0

This allows to minimize the terms $E^{3,M}_{\rm bs}$ independently from one another, and to identify the overall minimum with the lowest $\bar{E}^{3,M}_{\rm bs}$:

$$\bar{E}^3_{\rm bs} = \min_M \bar{E}^{3,M}_{\rm bs}(\bar{\mathbf{a}}^M,\bar{\alpha}^M). \tag{5}$$

The dependence of $E^{3,M}_{\rm bs}$ on the variables A^M_S is derived as follows. The first contribution in Eq. (4) is proportional to $f_M = \langle s_{2,z}\rangle = \sum_{S,S'}(A^M_S)^*(A^M_{S'})\langle S,M|s_{2,z}|S',M\rangle$. Here, the matrix element can be expressed in terms of the Clebsch-Gordan coefficients [21]: $\langle S,M|s_{2,z}|S',M\rangle = \sum_{m_2}\langle S,M|m_2,m_3\rangle\langle m_2,m_3|S',M\rangle m_2$ (with $m_3 = M - m_2$). The second contribution in Eq. (4) is instead diagonal in the basis $|S,M\rangle$, and reads $g_M = \langle \mathbf{s}_2 \cdot \mathbf{s}_3\rangle = \sum_S (a^M_S)^2[S(S+1) - s_2(s_2+1) - s_3(s_3+1)]/2$.

To analytically minimize—for $s \leqslant 3/2$—the function $E^{3,M}_{\rm bs}$ subject to the normalization constraints, we apply the method of Lagrange multipliers. The stationary points of the Lagrange function $\Lambda_M(A^M_S,\lambda) = E^{3,M}_{\rm bs} + \lambda[\sum_S (a^M_S)^2 - 1]$ are identified by the equations $\partial\Lambda_M/\partial a^M_S = \partial\Lambda_M/\partial\alpha^M_S = \partial\Lambda_M/\partial\lambda = 0$ for $|M| \leqslant S \leqslant s_2 + s_3$. In all the cases considered below, the lowest minima correspond to $M = 0$: $\bar{E}^3_{\rm bs} = \bar{E}^{3,M=0}_{\rm bs}$. We shall thus refer only to this subspace, and omit the superscripts M from the notation. In addition, 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 [9]. Here we show that such a value actually corresponds to a minimum, and derive the corresponding biseparable state. The dependence of $E^3_{\rm bs}$ on the parameters a_S and α_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 α_S are concerned, $E^3_{\rm bs}$ is minimized by $\bar{\alpha}_1 - \bar{\alpha}_0 = 0$. The remaining conditions give rise to the energy minimum $\bar{E}^3_{\rm bs} = -(1+\sqrt{5})/4$, which coincides with the lower bound derived in Ref. [9]. The corresponding biseparable state is given by

$$\bar{a}_0 = (1/2 + 1/\sqrt{5})^{1/2},\ \bar{a}_1 = (1/2 - 1/\sqrt{5})^{1/2}. \tag{6}$$

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 $\bar{\alpha}_{S+1} - \bar{\alpha}_S = 0$, derived from $\partial\Lambda_M/\partial\alpha_S = 0$, have already been included. The analytic expression of the energy minimum is

$$\bar{E}^3_{\rm bs} = -2/3\{1 + \sqrt{5/2}[\cos(\varphi/3) + \sqrt{3}\sin(\varphi/3)]\}, \tag{7}$$

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

For the spin values $s = 3/2$, 2, and 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 ($\bar{a}_0$) decreases with increasing s, as well as the ratio between the energies of the entangled and unentangled spin pairs ($\bar{E}_{23}/\bar{E}_{12}$). In all cases, the inequality $\langle H_{123}\rangle < \bar{E}^3_{\rm bs}$ implies tripartite entanglement in the three-spin system. The criterion becomes $\langle H\rangle < n_3\bar{E}^3_{\rm bs}$ 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 $2n_3$. Here, the violation of the above inequality implies 3-producibility [9].

II. QUADRIPARTITE ENTANGLEMENT

We consider the expectation values of the four-spin Hamiltonian $H_{1234} = \mathbf{s}_1\cdot\mathbf{s}_2 + \mathbf{s}_2\cdot\mathbf{s}_3 + \mathbf{s}_3\cdot\mathbf{s}_4$, corresponding to the biseparable states $|\psi^4_{22}\rangle = |\psi_{12}\rangle \otimes |\psi_{34}\rangle$ and $|\psi^4_{13}\rangle = |\psi_1\rangle \otimes |\psi_{234}\rangle$. In the former case, we compute

$$\bar{E}^4_{22} = \min_{|\psi_{12}\rangle,|\psi_{34}\rangle}\{\langle\psi_{12}|\mathbf{s}_1\cdot\mathbf{s}_2|\psi_{12}\rangle + \langle\psi_{34}|\mathbf{s}_3\cdot\mathbf{s}_4|\psi_{34}\rangle + \langle\psi_{12}|s_{2,z}|\psi_{12}\rangle\langle\psi_{34}|s_{3,z}|\psi_{34}\rangle\}, \tag{8}$$

where z is defined as the direction of $\langle\psi_{34}|s_{3,z}|\psi_{34}\rangle$. The states $|\psi_{12}\rangle$ and $|\psi_{34}\rangle$ are expanded in the bases $|S = S_{12}, M = M_{12}\rangle$ and $|S' = S_{43}, M' = M_{43}\rangle$, respectively. For $|\psi_{12}\rangle$, we use the expression in Eq. (3), and replace the indices 23 with 21. Similarly, $|\psi_{34}\rangle$ is expressed as $|\psi_{34}\rangle = \sum_{M'}\sqrt{Q_{M'}}\sum_S B^{M'}_{S'}|S',M'\rangle$, with $B^{M'}_{S'} = b^{M'}_{S'}e^{i\beta^{M'}_{S'}}$, $\sum_{M'}Q_{M'} = \sum_{S'}(b^{M'}_{S'})^2 = 1$. The indices 23 in Eq. (3) are replaced here by 34. Being both M and M' good quantum numbers, one can write $E^4_{22} = \sum_M\sum_{M'}P_M Q_{M'}E^{4,MM'}_{22}$, where

$$E^{4,MM'}_{22} = g_M(\mathbf{A}^M) + f_M(\mathbf{A}^M)f_{M'}(\mathbf{B}^{M'}) + g_{M'}(\mathbf{B}^{M'}) \tag{9}$$

and the functions $f_M = \langle s_{2,z}\rangle$ and $g_M = \langle s_{3,z}\rangle$. The energy $E^{4,MM'}_{22}$ is minimized numerically by the conjugate gradient approach as a function of $\mathbf{a}^M$ and $\mathbf{b}^M$, while the minimization with respect to α^M and β^M is straightforward. The minimum $\bar{E}^4_{22}$ is then identified with the lowest $\bar{E}^{4MM'}_{22}$:

$$\bar{E}^4_{22} = \min_{M,M'}\bar{E}^{4,MM'}_{22}(\bar{\mathbf{a}}^M,\bar{\alpha}^M,\bar{\mathbf{b}}^{M'},\bar{\beta}^{M'}). \tag{10}$$

For all values of s, the lowest minima belong to the subspace $M = M' = 0$. The minimum of $\bar{E}^4_{13}$ is instead identified with the ground state energy of the three-spin Hamiltonian $\tilde{H}_{234} = -s_1 s_{2,z} + \mathbf{s}_2\cdot\mathbf{s}_3 + \mathbf{s}_3\cdot\mathbf{s}_4$, which belongs, in all the considered cases, to the subspace with $M = s$. The energy minima and the corresponding states are reported in the left

TABLE II. Left: minima $\bar{E}^4_{22}$ and $\bar{E}^4_{13}$ for biseparable four-spin states $|\psi_{12}\rangle \otimes |\psi_{34}\rangle$ and $|\psi_1\rangle \otimes |\psi_{234}\rangle$, respectively. The states corresponding to the former partition are given by the displayed values of $\bar{a}_S$, and by $\bar{\mathbf{b}}_S = \bar{\mathbf{a}}_S$, $\bar{\alpha}_{S+1} - \bar{\alpha}_S = \pi$, and $\bar{\beta}_{S'+1} - \bar{\beta}_{S'} = 0$. Right: energy minima $\bar{E}^N_{\rm bs}$ of N-spin systems.

s	$\bar{a}_0$	$\bar{a}_1$	$\bar{a}_2$	$\bar{a}_3$	$\bar{a}_4$	$\bar{a}_5$	$\bar{E}^4_{\rm bs} = \bar{E}^4_{22}$	$\bar{E}^4_{13}$	$\bar{E}^5_{\rm bs}$	$\bar{E}^6_{\rm bs}$	$\bar{E}^7_{\rm bs}$	$\bar{E}^8_{\rm bs}$
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

part of Table II. We note that the bipartition $|\psi_{12}\rangle \otimes |\psi_{34}\rangle$ always gives lower minima with respect to $|\psi^4_{13}\rangle = |\psi_1\rangle \otimes |\psi_{234}\rangle$: therefore, $\bar{E}^4_{\rm bs} = \bar{E}^4_{22}$. For the four-qubit system, the expectation value of energy is minimized by the dimerized state [9]. 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'. In addition, the energy is minimized by the state with $\langle s_{2,z}\rangle = -\langle s_{3,z}\rangle$ ($\bar{\mathbf{a}}^0 = \bar{\mathbf{b}}^0$, $\bar{\beta}^0_{S'+1} - \bar{\beta}^0_{S'} = 0$, and $\bar{\alpha}^0_{S+1} - \bar{\alpha}^0_S = \pi$). We thus conclude that, for all the considered spin values, the inequality $\langle H_{1234}\rangle < \bar{E}^4_{\rm bs}$ implies quadripartite entanglement in the four-spin system. The criterion generalizes to $\langle H\rangle < n_4 \bar{E}^4_{\rm bs}$ for any H that can be written as the sum of n_4 four-spin Hamiltonians, such as chains of $3n_4 + 1$ spins or rings with $3n_4$, where the violation of the above inequality implies 4-producibility.

III. *N*-PARTITE ENTANGLEMENT

For larger spin numbers N, the analytic derivation 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 $H_A = \sum_{i=1}^{N_A-1} \mathbf{s}_i \cdot \mathbf{s}_{i+1}$, $H_B = \sum_{i=N_A+1}^{N-1} \mathbf{s}_i \cdot \mathbf{s}_{i+1}$, and $H_{AB} = \mathbf{s}_{N_A} \cdot \mathbf{s}_{N_A+1}$. The energy minima for biseparable states $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$ are

$$\bar{E}^N_{N_A N_B} = \min_{|\psi_A\rangle,|\psi_B\rangle} \{\langle\psi_A|H_A|\psi_A\rangle + \langle\psi_B|H_B|\psi_B\rangle + \langle\psi_A|\mathbf{s}_{N_A}|\psi_A\rangle \cdot \langle\psi_B|\mathbf{s}_{N_A+1}|\psi_B\rangle\}. \quad (11)$$

We identify the z direction with that of $\langle\psi_A|\mathbf{s}_{N_A}|\psi_A\rangle$, and define $z_A \equiv \langle\psi_A|s_{N_A,z}|\psi_A\rangle \geqslant 0$ and $z_B \equiv \langle\psi_B|s_{N_A+1,z}|\psi_B\rangle$. In addition, the state $|\bar{\psi}_B\rangle$ that minimizes $E^{N_A,N_B}_{\rm bs}$ necessarily has an expectation value $\langle\mathbf{s}_{N_A+1}\rangle$ antiparallel to $\hat{\mathbf{z}}$ (and thus $z_B \leqslant 0$): any rotation of the subsystem B with respect to such orientation would in fact increase $\langle H_{AB}\rangle$ while leaving $\langle H_A + H_B\rangle$ unaffected. The minimization can now be split into two correlated eigenvalue problems that consist in finding the ground states of $\tilde{H}_A(z_B) = H_A + z_B s_{N_A,z}$ and $\tilde{H}_B(z_A) = H_B + z_A s_{N_A+1,z}$. The self-consistent solution of the minimization problem Eq. (11) is thus represented by the state $|\bar{\psi}\rangle = |\psi^0_A(\bar{z}_B)\rangle \otimes |\psi^0_B(\bar{z}_A)\rangle$ with

$$\bar{z}_A = \langle\psi^0_A(\bar{z}_B)|s_{N_A,z}|\psi^0_A(\bar{z}_B)\rangle, \quad (12)$$

$$\bar{z}_B = \langle\psi^0_B(\bar{z}_A)|s_{N_A+1,z}|\psi^0_B(\bar{z}_A)\rangle, \quad (13)$$

where $|\psi^0_A(\bar{z}_B)\rangle$ is the ground state of $\tilde{H}_A(\bar{z}_B)$ and $|\psi^0_B(\bar{z}_A)\rangle$ is that of $\tilde{H}_B(\bar{z}_A)$. The corresponding value of energy is given by

$$\bar{E}^N_{N_A N_B} = E^0_A(\bar{z}_B) + E^0_B(\bar{z}_A) - \bar{z}_A \bar{z}_B, \quad (14)$$

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

$$\bar{E}^N_{\rm bs} = \min_{N_A,N_B} \bar{E}^{N_A N_B}_N, \quad (15)$$

are reported in the right part of Table II for $N \leqslant 8$. For all the considered values of s and N, the partition with the 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 tripartite and quadripartite entanglement, these minima provide a criterion, namely $\langle H\rangle < n_k \bar{E}^k_{\rm bs}$, 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.

Theorem. The ground state $|\psi_0\rangle$ of the spin Hamiltonian $H = \sum_{i=1}^{N-1} \mathbf{s}_i \cdot \mathbf{s}_{i+1}$, 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. The same applies to any nondegenerate eigenstate of H.

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 $S_\chi = 0$ ($\chi = A,B$). In fact, one can write $|\psi_\chi\rangle$ as a linear superposition of eigenstates of $\mathbf{S}^2_\chi$: $|\psi_\chi\rangle = \sum_{S_\chi} C^\chi_{S_\chi} |\phi^\chi_{S_\chi}\rangle$. The following inequality applies: $\langle\mathbf{S}^2\rangle \geqslant \sum_{S_A,S_B} |C^A_{S_A} C^B_{S_B}|^2[(S_A - S_B)^2 + S_A + S_B] \geqslant \sum_{S_A,S_B} |C^A_{S_A} C^B_{S_B}|^2(S_A + S_B)$, where we make use of $\langle\phi^A_{S_A}|\mathbf{S}_A|\phi^A_{S_A}\rangle \cdot \langle\phi^B_{S_B}|\mathbf{S}_B|\phi^B_{S_B}\rangle \geqslant -S_A S_B$. Therefore, $\langle\mathbf{S}^2\rangle$ can only vanish if $C^A_{S_A} = \delta_{S_A,0}$ and $C^B_{S_B} = \delta_{S_B,0}$.

We now prove that the state $|\psi_A\rangle \otimes |\psi_B\rangle$, with $S_A = S_B = 0$, cannot be the ground state of H by showing that $H|\psi_{AB}\rangle$ has a component $|\psi^\perp_{AB}\rangle$ which is orthogonal to $|\psi_{AB}\rangle$. To this end, we write $H_{AB} = s_{z,N_A} s_{z,N_A+1} + (s_{+,N_A} s_{-,N_A+1} + \text{H.c.})/2$. We first show that $|\psi^\perp_{AB}\rangle \equiv s_{z,N_A} s_{z,N_A+1} |\psi_{AB}\rangle$ is finite and belongs to the subspace $S_A = S_B = 1$ and $M_A = M_B = 0$. In the partial spin sum basis [21], the state of A reads $|\psi_A\rangle = \sum_\alpha D^A_\alpha |\alpha, S_A, M_A\rangle$, where α denotes the quantum numbers $S_1, \ldots, S_{N_A-1}$ corresponding to the partial spin sums $\mathbf{S}_k \equiv \sum_{i=1}^k \mathbf{s}_k$, and $S_A = 0$ implies $S_{N_A-1} = s$.

The operator $s^z_{N_A}$ commutes with all $\mathbf{S}_k^2$ with $k \leqslant N_A - 1$. The matrix elements of the N_Ath spin can thus be reduced to those between the states of two spins s: $\langle \alpha', S'_A, M'_A | s^z_{N_A} | \alpha, S_A, M_A \rangle = \delta_{\alpha,\alpha'} \langle S'_A, M'_A | s^z_{N_A} | 0,0 \rangle$. The latter matrix element is only finite, and equals $-\eta_s$, for $S'_A = 1$ and $M'_A = 0$; therefore, $s^z_{N_A} |\psi_A\rangle = -\eta_s \sum_\alpha D^A_\alpha |\alpha, 1, 0\rangle$, with $\eta_s = [(\sum_{m=-s}^{s} m^2)/(2s+1)]^{1/2} > 0$. The same procedure can be applied to B, resulting in $s^z_{N_A+1} |\psi_B\rangle = -\eta_s \sum_\beta D^B_\beta |\beta, 1, 0\rangle$. Here $|\psi_B\rangle = \sum_\beta D^B_\beta |\beta, S_B = 0, M_B = 0\rangle$, and β denotes the quantum numbers $S_1, \ldots, S_{N_B - 1}$ corresponding to $\mathbf{S}_k = \sum_{i=1}^{k} \mathbf{s}_{N+1-i}$. As a result, $|\psi^\perp_{AB}\rangle = \eta_s^2 \sum_{\alpha,\beta} D^A_\alpha D^B_\beta |\alpha, 1, 0\rangle \otimes |\beta, 1, 0\rangle$ has finite norm, belongs to the subspace $S_A = S_B = 1$ and $M_A = M_B = 0$, and is thus orthogonal to $|\psi_{AB}\rangle$.

We now show that $|\psi^\perp_{AB}\rangle$ coincides with the component of $H|\psi_{AB}\rangle$ with $S_A = S_B = 1$ and $M_A = M_B = 0$. In fact, $(H_A + H_B)|\psi_{AB}\rangle$ belongs to the $S_A = S_B = 0$ subspace, being $[H_\chi, \mathbf{S}^2_{\chi'}] = 0$ for $\chi, \chi' = A, B$. The states $s^\pm_{N_A} s^\mp_{N_A+1} |\psi_{AB}\rangle$ belong instead to the subspaces $M_A = -M_B = \pm 1$. Therefore, $H|\psi_{AB}\rangle$ has a finite component $|\psi^\perp_{AB}\rangle$, and cannot be an eigenstate of H.

We finally consider the case in which the spins of the subsystems are not consecutive. In the simplest case, the spins of A are split into two sequences of N_{A_1} and N_{A_2} 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 ρ_{A_k} for A_1 and A_2; this is because correlations between uncoupled spins do not 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 do not consist of consecutive spins by recursively applying the above argument. ■

IV. CONCLUSION

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 applied here to spin chains of up to eight spins s, with $s \leqslant 5/2$. 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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