Separability and parity transitions in XYZ spin systems under nonuniform fields

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We examine the existence of completely separable ground states (GS) in finite spin-\(s\) arrays with anisotropic XYZ couplings immersed in a non-uniform magnetic field along one of the principal axes of the coupling. The general conditions for their existence are determined. The separability curve in field space for alternating solutions is then derived, together with simple analytic expressions for the ensuing factorized state and GS energy, valid for any spin and size. It is also shown that such curve corresponds to the fundamental \(S_z\)-parity transition of the GS, present for any spin, in agreement with the breaking of this symmetry by the factorized GS, and that two different types of GS parity diagrams in field space can emerge, according to the relative strength of the couplings. The role of factorization in the magnetization and entanglement of these systems is also analyzed, and analytic expressions for observables at the borders of the factorizing curve are derived. Illustrative examples for spin pairs and chains are as well discussed.

I. INTRODUCTION

Interacting spin chains and arrays constitute paradigmatic many-body quantum systems characterized by strong quantum correlations. They conform an ideal scenario for probing and analyzing entanglement, critical behavior and other nontrivial cooperative phenomena [1][8]. Interest on these systems has been recently stimulated by the advances in quantum control techniques [4][5], which make it possible to simulate finite quantum spin systems with tunable couplings and magnetic fields through different platforms [6], including cold atoms in optical lattices [5][8], trapped ions [6][9][12] and superconducting Josephson junctions [13][15].

The GS of these systems is normally entangled, even if immersed in a finite external magnetic field. However, due to the competition between spin interactions and the external magnetic field, the GS may become *exactly* separable, i.e. a product state, under certain conditions. This remarkable phenomenon occurs at particular finite values and orientations of the magnetic field, denoted as *factorizing fields*. It was first analyzed in [16] for spin chains with antiferromagnetic first neighbor XYZ couplings under a uniform field, and since then studied in different spin models, mostly under uniform magnetic fields [17][31], with a general treatment provided in [22] and [31].

A remarkable aspect of GS factorization is that it corresponds to a GS *entanglement transition*, in which entanglement changes its type and, moreover, reaches full range in its immediate vicinity [18][19][21][24][31].

The case of non transverse factorizing fields in systems with XYZ Heisenberg couplings was discussed in [31], while nonuniform transverse factorizing fields in XY systems were explicitly considered in [21][24] and [32]. On the other hand, GS separability in chains and arrays with XXZ couplings under a non-uniform field along the \(z\) axis was recently examined in [33]. In addition to the fully aligned phases, an exceptional multicritical factorization point where all magnetization plateaus merge was shown to exist [33], for a wide range of nonuniform factorizing field configurations and any spin and size, at which a continuous set of symmetry-breaking factorized GS’s exists. Moreover, under non uniform fields XXZ systems may exhibit novel and nontrivial magnetization diagrams and critical behavior [34].

Motivated by these results our aim here is to examine the GS factorization in finite anisotropic XYZ systems of arbitrary spin under a non uniform field along one of the principal axes (i.e. the \(z\) axis). In contrast with the XXZ case in a similar field, the eigenstates of an XYZ system no longer possess a definite magnetization along \(z\), but still have a definite \(S_z\)-parity \(P_z \propto e^{-i\pi S_z}\). And the magnetization transitions of the XXZ GS become replaced in a finite array by parity transitions. Non-trivial factorization in an XYZ system will require, as will be seen, the breaking of this symmetry, entailing that factorization will emerge at a fundamental GS parity transition arising for any spin. This will lead to a factorization curve in the field space, which will be analytically determined for alternating solutions, where a pair of separable parity breaking GS’s become feasible for any spin \(s\). Special entanglement properties will hold in its immediate vicinity. The GS parity diagram in field space will also exhibit other parity transitions, which depend on the total spin. Two distinct regimes are identified according to the relative strength of the couplings, separated by the critical XZZ case \((J_y = J_z)\) where all parity transition curves, including the factorizing curve, merge at zero field.

The formalism is presented in section II, where analytic results for the factorizing curve and GS are derived, first for spin pairs and then for spin chains and arrays. GS parity diagrams are also discussed. Illustrative results for the XXZ magnetization and entanglement are provided in section III for spin pairs and chains, in order to disclose the different role played by factorization in these systems. Analytic results at the borders of factorization are also determined. Conclusions are finally given in IV.
II. SEPARABILITY IN XYZ SYSTEMS

A. General separability equations

We consider an array of \( n \) spins \( s_i \) interacting through anisotropic XYZ Heisenberg couplings in the presence of a nonuniform external magnetic field along the \( z \) axis. The Hamiltonian reads

\[
H = -\sum_{i,\mu} h^i S^\mu_i - \sum_{i<j} \left( J_{1}^{ij} S^x_i S^x_j + J_{y}^{ij} S^y_i S^y_j + J_{z}^{ij} S^z_i S^z_j \right),
\]

where \( h^i \) and \( S^\mu_i, \mu = x, y, z \), denote the field and spin components at site \( i \) and \( \mu \). \( J_{1}^{ij} \) and \( J_{y}^{ij} \) are the coupling strengths. \( H \) commutes with the global \( S^z \) parity

\[
P_z = \exp[i\pi \sum_i (S^z_i - s_i)],
\]

for any value of the fields or couplings, as \( P_z \) just changes the sign of all \( S^x_i \) and \( S^y_i \). Any nondegenerate eigenstate will then have a definite parity \( P_z = \pm 1 \).

We now examine the possibility of a fully separable exact GS \( |\Theta\rangle \) of \( H \), of the form

\[
|\Theta\rangle = \otimes_{i=1}^n (R_i |\uparrow_i\rangle) = |\theta_1\phi_1, \theta_2\phi_2, \ldots\rangle,
\]

\[
R_i = \exp[-i\phi_i S^z_i] \exp[-i\theta_i S^\mu_i],
\]

where \( |\uparrow_i\rangle \) is the state with maximum spin along the \( z \) axis \( (S^z_i |\uparrow_i\rangle = s_i |\uparrow_i\rangle) \) and \( R_i \) rotates spin \( i \) to direction \( n_i = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i) \). Such GS will break parity symmetry unless \( \sin \theta_i = 0 \quad \forall \, i \), and can then only arise at fields where the GS becomes degenerate, i.e. where a GS parity transition takes place.

The eigenvalue equation \( H |\Theta\rangle = E_{\Theta} |\Theta\rangle \) can be rewritten as \( \otimes_{i=1}^n (R_i |\uparrow_i\rangle) H |\Theta\rangle = E_{\Theta} |\Theta\rangle \), with \( |\Theta\rangle = \otimes_{i=1}^n |\uparrow_i\rangle \) the fully aligned state, which implies replacing all \( S^\mu_i \) in \( H \) by the rotated operators \( S'^\mu_i = R_i S^\mu_i R_i \). We then obtain two sets of equations, which together constitute the necessary and sufficient conditions ensuring that \( |\Theta\rangle \) is an exact eigenstate. The first set comprises the field independent equations

\[
J_{1}^{ij} (\cos \theta_i \cos \phi_j - \cos \theta_j \sin \phi_i \cos \phi_j) = J_{x}^{ij} (\cos \theta_i \cos \phi_j \cos \phi_j - \sin \phi_i \sin \phi_j) + J_{y}^{ij} \sin \theta_i \sin \theta_j,
\]

\[
J_{y}^{ij} (\cos \theta_i \sin \phi_j \cos \phi_j + \cos \phi_i \cos \phi_j \sin \phi_j) = J_{x}^{ij} (\cos \theta_i \cos \phi_j \sin \phi_j + \sin \phi_i \cos \theta_j \cos \phi_j),
\]

(5a)

(5b)

to be satisfied for all coupled pairs \( i, j \), which are also spin independent and cancel all elements of \( H \) connecting \( |\Theta\rangle \) with two-spin excitations (terms \( \propto S^z_i S^z_j \)). The second set contains the field dependent equations, which in the absence of fields along the \( x \) and \( y \) axes become

\[
h^i \sin \theta_i = \sum_{j \neq i} s_j [\cos \theta_j \sin \phi_j J_{x}^{ij} \cos \phi_i \cos \phi_j + J_{y}^{ij} \sin \phi_j] - J_{y}^{ij} \sin \theta_j \cos \theta_j,
\]

(6a)

\[
0 = \sum_{j \neq i} s_j \sin \theta_j [J_{x}^{ij} \sin \phi_j \cos \phi_j - J_{y}^{ij} \cos \phi_j \sin \phi_j] + J_{y}^{ij} \sin \phi_j \cos \phi_j,
\]

(6b)

determine the factorizing fields \( h^i \). They cancel all elements connecting \( |\Theta\rangle \) with single spin excitations and coincide with the mean field equations \( \partial (H)_{\Theta}/\partial \theta_i = 0 \), \( \partial (H)_{\Theta}/\partial \phi_i = 0 \), where \( (H)_{\Theta} = \langle \Theta | H | \Theta \rangle \).

With the replacements \( h^i = s h^i / s_i \), \( J_{1}^{ij} = s h_{ij} / (s_i s_j) \), where \( s > 0 \) (in principle arbitrary) can represent an average spin, Eqs. (5) also become spin-independent at fixed values of \( h^i \) and \( j_{ij}^s \). Therefore, the present factorization is essentially a spin independent phenomenon: If present, for instance, in a spin 1/2 array at fields \( h^i \) and couplings \( j_{ij}^s \), it will also arise in a similar array of arbitrary spins \( s_i \) at each site, at fields \( s h^i / (2 s_i) \) and couplings \( s J_{1}^{ij} / (4 s_i s_j) \). In this sense it is universal.

In what follows we then consider for simplicity a common spin \( s_i = s \quad \forall \, i \) and set

\[
J_{1}^{ij} = j_{ij}^s / s,
\]

such that Eqs. (5)–(6), as well as the scaled energy

\[
\langle H \rangle_{\Theta}/s = -\sum_{i} h^i n_i^z - \sum_{i<j} n_i^z n_j^z,
\]

(7)

(8)

where we used \( \langle S_i \rangle_{\Theta} = s n_i \) are \( s \)-independent at fixed fields \( h^i \) and couplings \( j_{ij}^s \).

B. The case of a spin pair

1. General results

We first consider a single spin-s pair \( i \neq j \), with \( j_{ij}^s = j_{jj}^s \), \( h_{ij}^{(1)} = h_{12} \). Without loss of generality we can choose the \( x, y \) axes such that \( |j_{y}| \leq |j_{x}| \) and set \( j_{x} > 0 \) (its sign can be changed by a rotation of one of the spins around the \( z \) axis). We then seek solutions with \( \phi_1 = \phi_2 = 0 \) and \( \theta_{1(2)} \in (-\pi, \pi) \), such that \( |S_i \rangle_{\Theta} \) lies in the \( x, z \) plane and \( |\Theta\rangle = |\theta_1, \theta_2\rangle \).

Eqs. (5b) and (6b) are then trivially satisfied whereas (5a) and (6a) become

\[
j_y = j_x \cos \theta_1 \cos \theta_2 + j_z \sin \theta_1 \sin \theta_2, \quad (9)
\]

\[
h_1 \sin \theta_1 = j_x \cos \theta_1 \sin \theta_2 - j_z \sin \theta_1 \cos \theta_2, \quad (10)
\]

\[
h_2 \sin \theta_2 = j_x \cos \theta_2 \sin \theta_1 - j_z \cos \theta_2 \cos \theta_1 \cos \theta_2, \quad (11)
\]

Since the system is linear in \( j_y \) and \( h_{12} \), it is first seen that given arbitrary angles \( \theta_{1(2)} \) with \( \sin \theta_{1(2)} \neq 0 \) \[39, unique \] values of \( j_y \) and \( h_{12} \) always exist such that previous equations are satisfied. Using \( (9) - (11) \) it can be shown that these values satisfy the constraints

\[
(h_1 \pm h_2)^2 + (j_y \pm j_z)^2 = (\varepsilon_{\Theta} \pm j_z)^2, \quad (12)
\]

with \( \varepsilon_{\Theta} = E_{\Theta}/s \) the scaled pair energy at factorization:

\[
\varepsilon_{\Theta} = -\sum_{i=1,2} h_i \cos \theta_i - j_x \sin \theta_1 \sin \theta_2 - j_z \cos \theta_1 \cos \theta_2 \quad (13a)
\]

\[
+j_z (\sin^2 \theta_1 + \sin^2 \theta_2 - \sin \theta_1 \sin \theta_2) + j_x \cos \theta_1 \cos \theta_2 \quad (13b)
\]

For \( \varepsilon_{\Theta} \leq |j_z|, \varepsilon_{\Theta} \pm j_z \leq 0 \) and Eq. (12) implies the following constraint on the fields and couplings:
which is the fundamental factorization condition for the GS, as will be shown. It determines the GS factorization curves in the field plane \((h_1, h_2)\), and hence the fundamental GS parity transition arising for any spin \(s\). Eq. 12 also enables to write the pair energy (13) as

\[
\mathcal{E}_\Phi = -\sqrt{(h_1 - h_2)^2 + (j_x + j_y)^2} + \sqrt{(h_1 + h_2)^2 + (j_x - j_y)^2}/2 \Rightarrow (14)
\]

(15a)

\[
= -\frac{h_1^2 + h_2^2 + j_x^2 + j_y^2 - 2j_x}{j_x}, \tag{15b}
\]

where Eq. (14) is assumed to be satisfied (for \(j_z \to 0\), Eq. 14 implies \(h_1h_2 = j_xj_y\) and (15b) approaches (15d)). Angles leading to other signs of \(\varepsilon_\Phi \pm j_z\) imply different signs of the square roots in (14)–(15b) and correspond to crossings of excited states of opposite parity, i.e., to factorization of excited states.

It is also possible to obtain from (9), (11) an expression for \(s_\Phi \) in terms of the couplings and its own field \(h_1:\)

\[
\cos^2 \theta_i = \frac{h_i^2 + j_x^2 - j_y^2}{h_i^2 - j_x^2}, \quad i = 1, 2, \tag{16}
\]

where Eq. (14) is again assumed to be fulfilled. The sign of \(\cos \theta_i\) is such that Eqs. (9)–(11) are satisfied. Note that \((\theta_1, \theta_2)\) and \((\pi - \theta_1, \pi - \theta_2)\) are solutions of (9)–(11) for the same \(j_y\) but opposite fields, while \((\theta_1, \theta_2)\) and \((-\theta_1, -\theta_2)\) are solutions for the same \(j_y\) and the same fields \(h_1(2)\), with the same energy \(\varepsilon_\Phi\), in agreement with parity symmetry \((P_2|\Theta\rangle = | -\Theta\rangle \Rightarrow | -\theta_1, -\theta_2\rangle\). This shows explicitly the degeneracy at factorization. We also remark that for \(j_z > 0\), minimum \(\langle H_\Phi\rangle\) (GS factorization) requires \(\theta_1, \theta_2\) of the same sign (in the interval \((\pi, \pi)\), as seen from (13a).

2. The spin 1/2 case

It can be easily verified that for a spin 1/2 pair, Eq. 14 determines precisely the fields where the GS parity transition takes place: The exact energies of the spin 1/2 pair, obtained from diagonalization, are

\[
E_{\pm}^\pm = \frac{1}{2}[\pm \sqrt{(h_1 + h_2)^2 + (j_x - j_y)^2} - j_z], \tag{17a}
\]

\[
E_{\pm}^- = \frac{1}{2}[\pm \sqrt{(h_1 - h_2)^2 + (j_x + j_y)^2} + j_z], \tag{17b}
\]

where \(E_{\pm}^+\) (\(E_{\pm}^-\)) correspond to the positive (negative) parity eigenstates

\[
|\Psi_{\pm}^\pm\rangle = \cos \gamma_{\nu}^\pm |\uparrow\uparrow\rangle + \sin \gamma_{\nu}^- |\downarrow\downarrow\rangle, \tag{18a}
\]

\[
|\Psi_{\pm}^-\rangle = \cos \gamma_{\nu}^\pm |\uparrow\downarrow\rangle + \sin \gamma_{\nu}^- |\downarrow\uparrow\rangle, \tag{18b}
\]

with \(\tan \gamma_{\nu}^- = -\nu \sqrt{(h_1 \pm h_2)^2 + (j_x \pm j_y)^2 \mp h_z}/j_x\) \((\nu = \pm)\). The lowest energies \(E_{\pm}^\pm\) for each parity then cross when \(E_{\pm}^\pm = E_{\pm}^\mp\), which leads to Eq. (14). And at the crossing, after solving for \(j_z\), the scaled GS energy \(E_{\pm}^\pm/s\) becomes identical with (15). Similarly, crossing of excited opposite parity levels leads to different signs of the square roots in (14), implying \(\varepsilon_{\pm} \neq j_z\), not both negative.

The connection between the entangled definite parity eigenstates (18) and the separable parity breaking eigenstates \(|\pm \Theta\rangle\), with \(| \pm \theta_i \rangle = \cos \theta_i |\uparrow\rangle \pm \sin \theta_i |\downarrow\rangle\) for \(s = 1/2\), is just parity projection:

\[
|\Psi_{\pm}^\pm\rangle = \frac{\langle \Theta | \pm | - \Theta \rangle}{\sqrt{2(1 + |\Theta| - | - \Theta|)}} \tag{19}
\]

Eq. (19) holds only at the GS factorization curve (14), where it can be verified that \(\tan \gamma_{\nu}^\pm = \tan \theta_i \pm \tan \theta_j \pm \frac{\pi}{2}\), with \(\theta_i(2)\) obtained from (16) and fulfilling (9)–(11).

3. The spin \(s\) case

Previous results remain valid for any spin \(s\). Namely, when \(|j_y| < j_x\) and the fields satisfy Eq. (14), a GS parity crossing takes place for any spin \(s\), at which the GS becomes twofold degenerate and a pair of product states \(|\pm \Theta\rangle = |\pm \theta_1, \pm \theta_2\rangle\) become GS’s.

Proof: For fields satisfying Eq. (14), we choose positive angles \(\theta_1(2) \in (0, \pi)\) fulfilling (16) and (9)–(11). The condition \(|j_y| < j_x\) and Eq. (14) ensure that the quotient in (16) is nonnegative and < 1. In such a case, \(|\Theta\rangle = |\theta_1, \theta_2\rangle\) is an exact eigenstate of \(H\), with \(|\theta_i\rangle = R_i|\uparrow\rangle\) given by

\[
|\theta_i\rangle = \sum_{m=-s}^{s} \sqrt{\frac{2s}{2s+m}} \cos^{s+m} \frac{\theta_i}{2} \sin^{s-m} \frac{\theta_i}{2} |m_i\rangle. \tag{20}
\]

Hence, the expansion coefficients of \(|\Theta\rangle\) in the standard product basis \(|m_1m_2\rangle\) \((S_{ij}^x|m_i\rangle = m_i|m_i\rangle\) are all non-zero and of the same sign. Since

\[
\sum_{\mu=x,y} j_{\mu} S_{ij}^{\mu} = \sum_{\nu=\pm} j_{\nu} (S_{ij}^+ S_{ij}^- + S_{ij}^- S_{ij}^+) \tag{21}
\]

where \(S_{ij}^\pm = S_{ij}^x \pm i S_{ij}^y\) and \(j_{\pm} = (j_x \pm j_y)/4\), the non-zero off-diagonal elements of \(H\) in the previous basis are all negative if \(|j_y| < j_x\), implying that a GS \(|\Psi\rangle = \sum_{m_1,m_2} C_{m_1m_2} |m_1m_2\rangle\) with \(C_{m_1m_2} \geq 0 \forall m_1, m_2\) exists, as different signs will not decrease the energy \(\langle \Psi | H | \Psi \rangle\). Therefore, \(|\Theta\rangle\) must be a ground state since it cannot be orthogonal to \(|\Psi\rangle\). The same holds for \(| - \Theta\rangle = P_2|\Theta\rangle\) since \([H, P_2] = 0\), implying GS degeneracy. For such angles (and \(|j_y| < j_x\), \(\varepsilon_{\Phi} \neq j_z\) < in (12), since Eq. (14) was originally fulfilled, implying that \(\varepsilon_{\Phi} = E_{\Phi}/s\) will be given by (15). The connection between the states \(|\pm \Theta\rangle\) and the crossing definite parity GS’s \(|\Psi_{\pm}^\pm\rangle\) will be given again by (19). These arguments can be directly extended to a pair with distinct spins \(s_i \neq s_j\).
curves intersect at the origin.

c) $|\pm\rangle$ and $\varepsilon = -j_x = j_y - j_z$ (Eq. 15). At these points the factored state is uniform ($\theta_1 = \theta_2$).

b) $j_z > j_y$ (bottom right panel): Here the GS has positive parity at zero field and vertices lie at opposite fields

$$h_1 = -h_2 = \pm \sqrt{(j_x - j_y)(j_z + j_y)},$$

(23)

where $\varepsilon = -(j_x + j_y - j_z)$ and $\theta_2 = \pi - \theta_1$ (Eq. 16).

c) $j_z = j_y$ (bottom left panel): In this limit case both curves intersect at the origin $h_{1(2)} = 0$, where all sectors meet. At this point $\varepsilon = -j_x$ and $\theta_1 = \theta_2 = \pm \pi/2$, implying that the factored GS’s $|\pm\rangle$ are here orthogonal for any spin $s$ (they are fully aligned states along the $\pm x$ directions). The parity restored states then become Bell-type states.

The curves asymptote lie at $h_{1(2)} = \pm j_z$ in all cases, since for strong field $h_{1(2)} \to \pm \infty$, Eq. 14 leads to $h_{2(1)} = \pm j_z + j_x j_y/h_{1(2)}$. For $0 < j_z < j_y$ and $|j_y| > j_x$ the separability curves then cross the axes (top right panel in Fig. 1), implying that GS factorization (and thus the GS parity transition) can in this case be achieved with just one field: Setting $h_{2(1)} = 0$ in Eq. 14, we obtain

$$h_{1(2)} = \pm \sqrt{(j_x^2 - j_z^2)(j_y^2 - j_z^2)/j_z} \quad (24)$$

On the other hand, for $j_z < 0 < j_y$, $|h_1| \geq -j_z$, implying that finite fields at both spins are required for factorization in order to overcome the antiferromagnetic $j_z$ coupling. This is also the case for $j_z > j_y > 0$ (ferromagnetic $j_z$ coupling) where $|h_1| \geq \sqrt{j_z^2 - j_z^2}$ along the factorizing curves, as implied by 16.

The positive angles $\theta_1, \theta_2$ determining the separable GS, obtained from 16, are depicted in Fig. 2 as a function of the scaled magnetic field $h_1$ along the right curve of the right panels of Fig. 1 ($j_y = 0.5 j_x$). Dashed vertical lines indicate the asymptote $h_1 = -j_z + j_x = 0.25$ (0.75).

![FIG. 1. The ground state (GS) factorization curves (solid lines) in the field plane ($h_1, h_2$) determined by Eq. 14, for $j_y = j_z/2 > 0$ and different values of $j_x/j_y$. At these curves the GS $S_z$-parity transition takes place. For a spin 1/2 pair, the lighter (darker) colored sectors separated by these curves correspond to positive (negative) GS parity $P_z = +1 (-1)$. The same factorization curves remain, nevertheless, valid for a general spin $s$ pair as well as for a spin chain or lattice.]

![FIG. 2. The angles $\theta_{1(2)}$ which determine the separable GS at factorization, obtained from Eq. 16, as a function of the scaled magnetic field $h_1$ along the right curve of the right panels of Fig. 1 ($j_y = 0.5 j_x$). Dashed vertical lines indicate the asymptote $h_1 = -j_z + j_x = 0.25$ (0.75).]
tions curves in each sector (4s curves in the whole plane) as seen on the left panels of Fig. 3 for $s = 1$. These transitions are reminiscent of the GS magnetization transitions arising in the XXZ limit [7]. For $j_z < j_y < j_x$, the factorization curves determine the last GS parity transition as the fields $(h_1, h_2)$ increase from 0 along the first or third quadrant, as seen on the top left panel.

On the other hand, for $j_x = j_y$ all GS parity transition curves intersect again at the origin (center left), where all GS parity sectors meet. Nevertheless, the GS remains here twofold degenerate for any spin (we recall that at the origin $\theta_1 = \theta_2 = \pm \pi/2$, so that the degenerate factorized GS’s are orthogonal maximally aligned states along the $\pm x$ directions). For $j_z > j_y$ the GS parity diagram becomes more complex (bottom panel). Here the second transition curve crosses the factorization curve (remnant in part of the behavior for $j_z = j_y$) so that the negative parity sector may be located above or below the latter. The behavior for higher spins is analogous and qualitatively similar to that of a spin chain with the same total spin (right panels, see next section).

C. Extension to spin arrays

1. General results

We now consider a general spin-$s$ array with couplings satisfying $|j^{ij}_y| \leq j^{ij}_x$ for all interacting pairs, and analyze the possibility of a product GS $|\Theta\rangle = |\theta_1, \theta_2, \ldots\rangle$ with $\phi_1 = 0 \forall i$. Eqs. (10–11) are to be replaced by

$$j^{ij}_y = j^{ij}_x \cos \theta_i \cos \theta_j + j^{ij}_z \sin \theta_i \sin \theta_j,$$

$$h^i \sin \theta_i = \sum_{j \neq i} j^{ij}_x \cos \theta_i \sin \theta_j - j^{ij}_z \cos \theta_j \sin \theta_i,$$

leading in general to a nonuniform total field $h^i = \sum_j h^{ij}$. The total GS energy at factorization will be

$$E_{\Theta} = s \sum_{i<j} \varepsilon^{ij}_{\Theta},$$

with $\varepsilon^{ij}_{\Theta}$ given by (15) in terms of the partial fields $h^{ij}$, i.e., $\varepsilon^{ij}_{\Theta} = -(j^{ij}_x j^{ij}_y - h^{ij} h^{ji})/j^{ij}_z$.

2. Alternating solutions

We will focus on alternating product eigenstates involving just two angles $\theta_1, \theta_2$, such that all coupled pairs are in the same product state. These states can be exact GS’s in spin chains and square-type lattices with uniform first neighbor couplings under alternating fields.

We start with a one-dimensional spin chain of $n$ spins with couplings

$$j^{ij}_\mu = \delta_{i,j+\pm 1} j_\mu,$$

It is apparent that the previous product GS $|\Theta\rangle = |\theta_1, \theta_2\rangle$ for a single pair turns into an alternating product GS

FIG. 3. GS spin parity phase diagram in the $(h_1, h_2)$ field space for a pair of spins 1 (left) and for a spin 1/2 chain of 8 spins (right), for $j_y = 0.5 j_x$, and three values of $j_z/j_x$. Solid lines depict the factorizing curves (the same as those of Fig. 1) while dashed lines the remaining GS parity transitions. Signs denote the GS parity in each sector, with dark coloured regions indicating negative parity. For $j_z = j_y$ (central panels) all curves and GS parity sectors meet at the origin.
FIG. 4. Examples of spin systems with first neighbor anisotropic XYZ couplings under a non uniform field (schematic representation), which possess an alternating separable GS for any spin s when the indicated fields h_1 and h_2 satisfy Eq. (13): a) Spin pair; b) open chain; c) cyclic chain; d) square lattice; e) ladder with non uniform couplings. Here the factorizing fields are r_1 h_{1/2} (r_2 h_{1/2}) in the lower (upper) row, with r = 2α + β (r’ = 2γ + β).

|(Θ)| = |θ_1, θ_2, ..., θ_i| for the whole chain under an alternating field (Fig. 4 b and c). Eq. (25) then reduces to Eq. (9) for all coupled pairs (i, i ± 1), while (26) leads to

\[ h^i \sin \theta_i = r_i (j_x \cos \theta_i \sin \theta_j - j_x \sin \theta_i \cos \theta_j), \]

(30)

where for i odd (even), θ_i = θ_{1(2)} while θ_j = θ_{2(1)}, and r_i is the number of spins coupled to spin i (coordination number). Eq. (30) is thus equivalent to Eqs. (10)–(11) except for the factor r_i, which implies a rescaling of the factorizing fields h^i:

\[ h^i = r_i h_{1/2}, \]

(31)

for i odd (even), where h_{1/2} are the single pair fields satisfying Eq. (14).

In a cyclic chain (n + 1 = 1, n even) r_i = 2 for all spins, implying alternating factorizing fields (2h_1, 2h_2, 2h_1, ...) (plot c). The same holds in an open chain for inner spins, while for edge spins (i = 1 or n) r_i = 1, implying factorizing fields (h_1, 2h_2, 2h_1, ...) (plot b). Thus, alternating product GS’s are feasible in both cyclic and open chains under alternating fields, provided border field corrections are applied in the open case.

These arguments also hold for 2d square lattices (plot d) in Fig. 4 as well as 3d cubic lattices with first neighbor uniform couplings, again of any size. In these cases a similar alternating product GS (Θ) remains exactly feasible since Eq. (25) reduces to Eq. (9) for all coupled pairs.

The coordination number in the square lattice is r_i = 4 for bulk spins and r_i = 3 (2) for edge (corner) spins (plot d) while in the cubic lattice r_i = 6 for bulk spins and r_i = 5, 4, 3 for side, edge and corner spins respectively. In these cases θ_{1(2)} are the angles at sites (i, j) with i + j even (odd) in the square lattice (i, j = 1, 2, ...), and sites (i, j, k) with i + j + k odd (even) in the cubic lattice.

Thus, if h_{1/2} denote the fields satisfying the original pair factorization equation (14), such that the angles θ_{1/2} can be obtained from Eq. (16), the factorizing fields h^i for alternating product states in such arrays will be r_i h_{1/2}. And the exact GS energy (28) along the factorization curves (14) becomes just

\[ E_Θ = N s \varepsilon_Θ, \quad N = \frac{1}{2} \sum_i r_i, \]

(32)

where ε_Θ is the pair energy (15) and N is the total number of coupling links. For instance, in a 1d cyclic array of n spins (n even), r_i = 2 ∀ i and N = n, whereas in an open chain of n spins (n arbitrary) N = n - 1. On the other hand, in a finite open 2d square lattice of n = m × l spins, N = 2n - m - l, while in open 3d cubic arrays of n = m × l × k spins, N = 3m - ml - mk - lk.

Previous alternating product GS’s remain valid for arrays with nonuniform first neighbor XYZ couplings with fixed anisotropy ratios, i.e.,

\[ J_{ij}^\mu = r_{ij} j_{xy}, \quad \mu = x, y, z, \]

(33)

for first neighbors i, j, since Eq. (25) still reduces to Eq. (9) for all coupled pairs. Assuming r_{ij} > 0 and |j_{xy}| < j_z, the final effect is again just a factor r_i = \sum_{j} r_{ij} in the factorizing fields h^i (Eq. (31)), as (26) reduces to (30) at all sites. This enables, for instance, direction dependent couplings in square-type arrays and lattices (panel e) in Fig. 4. The total GS energy will still be given by Eq. (32) with the present values of r_i.

3. GS parity diagrams and particular cases

The exact GS parity diagram of a spin chain exhibits 2 × ns parity transition curves in the whole field plane h_1, h_2, as seen in the right panels of Fig. 3 resembling those of a spin pair with the same total spin. For j_z < j_y the factorization curve represents the last GS parity transition as the fields h_1, h_2 increase from 0 within the first or third quadrant, with the GS reaching the final P_z = +1 phase beyond this curve (top right panel in Fig. 3). This behavior holds up to the limit case j_z = j_y, where all curves, and hence all GS parity sectors, coalesce at the origin (central right panel). The diagram becomes again more complex for j_z > j_y, with the trend seen for the spin 1 pair becoming more notorious. The negative parity sectors can arise at both sides of the factorization curves (bottom right panel). It should be noticed that the energy splitting between opposite parity states in the
narrow regions between curves are small and rapidly decrease with size. Hence, the factorization curve can be associated with the onset of a cascade of GS parity transitions, which in a large system corresponds to the onset of GS quasi degeneracy.

We also remark that the factorization equation (14) generalizes separability equations for spin chains and arrays obtained for particular more symmetric cases, unifying them in a single equation. For example, in the case of a uniform factorizing field $h_1 = h_2 = h$, feasible for $j_z < j_y$, Eq. (14) leads to the field (22), which coincides with the known result for this case [21][26], with Eq. (16) implying $\cos \theta = \sqrt{(j_y-j_z)/(j_x-j_z)}$.

On the other hand, if $j_z = 0$ (XY case) Eq. (14) becomes an hyperbola in the field plane $h_1, h_2$, namely

$$h_1 h_2 = j_x j_y \quad (j_z = 0),$$

in agreement with the results of [20][32] for chains in an alternating field. And in the XXZ limit $j_y \to j_x$, Eq. (14) reduces to the two hyperbola branches

$$(h_1 \pm j_z)(h_2 \pm j_z) = j^2, \quad (j_x = j_y)$$

where the $+$ $-$ sign holds for $h_1 + h_2 > 0 (< 0)$. These hyperbolas are precisely those defining the fully aligned phases ($S_i^z = s$ or $-s \forall i$) in the XXZ system under a nonuniform alternating field [33]. Note that in this limit Eq. (16) leads to $\cos^2 \theta_i \to 1$, i.e., $\theta_i \to 0$ or $\pi$. Finally, if $j_z > j_y$ and $h_1 = -h_2 = h$, Eq. (14) reduces to (23), which in the XXZ limit $j_y = j_x$ coincides with the factorizing field $h = \pm \sqrt{j^2 - j_z^2}$ that determines the multicritical point present in XXZ systems [33][34].

An important final remark is that the present factorization offers the possibility to “extract” a separable nondegenerate GS just by applying an additional non uniform field $h_2$, parallel to the spins alignment directions $\mathbf{n}_i$ of one of the factorized GS’s. This field will remove the GS degeneracy and lower the chosen product state energy by an amount $-s \sum_i h_2^i$ (it will remain an exact GS for any strength $|h_2^i|$, enabling an arbitrarily large gap with the first excited state.

### III. ENTANGLEMENT AND MAGNETIZATION

#### A. Expressions at factorization

As the factorization curve is approached in the field plane $(h_1, h_2)$, the side-limits of physical observables and entanglement measures will be determined by the parity restored GS’s [19], i.e. $|\Psi^\pm\rangle = \frac{|\Theta_j\rangle \Psi_{ji} + |\Theta_k\rangle \Psi_{kj}}{\sqrt{2(1 \pm (-1)^\Theta)}}$, since the exact GS possesses definite parity in the immediate vicinity. These states are entangled and lead to critical entanglement properties [21], significant in small systems.

The reduced state of a single spin $i$ in the states $|\Psi^\pm\rangle$ is given by

$$\rho_{ij}^\pm = \frac{|\Theta_j\rangle\langle\Theta_j| + |\Theta_k\rangle\langle\Theta_k| + \gamma_{ij}(|\Theta_j\rangle\langle\Theta_k| + |\Theta_k\rangle\langle\Theta_j|)}{2(1 \pm (-1)^\Theta)}$$

where $(-\Theta) = \prod_i \cos^2 \theta_i$ is the overlap of the two factorized GS’s and $\gamma_{ij} = \prod_{j \neq i} \cos^2 \theta_j = (-\Theta)/\cos^2 \theta_i$ is the complementary overlap. Thus, for any $s$, $\rho_{ij}^\pm$ is always a rank 2 mixed state with two non-zero eigenvalues

$$p_{ij}^\pm = \frac{(1 + \nu \cos^2 \theta_i)(1 \pm \nu \gamma_{ij})}{2(1 \pm (-1)^\Theta)}, \quad \nu = \pm 1,$$

with $p_{ij}^+ + p_{ij}^- = 1$. The ensuing single spin magnetization $\langle S_i \rangle = \text{Tr} \rho_{ij}^+ S_i$, which in a definite parity state always points along $z$ (Tr$\rho_{ij}^+ S_i^\mu = 0$ for $\mu = x, y$), is

$$\langle S_i \rangle = \text{Tr} \rho_{ij}^+ S_i^z = \frac{\cos \theta_i (1 \pm \gamma_{ij} \cos^2 2 \theta_i)}{1 \pm (-1)^\Theta}.$$  

This result leads to a magnetization step at the parity transition, visible for small sizes and spin. If $(-\Theta)$ and $\gamma_{ij}$ are neglected, we obviously obtain $\langle S_i \rangle = s \cos \theta_i$.

The entanglement of spin $i$ with the rest of the chain can be conveniently measured through the linear entropy $S_2(\rho_i) = 2(1 - \text{Tr} \rho_{ij}^2)$, which becomes

$$S_2(\rho_{ij}^\pm) = 4 p_{ij}^+ p_{ij}^- = \frac{(1 - \cos^4 \theta_i)(1 - \gamma_{ij}^2)}{(1 \pm (-1)^\Theta)^2}.$$  

For $s = 1/2$, the entropy [39] and the magnetization [38] are directly related: In this case Eq. (36) becomes diagonal in the standard basis $\{|0\rangle = |\uparrow_i\rangle, |1\rangle = |\downarrow_i\rangle\}$, i.e. $\rho_{ij}^+ = p_{ij}^+ |0\rangle\langle 0| + p_{ij}^- |1\rangle\langle 1|$, and hence $\langle S_i \rangle = p_{ij}^+ - p_{ij}^-$, implying

$$S_2(\rho_{ij}^\pm) = 1 - 4(S_i^\pm)^2 \quad (s = 1/2).$$  

Thus, zero local magnetization is associated with maximum spin-rest entanglement. Eq. (40) actually holds for any state $|\Psi^\pm\rangle$ with definite party $P_z$ whenever $s_i = 1/2$.

On the other hand, the reduced state $\rho_{ij} = \text{Tr}_{k \neq ij} |\Psi^\pm\rangle\langle \Psi^\pm|$ of two spins $i \neq j$ is

$$\rho_{ij}^\pm = \frac{|\Theta_{ij}\rangle \Theta_{ij} + |\Theta_{ij}\rangle \Theta_{ij} + \gamma_{ij} (|\Theta_{ij}\rangle \Theta_{ij} + |\Theta_{ij}\rangle \Theta_{ij})}{2(1 \pm (-1)^\Theta)},$$

where $|\Theta_{ij}\rangle = |\theta_i, \theta_j\rangle$ and $\gamma_{ij} = \prod_{i \neq j} \cos^2 \theta_k$. It is again a rank 2 mixed state with eigenvalues similar to [37] and [39] ($\gamma_{ij} \to \gamma_{ij}$, cos $^2 \theta_i \to \cos^2 \theta_i$, cos $^2 \theta_j$). Its quadratic entropy, measuring the entanglement of the pair with the rest of the chain, is then given by an expression similar to [39]. Analogous expressions hold for reduced states of any group of spins [21].

A remarkable property of the pair state [41] is that it depends on the angles $\theta_i$ and $\theta_j$ but not on the actual distance between the spins. Hence, the entanglement between spins $i$ and $j$ in the state [41], though weak, will be independent of the spin separation for fixed angles.
\[ C(\rho_{ij}^\pm) = \gamma_{ij} \sqrt{1 \cos^2 \theta_i (1 \cos^2 \theta_j)} \frac{1 \pm (-\Theta \theta)}{1 \pm \Theta \theta}, \]  

which is of parallel (antiparallel) type \cite{[19]} for positive (negative) parity, with \( C(\rho_{ij}^+ \geq C(\rho_{ij}^-). \) It is thus verified to be independent of the separation, being determined just by the angles \( \theta_i, \theta_j \) and the complementary overlap \( \gamma_{ij}. \) For an alternating state [\( \Theta \)], just three concurrences are then obtained at factorization: \( C_{11} \) and \( C_{22} \) for \( \theta_i = \theta_j = \theta_1 \) or \( \theta_2 \) and \( C_{12} \) for \( \theta_i = \theta_1, \theta_j = \theta_2, \) irrespective of the actual distance between the spins. Pairwise entanglement then reaches full range at the factorizing curve, although it becomes rapidly small as size increases due to the factor \( \gamma_{ij}, \) in agreement with monogamy \cite{[35]}. We finally note that if the whole system reduces to a single spin-s pair, Eqs. \( \text{(45)} \) and \( \text{(42)} \) become

\[ \langle S_i^z \rangle = s \cos \theta_s \cos^2 \theta_j \cos^2 \theta_j, \]  

\[ C(\rho_{ij}^\pm) = \sqrt{\cos^2 \theta_i (1 - \cos^4 \theta_j)} / (1 \pm \Theta \theta_j), \]  

with \( \rho_{ij}^\pm \) obviously isospectral since \( \rho_{ij}^\pm \) is pure. In this case the concurrence \( \text{(42)} \) reduces to the square root of the linear entropy \( \langle \text{Eq. (39)} \rangle, \) in agreement with the general result for pure two-qubit states \( \text{[37]} \). For \( s = 1/2 \) Eq. \( \text{(40)} \) is again verified. These expression can be directly expressed in terms of the factorizing fields and coupling strengths through Eq. \( \text{(16)} \).

**B. Results**

We now show results for the GS magnetization and entanglement in some selected spin pairs and chains, in order to visualize the role of the factorizing transition.

Fig. 5 depicts the total GS magnetization \( M = \langle S_i^z + S_j^z \rangle \) and concurrence \( C(\rho_{12}) \) of a spin 1/2 pair. The negative parity sectors coincide in this case exactly with the zero magnetization plateau, as is apparent from Eqs. \( \text{(18)} \) and also \( \text{(43)} \) \( \langle S_i^z \rangle = \langle S_j^z \rangle - \). For \( j_z < j_y \) (top left), we see that the positive parity sectors are also associated with approximate magnetization plateaus, with the factorizing curves coinciding with their borders. On the other hand, for \( j_z > j_y \) (top right) the magnetization in the positive parity sector evolves continuously from maximum (1) to minimum (-1).

The exact concurrence \( C(\rho_{12}) \) is in this case \( | \sin 2 \gamma_{i,j}^\pm | \), where \( \gamma_{i,j}^\pm \) are the angles in the states \( \text{[18]} \). It is larger for negative parity when \( j_z < j_y \) (bottom left panel), saturating in this sector for \( h_1 = h_2 \), where \( C(\rho_{12}) = 1 \).

FIG. 5. Ground state magnetization (top) and entanglement (bottom), measured through the concurrence, of a spin 1/2 pair as a function of the scaled magnetic fields \( h_1, h_2 \). The XYZ couplings are \( j_x = 0.5 \) and \( j_y = 0.25 \). The entanglement then reaches full range at the factorizing curve, although it becomes rapidly small as size increases due to the factor \( \gamma_{ij} \), in agreement with monogamy \cite{[35]}. The exact concurrences of first, second and third neighbors are depicted in Fig. 8. Now the values at

\( (\gamma_{i,j}^\pm = \pi/4). \) In contrast, for \( j_z > j_y \) the maximum value is attained along the \( h_1 = h_2 \) line in the positive parity sector, where again \( C(\rho_{12}) = 1 \). Note that for \( s = 1/2 \) Eqs. \( \text{[13]} - \text{[14]} \) lead to the values (side-limits) \( M_{\pm} = \left\{ \begin{array}{ll} \cos \theta_1 \cos \theta_2 & 1 + \cos \theta_1 \cos \theta_2, \\ 0 & 1 - \cos \theta_1 \cos \theta_2, \end{array} \right. \) at the factorizing curves, with \( \theta_{1,2} \) determined by \( \Theta \). For \( j_z < j_y \), it is then verified that \( C_{-} = 1 \) when \( h_1 = h_2 \) \( (\theta_1 = \theta_2) \) and \( C_{+} = 1 \) when \( h_1 = -h_2 \) \( (\theta_1 = \pi - \theta_2) \).

Results for the spin 1 pair are shown in Fig. 6. In agreement with the parity diagrams of the left panels in Fig. 3, the plots show now four steps and five approximate plateaus, with the factorization curves determining one of the steps (the last one for \( j_z < j_y \) when viewed from the origin). The discontinuities at the factorization curve are now smaller due to the decreased overlap \( -\Theta \Theta \), and the (approximate) zero magnetization plateau \( M \) is now not strictly constant in any sector) corresponds to the first even parity sector. Results are otherwise similar to the previous case. We have measured the pair entanglement through the square root of the linear entropy, \( C = \sqrt{S_2(\rho_i)}, \) such that the values at the border of the factorization are given by Eq. \( \text{(41)} \).

Finally, Figs. 7–8 depict results for a cyclic spin 1/2 chain of \( n = 8 \) spins. The magnetization plots (Fig. 7) are similar to those of previous figures. The steps associated with the parity transitions of the right panels in Fig. 3 are very small due to the small overlap. Accordingly, the factorization curves are now very close since results from the states \( |\Psi^{\pm} \rangle \) (Eq. \( \text{(41)} \)) become almost coincident.

The corresponding concurrences of first, second and third neighbors are depicted in Fig. 8. Now the values at
FIG. 6. Ground state magnetization (top) and entanglement (bottom), measured through \( C = \sqrt{\text{Tr}(\rho_i^2)} \), for a spin 1 pair as a function of the scaled magnetic fields \( h_i/j_x \) for \( j_y/j_x = 0.5 \) and \( j_z/j_x = 0.25 \) (left) and 0.75 (right). Details are similar to those of Fig. 5.

FIG. 7. Ground state magnetization for a spin 1/2 cyclic chain of 8 spins and XYZ Heisenberg couplings with \( j_y/j_x = 0.5 \) and \( j_z/j_x = 0.25 \) (left) and 0.75 (right), for the same chain of Fig. 7, as a function of the scaled magnetic fields \( h_i/j_x \). Solid lines depict the magnetization at the factorization curves.

FIG. 8. Ground state pairwise concurrence for first (top), second (center) and third (bottom) neighbors for \( j_y/j_x = 0.5 \) and \( j_z/j_x = 0.25 \) (left) and 0.75 (right), for the same chain of Fig. 7, as a function of the scaled magnetic fields \( h_i/j_x \). Solid lines depict the side-limits at the factorizing fields.

IV. CONCLUSIONS

We have analyzed GS factorization in finite spin arrays of arbitrary spin with anisotropic XYZ couplings under nonuniform transverse magnetic fields. We have shown that it is essentially a spin-independent phenomenon arising at a fundamental GS parity transition present for any spin, where the GS becomes two-fold degenerate and a pair of parity breaking product GS’s become exactly feasible. Starting with the case of a spin pair, the equation for the factorizing fields was derived, together with simple analytic expressions for the GS energy and the parameters of the factorized GS. These results directly imply the existence of alternating product GS’s in spin chains and square-type arrays with first neighbor XYZ couplings under essentially alternating factorizing fields with border corrections, which satisfy the same equation when adequately scaled.

We have also determined the GS parity diagrams in field space. They show a cascade of \( 2 \times ns \) parity transition curves, the “first” one corresponding to the factorization curve. Eq. (14) actually implies two different types of GS parity diagrams, according to the ratio of the coupling strengths, with the XZZ case representing an intermediate critical case where all GS parity transition curves intersect at zero field.
tion and their relation with factorization were also analyzed. The factorization curves also represent an entanglement transition and lead to critical entanglement properties in their immediate vicinity. Analytic expressions for these limits were provided.

In summary, the present results unveil new features of the factorization phenomenon in finite XYZ systems under nonuniform fields and their relation with parity symmetry. Factorization enables the knowledge of the exact GS of these strongly correlated systems at least at certain curves in field space, allowing insights into the magnetic properties in their immediate vicinity. Analytic expressions for these limits were provided.

The factorization curves also represent an useful mean for testing and extending the present results. The increasing possibilities of simulating spin systems with tunable couplings and fields through different platforms could provide a useful mean for testing and extending the present results.

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