Generalized mean field description of entanglement in dimerized spin systems

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We discuss a generalized self-consistent mean field (MF) treatment, based on the selection of an arbitrary subset of operators for representing the system density matrix, and its application to the problem of entanglement evaluation in composite quantum systems. As a specific example, we examine in detail a pair MF approach to the ground state (GS) of dimerized spin 1/2 systems with anisotropic ferromagnetic-type XY and XYZ couplings in a transverse field, including chains and arrays with first neighbor and also longer range couplings. The approach is fully analytic and able to capture the main features of the GS of these systems, in contrast with the conventional single spin MF. Its phase diagram differs significantly from that of the latter, exhibiting ($S_z$) parity breaking just in a finite field window if the coupling between pairs is sufficiently weak, together with a fully dimerized phase below this window and a partially aligned phase above it. It is then shown that through symmetry restoration, the approach is able to correctly predict not only the concurrence of a pair, but also its entanglement with the rest of the chain, which shows a pronounced peak in the parity breaking window. Perturbative corrections allow to reproduce more subtle observables like the entanglement between weakly coupled spins and the low lying energy spectrum. All predictions are tested against exact results for finite systems.

PACS numbers: 03.65.Ud,03.67.Mn,75.10.Jm,64.70.Tg

I. INTRODUCTION

The analysis of correlations and entanglement in interacting quantum many body systems has attracted strong attention in recent years, motivated by their deep implications for quantum information processing and transmission, the impressive advances in techniques for controlling and measuring quantum systems and the new perspective they provide for the analysis of quantum phase transitions. While the conventional mean field (MF) approximations provide a basic starting point for studying such systems over a broad range of the pertinent control parameters, they are not directly suitable for the description of entanglement, since they are based on completely factorized states. More sophisticated treatments have been developed to include and compute quantum correlations, like for instance density matrix renormalization group (DMRG) techniques, matrix product states and tensor network methods, variational valence bond based approximations, quantum Monte Carlo calculations, and inclusion of static and quantum fluctuations around MF. In addition, non-conventional MF approaches, able to intrinsically include some essential correlations, have also been proposed and recently improved and revisited, which start from the so-called cluster MF approach, also known as BPW (Bethe-Peierls-Weiss) approximation. The essential point in these schemes is the consideration of composite sites containing more than one “body” as the basic independent units. Their application to specific spin systems has shown their capability for determining phase diagrams and critical temperatures, as well as for describing the main features of observables such as magnetization and susceptibility. Their ability to predict entanglement measures has so far not been investigated.

The aim of this work is to investigate a general self-consistent variational MF treatment, based on the selection of an arbitrary subset of operators for representing the system density matrix, and its potential for describing basic entanglement measures in spin systems. The approach can be applied at both zero or finite temperatures and contains as particular cases the conventional as well as the cluster-type MF approaches. In contrast with other variational treatments, the generalized MF scheme does not require an explicit ansatz for the approximate GS, as the latter is naturally determined by the self-consistency relations according to the chosen set of operators. The scheme may be also used as a convenient starting point for more sophisticated treatments. We will examine in particular its capability for describing entanglement, both within the defined units as well as between them, the latter emerging through symmetry restoration or perturbative corrections.

As a specific example, we will consider a pair MF approximation to the ground state (GS) of dimerized spin 1/2 systems with anisotropic XY or XYZ couplings in a transverse field. In order to test its accuracy, we first examine the case of dimerized XY chains with first neighbor couplings, where the exact results for any size can be obtained through the Jordan-Wigner fermionization. We then examine dimerized chains with longer range couplings, dimer lattices and dimerized XYZ systems, where exact results for finite samples were obtained by numerical diagonalization. Dimerized systems are of great interest in both condensed matter physics and quantum information, and can be realized in different ways, including recently cold atoms trapped in optical lattice. Spin 1/2 systems have the additional advantage of permitting a direct computation of the pairwise entanglement through the concurrence.
the latter, the pair MF approach is able to provide a reliable yet still analytic and simple description of dimerized arrays. Its phase diagram differs significantly from that of the conventional MF, and clearly identifies, for a wide range of systems, a fully dimerized phase for weak fields, a partially aligned phase for strong fields and an intermediate $S_z$-parity breaking degenerate phase. It then predicts, in particular, the two transitions exhibited by the GS of the dimerized XY chain for increasing fields\cite{Paulo}, providing a clear approximate picture of the GS in each phase. The approach also leads to a reduced pair density which correctly describes not only the internal entanglement of the pair, but also (through symmetry restoration) its entanglement with the rest of the system, which shows a prominent peak precisely in the parity breaking sector. By means of simple perturbative corrections, the approach can predict the tails of this entanglement between weakly coupled spins and the low lying energy spectrum. 

The formalism is described in sec. II while the application to dimerized XY and XY Z systems is developed in sec. III with the exact analytic solution to the approach can predict the tails of this entanglement discussed in the Appendix. Conclusions are given in IV.

II. FORMALISM

A. General self-consistent approximation

The mixed state $\rho$ of a system at temperature $T = 1/k\beta$ described by a Hamiltonian $H$, minimizes the free energy functional $F (\rho) = \langle H \rangle_\rho - TS (\rho)$, where $\langle H \rangle_\rho = \text{Tr} \rho H$ and $S (\rho) = -k \text{Tr} \rho \ln \rho$ is the entropy. One can then formulate a general variational approximation to $\rho$ based on the trial mixed state

$$\rho_h = \exp[-\beta h]/Z_h, \quad h = \sum_i \lambda_i O_i,$$

where $Z_h = \text{Tr} \exp[-\beta h]$ and $\{O_i, \ i = 1, \ldots, m\}$ is an arbitrary set of linearly independent operators, with $\lambda_i$ parameters determined through the minimization of $F (\rho_h)$. Considering the averages $\langle O_i \rangle \equiv \text{Tr} \rho_h O_i$, functions of the $\lambda_i$’s, as the independent parameters, the equations

$$\frac{\partial F (\rho_h)}{\partial \langle O_i \rangle} = 0 \quad \text{lead to} \quad \lambda_i = \frac{\partial H}{\partial \langle O_i \rangle},$$

hence, to the self-consistent approximate Hamiltonian

$$h = \sum_i \frac{\partial H}{\partial \langle O_i \rangle} O_i,$$

where $\langle H \rangle = \text{Tr} \rho_h H$. If the $O_i$’s form a complete set, $H$ is a linear combination of them and Eq. (2) leads to $h = H$. Otherwise, $\langle H \rangle$ will in general be a non-linear function of the $\langle O_i \rangle$’s and the $\lambda_i$’s, leading to a non-linear set of equations for the $\lambda_i$’s. While the basic MF approximations are obtained when the $O_i$’s are restricted to one-body operators and traces are taken in the grand canonical ensemble (with $H \rightarrow H - \mu N$), Eq. (3) holds for any restricted set, which may include some two-body (or in general $n$-body) operators, and for traces taken in any subspace $S$ invariant under $H$ and all $O_i$'s.

Here we will apply this general scheme to a composite system formed by $N$ distinguishable subsystems, such as an array of spins $s_i$ located at different sites, where the total Hilbert space is $\otimes_{1 \leq i \leq S_i}$, with $S_i$ that of subsystem $i$. We will consider Hamiltonians containing local terms and two-body couplings,

$$H = \sum_i B_\mu^i O_i^\mu - \frac{1}{2} \sum_{i \neq j} J_i^{\mu \nu} O_i^\mu O_j^\nu,$$

where $O_i^\mu$ are local operators pertaining to subsystem $i$ ($\langle O_i^\mu, O_j^\nu \rangle = 0$ if $i \neq j$) and sum over repeated labels $\mu, \nu$ is implied. The standard MF arises when the $O_i$’s in Eq. (3) are restricted to local operators $O_i^\mu$, i.e., when a “site” is identified with a single subsystem $i$. The present scheme enables, however, to consider as well composite sites $C_k$, such as pairs or clusters of spins in a spin system, where products $O_i^\mu O_j^\nu$ for sites $i, j$ in the same cluster are also included within the operators $O_i$ of Eq. (3). This is convenient when such pairs or clusters are internally strongly coupled but interact only weakly between them. The ensuing self-consistent scheme will treat the internal couplings exactly, leaving the MF for the weak couplings.

In this approach, $h = \sum_k h_k$, with $h_k$ local in $C_k$, such that $\rho_h = \otimes_k \rho_k$, with $\rho_k = \exp[-\beta h_k]/Z_{h_k}$. Hence,

$$\langle H \rangle = \sum_{k, i \in C_k} [B_{\mu i}^k (O_i^\mu) - \frac{1}{2} \sum_{j \in C_k} J_{ij}^{\mu \nu} (O_i^\nu O_j^\mu - \frac{1}{2} \sum_{j \notin C_k} J_{ij}^{\mu \nu} O_i^\mu O_j^\nu)],$$

and Eq. (4) leads to

$$h_k = \sum_{i \in C_k} [B_{\mu i}^k (O_i^\mu) - \frac{1}{2} \sum_{j \notin C_k} J_{ij}^{\mu \nu} (O_i^\nu O_j^\mu - \frac{1}{2} \sum_{j \notin C_k} J_{ij}^{\mu \nu} O_i^\mu O_j^\nu)],$$

which contains the exact internal two-body terms, as opposed to the standard MF. Eq. (5) implies the self-consistent conditions

$$\langle O_i^\mu \rangle = \text{Tr} \rho_k O_i^\mu, \quad i \in C_k,$$

to be fulfilled for all $C_k$, which can be solved, for instance, iteratively, after starting from an initial guess for the $\langle O_i^\mu \rangle$’s or the associated parameters $\lambda_i^\mu$. We will denote this approach as generalized MF (GMF). Eq. (6) can now be rewritten as

$$H = \langle H \rangle + \sum_k [h_k - \langle h_k \rangle - \frac{1}{2} \sum_{i \in C_k, j \notin C_k} J_{ij}^{\mu \nu} (O_i^\nu - \langle O_i^\nu \rangle) (O_j^\mu - \langle O_j^\mu \rangle)],$$

where the last term is the residual interaction.

For $T \rightarrow 0$, $\rho_k \rightarrow |0_k\rangle \langle 0_k|$, with $|0_k\rangle$ the GS of $h_k$. The present scheme will then lead in this limit to the state

$$|0_h\rangle = \otimes_k |0_k\rangle,$$

which minimizes $\langle H \rangle \equiv \langle \Psi | H | \Psi \rangle$ among all cluster product states $|\Psi\rangle = \otimes_k |\psi_k\rangle$. Let us remark that an explicit
ansatz for the states \( |0_k\rangle \) is not required, since they can be obtained as the GS of \( h_k \), Eq. (5), in each iteration. Nonetheless, in certain cases (see sec. III) the explicit form of \( |0_k\rangle \) may become apparent from the form of \( h_k \) and a direct minimization of \( \langle H \rangle \) becomes feasible.

B. Perturbative corrections and symmetry restoration

While in-cluster correlations are already described by \( \rho_k \) or \( |0_k\rangle \), those between clusters can in principle be estimated through perturbative corrections. At \( T = 0 \), it follows from Eq. (6) that \( H \) will connect \( |0_k\rangle \) just with two-cluster excitations \( |n_k\rangle |n_k\rangle \), \( k \neq k' \), \( nn' \neq 0 \), where \( |n_k\rangle \) are the eigenstates of \( h_k \) (\( h_k |n_k\rangle = \varepsilon_{n_k} |n_k\rangle \)). Consequently, first order (in the residual interaction) corrections will lead to the perturbed GS

\[
|0_H^1\rangle \propto |0_k\rangle + \sum_{k < k', n, n'} \alpha_{kn, k'n'} |n_k\rangle |n_{k'}\rangle ,
\]

(9)

which contains just two-cluster excitations.

For instance, the reduced state of cluster \( k \) derived from \( |0_H\rangle \) is (\( \tilde{k} \) denotes the complementary system)

\[
\rho_k = \text{Tr}_k|0_H\rangle \langle 0_H| \propto |0_k\rangle \langle 0_k| + \sum_{\mu, m} (\alpha \alpha^\dagger)_{kn, km} |n_k\rangle \langle m_k| ,
\]

(11)

which is a \textit{mixed} state. Its entropy \( S(\rho_k) \) represents the entanglement of the cluster with the rest of the system.

Beyond the weak coupling limit, the actual potential of the GMF lies in the possibility of breaking some essential symmetry of \( H \), which will enable it to describe non-perturbative coupling effects between the composite sites. We will be here concerned with a discrete broken symmetry, namely spin parity symmetry \( P_z \) (see next section), such that GMF will yield in some sectors a pair of parity breaking degenerate solutions \( h_{\pm} \), with \( h_{-} = h_{+} \). We can then construct from the parity breaking GS \( |0_{h_{+}}\rangle = \otimes_k |0_{k+}\rangle \) and \( |0_{h_{-}}\rangle = P_{\tilde{k}} |0_{h_{+}}\rangle \), the definite parity states

\[
|0_{\pm}\rangle = \frac{|0_{h_{+}}\rangle \pm |0_{h_{-}}\rangle}{\sqrt{2(1 \pm \text{Re}(\langle 0_{h_{+}}|0_{h_{-}}\rangle))}} ,
\]

(12)

which will normally be not strictly degenerate in finite systems and which lead to a non-perturbative entanglement between composite sites: Neglecting the complementary overlap \( \prod_{k' \neq k} (|0_{k'}\rangle \langle 0_{k'}|) \), typically small, the ensuing reduced state of the cluster \( k \) \( \pm \) given by

\[
\rho_k = \text{Tr}_k|0_{\pm}\rangle \langle 0_{\pm}| \approx \frac{1}{2} (|0_{k+}\rangle \langle 0_{k+}| + |0_{k-}\rangle \langle 0_{k-}|) ,
\]

(13)

which is a rank 2 mixed state with eigenvalues

\[
p_{\pm} = \frac{1}{2} (1 \pm |0_{k+}\langle 0_{k-}|) ,
\]

(14)

and non-zero entropy \( S(\rho_k) \). A parity breaking GMF is then a signature of a non-perturbative entanglement \( S(\rho_k) \) between the composite site and the rest of the system in the exact (definite parity) GS. Similar considerations hold for a group \( G \) of clusters, for which the reduced state will again be a similar rank 2 mixed state with \( p_{\pm} = \frac{1}{2} (1 \pm \prod_{k \in G} |\langle 0_{k+}|0_{k-}\rangle|) \). For a large group, \( p_{\pm} \to 1/2 \) and \( S(\rho_G) \to \ln 2 \). Such contribution is analogous to a “topological” entropy\(^{36} \).

III. APPLICATION TO DIMERIZED SPIN SYSTEMS

A. Dimerized \( XY \) spin chain

We first consider a cyclic spin \( 1/2 \) chain of \( \text{N} = 2n \) spins in a transverse uniform field \( B \), coupled through alternating first neighbor anisotropic \( XY \) couplings\(^{21,22,24,26} \), such that the system can be viewed, at least for weak fields, as strongly coupled pairs weakly interacting with their neighboring pairs (Fig. 1). The Hamiltonian can be written as

\[
H = \sum_{i=1}^{n} (B(s_{2i-1}^z + s_{2i}^z) - \sum_{\mu=x,y} J_{\mu}(s_{2i-1}^{\mu} s_{2i}^{\mu} + \alpha_{\mu} s_{2i}^{\mu} s_{2i}^{\mu} + 1)) ,
\]

(15)

where \( s_i^{\mu} \) denotes the (dimensionless) spin component at site \( i \). We will focus on the case \( \alpha_x = \alpha_y = \alpha \) (common anisotropy). We can suppose, without loss of generality, \( |\alpha| \leq 1 \) and, moreover, \( \alpha \geq 0 \), both in a cyclic chain \( \{s_{2n+1}^\mu = s_i^\mu\} \) with an even number \( n \) of pairs or in an open chain with \( n \) pairs, as its sign can be changed by a rotation of angle \( \pi \) around the \( z \) axis at even pairs (sites \( 2i - 1, 2i \), \( i \) even\(^{26} \)). A similar rotation at all even sites changes the sign of \( J_x \) and \( J_y \), so that we can also assume \( J_x \geq 0 \), with \( |J_y| \leq J_x \). We set here \( |J_y| < J_x \). Finally, we set \( B \geq 0 \), as its sign can be changed by a global rotation of angle \( \pi \) around the \( x \) axis, which leaves the couplings unchanged. These arguments also hold for arbitrary spin \( s \).

Eq. (15) commutes with the total \( S_z \) parity

\[
P_z = \exp[-i\pi (S_z + 2ns)] ,
\]

(16)

where \( S_z = \sum_{i=1}^{2n} s_i^z \). This implies \( \langle s_i^{\mu}\rangle = 0 \) for \( \mu =
in the cyclic case, with independent spin pairs $B \neq a$ degenerate in MF descriptions, at least within some field intervals.

The conventional MF is based on a product state
$$ρ_h = \otimes_{i=1}^{2n} ρ_i, \quad ρ_i = \exp[-β h_{i}] / Z_{h_{i}},$$
where, for the chosen signs of couplings, we may assume all $ρ_i$ identical in the cyclic case, such that $(s_i^x) = (s_i^y)$ and
$$⟨H⟩ = n[2B(s^2) - (1 + α) \sum J_μ(s_μ^x s_μ^y)],$$
with
$$h_i = λ \cdot s_i = B s_i^z - (1 + α) \sum J_μ(s_μ^x s_μ^y).$$

Considering now $T = 0$, the GS $|0_h⟩$ will be a state with maximum spin along $-λ$, leading to $⟨s^2⟩ = -s \cos θ$, $⟨s^y⟩ = s \sin θ \cos φ$, $⟨s^y⟩ = s \sin θ \sin φ$. Minimization of $⟨H⟩$ for $|J_y| < J_x$ leads then to $φ = 0$ ($⟨s^y⟩ = 0$) and
$$\begin{cases} \theta = 0, \\ \cos θ = B / B^c_x, \\ B \geq B^c_x \rightarrow J_x(1 + α) s, \\ B \leq B^c_x, \end{cases}$$
with parity broken for $B < B^c_x$, where the solution is degenerate ($θ = ±|θ|$). For $s = 1/2$ we then obtain
$$⟨0_h | H | 0_h⟩ = -n \left\{ \begin{array}{ll} B & B \geq B^c_x \\ B^c_x & B < B^c_x \end{array} \right.,$$
with $|0_h⟩ = \otimes_{i=1}^{2n} |0⟩$ with (Fig. 2)
$$|0⟩ = \cos \frac{θ}{2} |↓↓⟩ + \sin \frac{θ}{2} |↑↑⟩. \quad (21)$$
This simple approach ignores the dimerized structure of the chain (it is the same as that for a chain with uniform coupling $J_x(1 + α)/2$), and is also blind to the weaker $J_y$ coupling. Yet, it is remarkable that if $J_y \geq 0$, $|0_h⟩$ does become an exact GS at the separability field
$$B^c_x \equiv \sqrt{J_y J_x(1 + α)} s = \sqrt{J_y / J_x} B^c_x, \quad (22)$$
where $\cos θ = \sqrt{J_y / J_x}$. At this field the system exhibits a degenerate GS, with the GS subspace spanned by the pair of degenerate MF product states.

No traces of dimerization are left at this point in the exact GS.

B. Pair Mean Field Approximation

In order to improve the conventional MF picture for $B \neq B^c_x$, we now examine a generalized MF approach based on independent spin pairs, such that
$$ρ_h = \otimes_{i=1}^{2n} ρ_i^ρ, \quad ρ_i^ρ = \exp[-β h_i^ρ] / Z_{h_i^ρ}, \quad (23)$$
with $ρ_i^ρ$ a pair state. Eq. (23) is exact in the fully dimerized limit $α \rightarrow 0$, and can then be expected to provide a good approximation at least for small $α$. For the chosen signs of couplings, we may again assume all $ρ_i^ρ$ identical in the cyclic case, with $(s_i^x) = (s_i^y)$, implying
$$⟨H⟩ = n[2B(s^2) - \sum_{μ=x,y} J_μ((s_μ^x s_μ^y) + α⟨s^y⟩^2)], \quad (24)$$
and
$$h_i^ρ = B(s_{2i-1}^x + s_{2i}^x) - \sum_{μ=x,y} J_μ[(s_μ^x s_μ^y) + α⟨s^y⟩(s_{2i-1}^x + s_{2i}^x)]. \quad (25)$$

For $|J_y| < J_x$, minimization of $⟨H⟩$ leads again to $⟨s^y⟩ = 0$.

In the case of arbitrary spin and temperature, one should start from an initial seed for $⟨s^y⟩$, diagonalize $h_i^ρ$, and then recalculate $⟨s^y⟩$ until convergence is reached. Considering now $T = 0$ and $s = 1/2$, it is apparent from (23) that the GS of $h_i^ρ$ will be of the form
$$|0_ρ⟩ = \cos \frac{θ}{2} (cos \frac{θ}{2} |↓↓⟩ + \sin \frac{θ}{2} |↑↑⟩) + \sin \frac{θ}{2} (|↑↑⟩ + |↓↓⟩). \quad (26)$$
which is just the most general symmetric pair state real in the standard basis. Eq. (22) becomes
$$⟨0_ρ | H | 0_ρ⟩ = -n[(B \cos φ + J_− \sin φ) \cos \frac{θ}{2} + J_+ \sin \frac{θ}{2} + \sqrt{\frac{B}{4} \alpha J_2 \sin \theta (1 + sin \phi)}], \quad (27)$$
where $|0_ρ⟩ = \otimes_{i=1}^{n} |0_ρ⟩$ and $J_± = J_x ± J_y / 4 \geq 0$. Minimization of $⟨H⟩$ with respect to $θ, φ$ can then be directly done, leading to
$$\begin{cases} \cos θ = 2B \cos φ + J_− \sin φ \frac{J_+}{B} \cdot \frac{J_+}{J_2} > B < B^c_2, & (28a) \\ \sin φ = \frac{J_+}{J_2} & (28b) \end{cases}$$
for $θ = \pi$ (φ arbitrary), $B \leq B^c_3$ (28c)
where the critical fields are given by
$$B^c_3 = \frac{1}{2} \sqrt{J_2 (J_y - 2α J_x)}, \quad (29)$$
$$B^c_4 = \frac{1}{2} \sqrt{J_2 [J_+ + \frac{J_2}{2} J_x + \sqrt{(J_+ + \frac{J_2}{2} J_x)^2 + 4α J_x J_2}]^2 - 4J_x^2}, \quad (30)$$
as obtained from (28b) for $θ → 0$ and $θ → π$. The solution of system (28) for $θ$ and $φ$ can in fact be determined analytically (it leads to a quartic equation for $cos φ$).

In contrast with the standard MF, it is first seen that a parity breaking solution ($θ \in (0, π/2)$) will now arise just within a field window $B^c_3 < B < B^c_2$ if $α$ is sufficiently small and $J_y > 0$, as depicted in Fig. 2 (bottom panel). For $B < B^c_3$, the pair MF leads to a fully dimerized phase, where the strongly coupled pairs are in a $P_z = -1$ Bell state $|↓↓⟩ + |↑↑⟩$ and hence maximally entangled. On the other hand, for $B > B^c_2$ the approach leads to an entangled $P_z = 1$ pair state $cos \frac{θ}{2} |↓↓⟩ + sin \frac{θ}{2} |↑↑⟩$, which is only partially aligned. The intermediate parity breaking phase (28b) is then a transition region between the previous opposite parity phases, in which the pair is in a combination of the previous states. In this region the pair MF GS is two-fold degenerate ($θ = ±|θ|$). It is verified that the actual exact GS obtained from the Jordan-Wigner fermionization also exhibits two transitions for increasing positive fields if $α$ is sufficiently
small, becoming in a finite chain nearly two-fold degenerate in the intermediate sector and leading as well to almost maximally entangled pairs for low fields (see appendix and next section).

In the parity preserving phases, the pair MF GS energy obtained from \( \langle \psi_0^\alpha_1 | H | \psi_0^\alpha_2 \rangle \) is just

\[
\langle \psi_0^\alpha_1 | H | \psi_0^\alpha_2 \rangle = -n \begin{cases} \sqrt{B^2 + J^2}, & B \geq B_{c1}^\alpha, \\ J_+, & B < B_{c1}^\alpha \end{cases}
\]

which is, of course, lower than the conventional MF energy in these intervals.

The factorizing field \( \frac{J_0}{B_{c2}^\alpha} \) lies within the parity breaking phase \( \forall \alpha > 0 \): \( B_{c1}^\alpha < B_{c2}^\alpha < B_{c2}^\alpha \). It is verified that at \( B = B_{c1}^\alpha \), Eq. \( \langle \psi_0^\alpha | H | \psi_0^\alpha \rangle \) leads to \( 0 = \frac{\tan \phi}{\tan J_+/\sqrt{J_x J_y}} \), which implies

\[
\tan^2 \phi/2 = \sin \phi,
\]

which is precisely the condition ensuring that the pair state \( \langle \psi_0^\alpha | \psi_0^\alpha \rangle \) reduces to a product of single spin states.

On the other hand, for \( \alpha \rightarrow 0 \) (where the pair MF becomes exact), \( B_{c1}^\alpha \) and \( B_{c2}^\alpha \) merge (Fig. 2), approaching both the \( \alpha = 0 \) factorizing field \( B_{c1}^\alpha = \sqrt{J_y J_x}/2 \) \((B_{c2}^\alpha \approx B_{c1}^\alpha(1 + \alpha J_y/J_x) \) for small \( \alpha \): The exact GS of an isolated pair undergoes, for \( J_y > 0 \), a sharp parity transition at \( B = B_{c1}^\alpha \), from the Bell state \( |\text{\uparrow\downarrow} + \text{\downarrow\uparrow}\rangle/\sqrt{2} \) for \( B < B_{c1}^\alpha \), with energy \( E_{J+} \) (Eq. \( 31 \)) to the state \( \sin \frac{x}{4} |\text{\uparrow\downarrow}\rangle + \sin \frac{\phi}{2} |\text{\downarrow\uparrow}\rangle \) for \( B > B_{c1}^\alpha \), with energy \( -\sqrt{B^2 + J^2} \). At \( B = B_{c1}^\alpha \) these states become degenerate and coincide with the definite parity combinations of the MF product states \( \otimes_{i=1}^n |\text{\uparrow\uparrow}\rangle \).

It is also seen from Eq. \( 29 \) that \( B_{c1}^\alpha \) vanishes for

\[\alpha = \alpha_c \equiv \frac{J_y}{2J_x}.\]

If \( \alpha > \alpha_c \) (or \( J_y < 0 \)) parity is broken for all \( B \leq B_{c2}^\alpha \), as in the standard MF. Nonetheless, important differences with the latter persist: \( B_{c2}^\alpha \) remains lower than the MF critical field \( B_{c2}^\alpha \), even for \( \alpha = 1 \), and strongly coupled pairs remain entangled even for strong fields \( B > B_{c2}^\alpha \). Full alignment occurs only for \( B \rightarrow \infty \), with \( \phi \approx J_+/B \) for \( B \gg J_+ \). The pair MF depends also on \( J_y \), which affects the critical fields and the values of \( \phi, \theta \).

If \( J_y < 0 \) (with \( |J_y| \leq J_z \)), \( B_{c2}^\alpha \) also vanishes at \( \alpha = -\frac{J_y}{2J_x} \geq 0 \), entailing no parity breaking phase in the pair MF if \( \alpha \leq -\frac{J_y}{2J_x} \). This is in qualitative agreement with the exact result (see appendix), but differs from the standard MF, where parity breaking still occurs \( \forall \alpha \).

If \( J_x > 0 \) but \( \alpha < 0 \), the pair MF state can be obtained by rotation of angle \( \pi \) around the \( z \) axis at even pairs of the \( \alpha > 0 \) pair state, which implies (ignoring in what follows overall phases) an alternating angle \( \theta \) in \( \frac{\pi}{2} \) (\( \theta_i = -\sin \frac{\phi}{2} \)) in the parity breaking phase. If \( \alpha > 0 \) but \( J_x < 0 \) (with \( J_y > |J_z| \)), such rotation should be applied to all even sites, entailing \( |\text{\uparrow\uparrow}\rangle \rightarrow \text{\uparrow\downarrow} \rightarrow \rightarrow \text{\downarrow\uparrow} \rightarrow \text{\downarrow\uparrow} \) and

\[
\sin \frac{x}{4} |\text{\uparrow\downarrow}\rangle + \sin \frac{\phi}{2} |\text{\downarrow\uparrow}\rangle \rightarrow \cos \frac{x}{4} |\text{\uparrow\downarrow}\rangle - \sin \frac{\phi}{2} |\text{\downarrow\uparrow}\rangle \text{ in } 29 \text{.}
\]

C. Entanglement predictions and comparison with exact results

We first show in Figs. 24 typical GS results for different entanglement observables related with spin pairs and single spins in a finite chain with \( n = 50 \) pairs, according to conventional and pair MF as well as exact results (see Appendix). The latter correspond to the exact GS of the finite chain (having then a definite \( S_z \) parity).

For a pair of strongly coupled neighboring spins (1-2 in Fig. 1), the pair MF approach \( 20 \), leads, after the symmetry restoration, to the reduced state

\[
\rho_{12}^{\text{GMF}} = \begin{pmatrix}
\cos^2 \frac{\theta}{2} \sin^2 \frac{x}{2} & 0 & 0 & \frac{1}{2} \cos^2 \frac{\theta}{2} \sin \phi \\
0 & \frac{1}{2} \sin^2 \frac{\theta}{2} & \frac{1}{2} \sin^2 \frac{x}{2} & 0 \\
0 & \frac{1}{2} \sin^2 \frac{\theta}{2} & \frac{1}{2} \sin^2 \frac{x}{2} & 0 \\
\frac{1}{2} \cos^2 \frac{\theta}{2} \sin \phi & 0 & 0 & \cos^2 \frac{\theta}{2} \cos^2 \frac{x}{2}
\end{pmatrix},
\]

(expressed in the std. basis) after neglecting the overlap \( |\langle \psi_0^\theta | \psi_0^\theta(-\theta) \rangle|^{n-1} \) in the parity breaking phase. In

\[
B/J_x
\]

\[
\frac{|\psi_+\rangle = \cos \frac{\phi}{2} |\uparrow\downarrow\rangle + \sin \frac{\phi}{2} |\downarrow\uparrow\rangle}{\alpha}
\]

\[
\frac{|\psi\rangle = \cos \frac{\phi}{2} |\uparrow\downarrow\rangle + \sin \frac{\phi}{2} |\downarrow\uparrow\rangle}{\alpha}
\]

\[
\frac{|\psi\rangle = \cos \frac{\phi}{2} |\uparrow\downarrow\rangle + \sin \frac{\phi}{2} |\downarrow\uparrow\rangle}{\alpha}
\]
this phase it is a rank 2 mixed state (and is pure otherwise), with eigenvalues \( \sin^2 \frac{\theta}{2}, \cos^2 \frac{\theta}{2} \) (Eq. \[14\]). It then leads within this phase to a non-zero entanglement entropy \( E_{12} = S(\rho_{12}) \) between the pair and the rest of the chain. As seen in the top panel of Fig. 3, this is in agreement with the exact result, which also exhibits a pronounced peak in this interval (we use \( S(\rho) = -\text{Tr} \rho \log_2 \rho \) in all panels). Parity breaking in the pair MF is then a signature of a non-negligible entanglement between this pair and the rest of the chain. The exact result presents as well small nonzero tails outside the parity breaking interval, which can be correctly predicted by the perturbed pair MF reduced state \([11]\).

Note that the entropy \( S(\rho_{12}) \) does not vanish as \( B \) approaches the factorizing field \( B_{s}^0 \) \((\approx 0.39 J_s\) in Fig. 3), since the exact GS remains with a definite parity (and hence entangled) in its immediate vicinity. In fact, for \( B \to B_{s}^0 \) the result obtained from \([34]\) becomes exact (except for the small neglected overlap), as the parity restored pair MF GS is exact in this limit. Actually, as stated before, at \( B = B_{s}^0 \) the exact GS is degenerate, so that GS entanglement will depend at this point on the choice of GS. The result obtained from \([34]\) corresponds to the definite parity GS’s \([12]\), which are the actual side limits of the exact GS for \( B \to B_{s}^0 \).

The single spin state derived from \([34]\) is just

\[
\rho_{1}^{\text{MF}} = \begin{pmatrix}
  p_+ & 0 \\
  0 & p_-
\end{pmatrix}, \quad p_{\pm} = \frac{1}{2}(1 \mp \cos^2 \frac{\theta}{2} \cos \phi),
\]

which is of the form \( \frac{1}{2}(\rho_1^1 + \rho_1^-) \) in the parity breaking phase, with \( \rho_1^\pm \) the single spin reduced states derived from the pair state \([26]\) before parity restoration. Its entropy, quantifying its entanglement with the rest of the chain, is non-zero for all fields and seen to be almost coincident with the exact result (center panel). It is obviously maximum in the dimerized phase \( B < B_{s1}^0 \), but decreases rapidly in the parity breaking phase (when the pair becomes entangled with the rest of the chain) and slowly in the partially aligned phase \( B > B_{s2}^0 \) (where \( p_+ \approx \phi^2/4 = J_s^2/(4B_s^2) \)). The result derived from \([34]\) is again fully exact for \( B \to B_{s}^0 \).

The entanglement entropy \( S(\rho_{23}) \) of a weakly coupled pair with the rest of the chain can again be correctly described by the pair MF approach, as seen in the bottom panel. Note that \( \rho_{23}^{\text{MF}} = \frac{1}{2}(\rho_1^1 \otimes \rho_1^1 + \rho_1^- \otimes \rho_1^-) \), so that in the parity preserving phases \( (\rho_1^1 = \rho_1^-) \), \( S(\rho_{23}^{\text{MF}}) \) is just twice the single spin entropy \( S(\rho_{1}^{\text{MF}}) \). This relation no longer holds, however, in the parity breaking phase.

In contrast, it is verified in all panels that the conventional MF \([17]\) does not lead to a proper picture of any of these measures, even after symmetry restoration. The ensuing reduced pair state is the same for any pair,

\[
\rho_{12}^{\text{MF}} = \frac{1}{4} \begin{pmatrix}
  \sin^4 \frac{\theta}{2} & 0 & 0 & \frac{1}{4} \sin^2 \theta \\
  0 & \frac{1}{4} \sin^2 \theta & \frac{1}{4} \sin^2 \theta & 0 \\
  0 & \frac{1}{4} \sin^2 \theta & \frac{1}{4} \sin^2 \theta & 0 \\
  \frac{1}{4} \sin^2 \theta & 0 & 0 & \cos^2 \frac{\theta}{2}
\end{pmatrix},
\]

which is a rank 2 state for \( \theta \in (0, \pi) \) with eigenvalues \( \frac{1 + \cos \theta}{2} \) \((\theta \) is here the MF angle \([19]\)\). Its entropy does not reflect the exact entanglement of the strongly nor the weakly coupled pair. The associated single spin reduced state is of the form \([35]\) but with \( p_+ = (1 + \cos \theta)/2 \), and cannot correctly reproduce either its entanglement with the rest of the chain (center panel in Fig. 3). It is seen, however, that there is one point where the conventional MF result is exact for all three quantities (i.e., where the MF curve crosses the exact curve), which is the factorizing field \( B_{s}^0 \). Here the reduced states \([30]\) and \([34]\) become identical and, moreover, exact.
fields $B < B^a_1$. Note that for $B < B^a_3$ and $B > B^a_2$, the state \((\rho_{12}^{\text{GMF}})\) is pure, implying that the pair MF concurrence is just a function of $S(\rho_{12}^{\text{GMF}})$, and given by

$$C_{12}^{\text{GMF}} = \begin{cases} 1, & B < B^a_1 \in \mathbb{R}^+, \\ \frac{J}{\sqrt{B^2 + J^2}} C, & B > B^a_2, \end{cases}$$

(38)

decreasing as $J_-/B$ for strong fields $B \gg J_-$. However, in the parity breaking phase the state \((\rho_{12}^{\text{GMF}})\) is mixed and the concurrence \((\rho_{12}^{\text{GMF}})\) is no longer a function of $S(\rho_{12}^{\text{GMF}})$. In fact, and as opposed to the previous entropies, it vanishes at the factorizing field $B^a_2$, as can be verified from Eqs. \ref{32}, \ref{41}, since the state \((\rho_{12}^{\text{GMF}})\) becomes separable (a convex combination of product states\ref{26}) at this point. Here the single spin ceases to be entangled with its partner (except for tiny overlap corrections) even though it remains entangled with the rest of the chain ($S(\rho_{12}^{\text{GMF}}) \neq 0$), indicating again that no traces of dimerization remain.

We also mention that the fidelity of the state \((\rho_{12}^{\text{GMF}})\) with the exact $\rho_{12}$, $F = \text{Tr} \sqrt{\rho_{12}^{\text{GMF}} \rho_{12}}$, is very high ($> 0.99$ for $\alpha = 0.1$ in all phases). In contrast, the conventional MF state \((\rho_{12}^{\text{MF}})\) has a low fidelity, especially for $B < B^a_2$, and leads to a zero concurrence $\forall B$, since it is a separable state even after parity restoration ($\rho_{12}^{\text{MF}} = \frac{1}{2}(\rho_{12}^{\text{1}} \otimes \rho_{12}^{\text{1}} + \rho_{12}^{\text{1}} \otimes \rho_{12}^{\text{1}})$, with $\rho_{12}^{\text{1}}$ the MF single spin state before parity restoration).

The concurrence of a weakly coupled neighboring pair is plotted in the central panel of Fig. 4. This quantity cannot be reproduced by the standard nor the pair MF, since even after parity restoration they lead to a separable state $\rho_{23}$. However, it can be correctly described by the reduced state $\rho_{23}^{\text{GMF}+P}$ derived from the perturbed pair MF state \((\rho_{12}^{\text{GMF}})\). This concurrence is small and starts to be non-zero just before the factorizing field $B^a_2$, having peaks at both sides of $B^a_2$. We should actually recall that at the immediate vicinity of $B^a_2$ (i.e., $B \rightarrow B^a_2^\pm$), the concurrence between any two spins acquires in a finite chain a common tiny yet non-zero value in the definite parity GS, which can be exactly predicted by both the conventional or pair MF after parity restoration if the overlap $|\langle \psi_{\alpha} | \psi_{\alpha} \rangle |^{n-1}$ is conserved\ref{16,25}.

While the general accuracy of the pair MF approach will decrease as $\alpha$ increases, it will still improve the conventional MF results, even in the uniformly coupled case $\alpha = 1$. In the bottom panel of Fig. 4 we depict the pair MF concurrence of a strongly coupled pair for increasing $\alpha$ at a fixed field, which is seen to remain accurate for all $\alpha \leq 1$. The conventional MF result vanishes $\forall \alpha$.

### D. Energy predictions

We plot in Fig. 5 some basic energy level predictions, in order to provide a general view of the pair MF approach. As seen in the top panel, the pair MF GS energy significantly improves the conventional MF result, especially for $B < B^a_2$. In the bottom panel, we depict for
FIG. 5. (Color online) Top: The difference $\Delta \varepsilon_0/n = (E_{\text{app}} - E_0^\alpha)/n$ between the approximate and exact GS energies per pair, according to conventional and pair MF approaches, for the chain of Fig. 4. The inset depicts for reference the corresponding intensive GS energies. Bottom: The first excitation energies of a small chain with 8 spins with the same parameters, according to pair MF and exact results. The inset depicts a blow up of the exact first excitation energy in the parity breaking region.

clarity the first four excitation energies in a small chain of 8 spins ($n = 4$). According to the pair MF approach, the lowest levels are single pair excitations, of energies $E_{\text{ex}} = \varepsilon_0 - \varepsilon_0$ (using the notation of Eq. 39), which in the present case will be independent of the site and hence $n$-fold degenerate. It is verified that for small $\alpha$, this is approximately the case. Moreover, the splitting of these levels due to the residual interaction can be correctly described by simple first order perturbative treatment. In the present cyclic case with a uniform pair MF, this leads to the perturbed pair excitation energies

$$E_{m}^{1k} = \varepsilon_m - \varepsilon_0 - 2\alpha \sum_{\mu=x,y} J_\mu \langle 0 | s_1^{\mu} | m \rangle \langle m | s_2^{\mu} | 0 \rangle \cos \frac{2\pi k}{n},$$

(39)

where $\varepsilon_m$ are the eigenvalues of the single pair Hamiltonian $24$ ($h^0 | m \rangle = \varepsilon_0 | m \rangle$), with $\varepsilon_0$ its GS energy, and $k = 1, \ldots, n$. These energies are those of the (discrete) Fourier transformed states $| \hat{m}_k \rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} e^{2\pi ik j/n} | m_j \rangle$, where $| m_j \rangle$ denotes the state with pair $j$ at excited level $m$. As seen in the bottom panel, the result obtained from Eq. 39 is practically exact in the parity preserving phases, where the energies $\varepsilon_m$ are $\pm J_+$ and $\pm \sqrt{B^2 + J^2}$, and the lowest energies (39) become

$$E_{1}^{1k} = \pm (J_+ - \sqrt{B^2 + J^2}) - \alpha (J_+ + \frac{J^2}{\sqrt{B^2 + J^2}}) \cos \frac{2\pi k}{n},$$

(40)

with $+$ for $B < B^x$ and $-$ for $B > B^x$. For $n = 4$, $E_{1}^{11} = E_{1}^{13} = E_{1}^{10}$, so that just three levels are seen. In contrast, the conventional MF leads to a single spin excitation energy $E_{1}^{\text{MF}} = B$ for $B < B_c$ and $J_+ (1 + \alpha/2)$ if $B > B_c$, which lies well above the previous levels.

The parity breaking phase of the pair MF approach is seen (bottom panel) to coincide approximately with the region where the exact GS of the finite chain becomes nearly degenerate $21,22,25,26$. The exact lowest energy levels of each parity sector become very close in this interval, actually crossing at $n$ fields (as seen in the inset), with the last crossing taking place exactly at the factorizing field $B_c$. This interval is enclosed by the fields $B_{c}^{\text{ex}}$ and $B_{c}^{\text{cs}}$ where the lowest quasiparticle energy of the Jordan-Wigner fermionized Hamiltonian vanishes (see appendix).

E. Longer range couplings and lattices

The pair MF approach remains directly applicable to more complex situations where exact analytic results are no longer available. For instance, if adjacent dimers in Fig. 4 are further connected by second and third neighbor couplings $-\alpha_2 J_\mu s^\mu_j s^\mu_{j+2}$ (for spins like 1-3 and 2-4) and $-\alpha_3 J_\mu s^\mu_{2j-1} s^\mu_{2j+2}$ (for spins like 1-4, such that

$$H = \sum_{j=1}^{n} \{ B (s^z_{2j-1} + s^z_{2j}) - \sum_{\mu=x,y} J_\mu (s^\mu_{2j-1} s^\mu_{2j})$$

$$+ \sum_{j=1}^{1,2} \{ \alpha_j s^\mu_{2j} s^\mu_{2j+1} + \alpha_{j+1} s^\mu_{2j-1} s^\mu_{2j+1}) \},$$

(41)

the Jordan-Wigner transformation will no longer lead to a quadratic (and hence analytically solvable) fermionic Hamiltonian. However, it is seen from Eqs. 39 that the previous MF and pair MF expressions and phase diagram (Fig. 2) remain valid with the replacement

$$\alpha = \alpha_1 + 2\alpha_2 + \alpha_3,$$

(42)
provided $\alpha_2$ and $\alpha_3$ are also positive (as $\alpha_1$) or sufficiently small. The system of Eq. (41) is equivalent to a ladder-type dimer chain (Fig. 2 left). A uniform factorizing field will still exist in this system for common anisotropy $J_{\mu}^i (\alpha_i^j = \alpha_j \forall j$, as considered in (41)), which will be again given by Eq. (42) with the previous value of $\alpha$. Similar considerations hold for longer range $XY$ couplings.

The phase diagram of Fig. 2 also applies, at the pair MF level, to ferromagnetic-type $XY$ dimer lattices like that of Fig. 4 right, described by the Hamiltonian

$$H = \sum_{i,j} \{ B(s_{2i-1,j}^z + s_{2i,j}^z) - \sum_{\mu=x,y} J_\mu [s_{2i-1,j}^\mu s_{2i,j}^\mu + \alpha_1 s_{2i,j}^\mu s_{2i+1,j}^\mu + \alpha_2 (s_{2i-1,j}^\mu s_{2i-1,j+1}^\mu + s_{2i,j}^\mu s_{2i,j+1}^\mu)] \},$$

(43)

where we assumed first neighbor couplings. For $\alpha_1 > 0$, $\alpha_2 > 0$, we should just replace

$$\alpha = \alpha_1 + 2\alpha_2,$$

(44)

in the MF and pair MF approaches. Similar considerations hold for 3D lattices or longer range couplings.

Fig. 7 depicts illustrative results for a finite spin ladder and lattice with cyclic conditions ($n + 1 = n$ in (41), $n_i + 1 = n_i$ for $i = 1, 2$ in (43)). We have computed the exact results by exact diagonalization for a total of $2n = 16$ spins ($2 \times 8$ ladder, $4 \times 4$ lattice). We have set a fixed value $\alpha = 0.2$ in Eqs. (42) and (43), with $\alpha_1 = \alpha_2 = \alpha_3$ in (42) and $\alpha_1 = \alpha_2$ in (43). For comparison, results for the chain of Eq. (15) with the same $\alpha$ and spin number are also depicted.

It is verified that for a common total $\alpha$, these systems do exhibit almost coincident values of the entanglement of a strongly coupled pair with the rest of the system, and of its concurrence, confirming the pair MF prediction. Moreover, the exact results are in very good agreement with the pair MF results. Those for the ladder are in fact almost indistinguishable from those of the chain, while those for the lattice are slightly closer to the pair MF result due to the larger connectivity, in agreement with the perturbative corrections of Eq. (14) (which can again predict the tails of $S(\rho_{12})$ in the parity preserving phases). Conventional MF results, not shown, are similar to those of Figs. 6,6. The concurrence $C(\rho_{12})$ remains close in the three systems also for higher values of the total $\alpha$, as seen in the bottom panel.

**F. XYZ coupling**

Let us now examine the effects of an additional $J_z$ coupling in (8), i.e.,

$$H = \sum_{i=1}^{n} B (s_{2i-1}^z + s_{2i}^z) - \sum_{\mu=x,y,z} J_\mu [s_{2i-1}^\mu s_{2i}^\mu + \alpha_1 s_{2i}^\mu s_{2i+1}^\mu].$$

(45)

As is well known, this model is no longer analytically solvable in the general anisotropic case (the added term does not lead to a quadratic fermionic operator in the Jordan-Wigner fermionization). We again assume $J_x > 0$ and $|J_y| < J_x$, with a common anisotropy $\alpha_\mu = \alpha > 0$.

For small values of $J_z$, the phase diagram of Fig. 8 remains essentially valid, with adequate shifts in the critical values of the field and $\alpha$. At the conventional MF level, Eq. (19) applies with $B_{\alpha}^z$ replaced by the critical field

$$B_{\alpha}^{\alpha z} = (J_z - J_{\alpha})(1 + \alpha)s,$$

with no parity breaking phase if $J_z > J_{\alpha}$ and a uniform
factorizing field still exists for common anisotropy if \( J_z < J_y \), given by
\[
B_x^{az} = \sqrt{(J_x - J_z)(J_y - J_z)(1 + \alpha)s}.
\] (46)

For \( B = B_x^{az} \), the uniform parity breaking MF state follows again an exact degenerate GS, with
\[
\cos \theta = \frac{J_y - J_x}{J_y + J_x} (\text{and } \theta = \pm |\theta|) \text{ if } J_z > J_x > J_y,
\]
and increasing \( \alpha \) will lower the energy of the dimerized state \( \cos \theta \). Equation (42) or (44) is to be replaced by
\[
\cos \theta = \frac{1}{2} \alpha J_z \cos \phi \cos \theta.
\] (47)

At the pair MF level, we may still use the same state \( \lvert \Psi \rangle \), which leads to
\[
\langle 0^p_h | H_{xy} | 0^p_h \rangle = \frac{n}{4} J_z [\cos \theta + \alpha \cos^2 \phi \cos^4 \frac{\theta}{2}],
\] (48a)

where \( \langle 0^p_h | H_{xy} | 0^p_h \rangle \) denotes Eq. (27). Hence, Eqs. (28) are to be replaced by
\[
\theta = 0, \quad \tan \phi = \frac{J_x}{B + \frac{1}{2} \alpha J_z \cos \phi}, \quad B \geq B_x^{az},
\] (48a)

\[
\cos \theta = \frac{2 B \cos \phi + J_x \sin \phi - J_y}{J_x + J_y (1 + \cos \phi)}, \quad B < B_x^{az}.
\] (48b)

\[
\tan \phi = \frac{J_x + J_y \cos \phi}{B + \frac{1}{2} \alpha J_z \cos \phi (1 + \cos \phi)}, \quad B > B_x^{az},
\] (48c)

where the critical fields depend now on \( J_z \). The first critical field, which delimits the maximally entangled dimerized phase, has still a simple exact expression, given by
\[
B_x^{az} = \frac{1}{2} \sqrt{(J_x - J_z)(J_y - J_z - 2 \alpha J_x)}.
\] (49)

Eq. (49) implies that for \( J_z < J_y \), this dimerized phase will exist for \( \alpha < \alpha_{cz} \), with
\[
\alpha_{cz} = \frac{J_y - J_z}{2 J_x}.
\] (50)

If \( \alpha > \alpha_{cz} \) (or \( J_z > J_y \)), parity will be broken for all \( B < B_x^{az} \). \( B_x^{az} \) will also vanish for sufficiently large \( J_z \).

A positive \( J_y \) in Eq. (46) obviously increases the energy of the dimerized state (\( \theta = \pi \) in Eq. (47)). Hence, its effect will be to decrease the critical fields, narrowing the dimerized phase as appreciated in Fig. 5. This phase will in fact disappear for \( J_z > J_y - 2 \alpha J_x \) (Eq. (49)), as also seen in Fig. 8. On the other hand, a negative \( J_y \) has the opposite effect, lowering the energy of the dimerized state and increasing \( B_x^{az} \), favoring dimerization. This picture will remain valid for sufficiently weak longer range XYZ couplings, employing the substitutions (12) or (14).

Results for a finite cyclic XYZ chain are depicted in Fig. 9. Exact results were again computed by diagonalization for \( n = 16 \) spins. It is verified that the pair MF predictions are fully confirmed. The addition of a small \( J_z \) coupling essentially shifts the results of the XY chain, in agreement with Eqs. (46) and (49). As previously stated, a reduced (extended) dimerized phase is obtained if \( J_z > 0 \) (\( J_z < 0 \)), together with a displaced parity breaking phase, which is still clearly visible through the peak in the dimer entanglement entropy \( S(\rho_{12}) \) with the rest of the chain. There is again a good agreement with the pair MF results, which can also be improved by adding the corrections of Eq. (11). For strong fields \( B \gg B_x^{az} \), we mention that the final effect is the replacement \( B \rightarrow B_{eff} = B + \frac{1}{4} \alpha J_z \) (Eq. (48a)), with \( \phi \approx J_y - B_{eff} \) for \( B \gg B_x^{az} \).

IV. CONCLUSIONS

We have investigated a general self-consistent variational MF approximation, based on the selection of an arbitrary subset of operators for representing the system density matrix, and its capability for describing entanglement in the GS of composite systems. While retaining the conceptual simplicity of the conventional MF, the generalization allows to significantly improve it by considering composite cells, such that couplings within the cell are treated exactly. The approach is then especially suitable for systems where a partition in composite cells with strong internal couplings but weak cell-cell couplings is feasible, although it is not limited to this case.

In the dimerized systems considered, the approach naturally leads to a pair MF approximation which is still analytic and simple, but which goes well beyond the plain single spin MF. Its phase diagram clearly identifies a dimerized phase for weak fields, together with a parity breaking phase in a transitional region between the latter and the strong field regime. The approach is thus able to accurately describe the entanglement of strongly coupled pairs, with parity breaking emerging as a signature of a non-negligible entanglement between these pairs and rest of system in the exact definite parity GS. With the addition of simple perturbative corrections, it is also pos-
where \( s_j^+ = s_j^z \pm is_j^y \). These operators fulfill the fermionic anticommutation relations \([c_j, c_k^+] = \delta_{jk}, [c_j, c_k] = 0\). The corresponding inverse transformation is

\[
   s_j^+ = c_j^i \exp[\mp \pi \sum_{k=1}^{j-1} c_k^i c_k]. \tag{A.2}
\]

We then obtain, setting \( J_{\mp} = J_{\pm} \pm J_{\pm} \),

\[
   H^P = \sum_{j=1}^{2n} B(c_j^i c_j - \frac{1}{2}) - \eta_j^P r_j (J_+ c_j^i c_{j+1} + J_- c_{j+1}^i c_j + h.c.)\tag{A.3}
\]

where \( r_j = \{1 \text{ (odd)}\} \) and \( \eta_j^P = 1 - 2\delta_{j2n} \), \( \eta_j^P = 1 \) in the cyclic case. Through separate parity dependent discrete Fourier transforms for even and odd sites,

\[
  \left( \begin{array}{c} c_{2j-1}^i \\ c_{2j}^i \end{array} \right) = \frac{1}{\sqrt{N}} \sum_{k \in K_P} e^{-i\pi kj/n} \left( \begin{array}{c} c_{k+}^i \\ c_{k-}^i \end{array} \right),
\]

where \( K_+ = \{\frac{1}{2}, \ldots, n - \frac{1}{2}\} \), \( K_- = \{0, \ldots, n - 1\} \), we may rewrite (A.3) as

\[
   H^P = \sum_{k \in K_P} \sum_{\sigma = \pm} B(\sigma c_{k \sigma}^i c_{k \sigma} - \frac{1}{2}) - (J_k^+ c_{k-}^i c_{k+} + J_k^- c_{k+}^i c_{k-} + h.c.)
\]

where \( J_k^\pm = J_{\mp}(1 \pm e^{-i\pi kn}) \) and \(-k \equiv n - k\). The final diagonal form (A.4) is obtained by means of a Bogoliubov transformation

\[
   c_{k \sigma}^i = \sum_{\nu = \pm} U_{k\sigma}^{\nu} a_{\nu k} + V_{k\sigma}^{\nu} a_{-\nu k}\text{ determined through the diagonalization of } 4 \times 4 \text{ blocks}
\]

\[
   \mathcal{H}_k = \begin{pmatrix}
   B & -J_k^+ & \mp J_k^- & 0 \\
   -J_k^+ & B & J_k^- & 0 \\
   -J_k^- & 0 & B & J_k^+ \\
   0 & J_k^- & -B & J_k^+
   \end{pmatrix}, \tag{A.5}
\]

whose eigenvalues are \( \pm \lambda_k^+, \pm \lambda_k^- \), with

\[
   |\lambda_k^\pm| = \sqrt{\Delta \pm \sqrt{\Delta^2 - |B^2 - (J_k^+ + J_k^-)(J_k^+ - J_k^-)|^2}}\tag{A.6}
\]

and \( \Delta = B^2 + |J_k^+|^2 + |J_k^-|^2 \). Care should be taken to select the correct signs of \( \lambda_k^\pm \) in order that the vacuum of the operators \( a_{\nu k} \) has the proper \( S_z \)-parity and represents the lowest state for this parity.

The spin correlations in the lowest states for each parity can then be obtained from the ensuing basic fermionic contractions \( f_{ij} = \langle c_i c_j \rangle - \frac{1}{2} \delta_{ij} \), \( g_{ij} = \langle c_i c_j^i \rangle \), which can be directly obtained from the inverse Fourier transform of \( \langle c_{k \sigma}^i c_{k' \sigma'} \rangle = \sum_{\nu=\pm} V_{k \sigma}^{\nu \nu'} V_{k' \sigma'}^{\nu} \), \( \langle c_{k \sigma}^i c_{-k' \sigma'} \rangle = \sum_{\nu=\pm} V_{k \sigma}^{\nu \nu'} U_{k' \sigma'}^{\nu} \). We then obtain, through the use of Wick’s theorem,

\[
   \langle s_i^z \rangle = f_{ii}, \langle s_i^z s_j^z \rangle = f_{ii} f_{jj} - f_{ij}^2 + g_{ij}^2, \text{ and } \langle s_i^z s_j^\pm \rangle = \frac{1}{2}(|\det(A_{ij}^z)| \pm |\det(A_{ij}^\mp)|), \text{ where } A_{ij}^z \text{ are } (j-i) \times (j-i)
\]
matrices of elements $2(f + g)_{i+p+q, i+q+b}$, with $p, q = 0, \ldots, j - i - 1$.

From Eq. (A.6) it is seen that for real $B \neq 0$ and finite $n$, $|\lambda^+_k| > 0$ while $\lambda^-_k$ vanishes just when $k = 0$ and

$$ B = B_{c2}^{ex} = \frac{1}{\alpha}(iJ_x + J_y)(iJ_x - \alpha J_y), $$

(A.7)

or $k = n/2$ and

$$ B = B_{c1}^{ex} = \frac{1}{\alpha}(J_y - \alpha J_x)(J_x - \alpha J_y), $$

(A.8)

remaining non-zero for other values of $k$. These critical fields coincide with those of refs.[22-25] for the present situation. For $0 \leq \alpha \leq 1$ and $J_x > 0$, Eq. (A.5) is real only for $J_y \geq 0$ and $\alpha \leq J_y/J_x$, while if $-J_x \leq J_y \leq 0$, Eq. (A.7) is real for $\alpha \geq -J_y/J_x$. The pair MF critical fields [20] correspond approximately to these fields and satisfy

$$ B_{c1} \leq B_{c1}^{ex} \leq B_s^{\alpha} \leq B_{c2}^{ex} \leq B_{c2}, \quad (A.9) $$

for $J_y \geq 0$, all approaching the factorizing field $B_{c1}^{ex}$ for $\alpha \rightarrow 0$ (where $B_{c1}^{ex} \approx B_{c1}^{0}[1 \mp \frac{x}{2}(\frac{J_x}{J_y} + \frac{J_y}{J_x})]$).

The fields [A.1] = [A.3] enclose the interval where the finite chain GS will be almost two-fold degenerate, i.e., where the lowest state with positive $S_z$ parity will have nearly the same energy as the lowest state with negative parity. Actually, starting at a field slightly above $B = B_{c1}^{ex}$, the exact GS of the finite chain will experience $n$ parity transitions [26,28] in the interval $(B_{c1}^{ex}, B_{c2}^{ex})$, with the last one taking place exactly at the factorizing field $B_{c2}^{ex}$.

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