Generalized mean field description of entanglement in dimerized spin chains

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We discuss a generalized self-consistent mean field (MF) treatment, based on an arbitrary subset of operators, 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 of a dimerized spin chain with XY couplings in a transverse field. The approach is fully analytic and able to capture the main features of the system, significantly improving the conventional single spin MF. Its phase diagram differs substantially from that of the conventional MF, 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 also allow to accurately reproduce more subtle observables like the entanglement between weakly coupled spins and the low lying energy spectrum. All predictions are tested against the exact results obtained from the Jordan-Wigner fermionization.

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I. INTRODUCTION

The analysis of correlations and entanglement in interacting quantum many body systems has attracted strong attention in recent years\(^\text{12}\), motivated in part by their deep implications for quantum information processing and transmission\(^\text{3}\), and the impressive advances in techniques for controlling and measuring quantum systems\(^\text{4}\). While the conventional mean field (MF) approximations\(^\text{5}\) 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 methods have been developed to describe correlations, like for instance density matrix renormalization group (DMRG) techniques\(^\text{6}\), matrix product and tensor network methods\(^\text{7}\) and inclusion of quantum fluctuations around MF\(^\text{8}\). In addition, non-conventional MF approaches, able to intrinsically include some essential correlations, have also been proposed and recently improved and revisited\(^\text{10,11}\), which start from the so-called cluster MF approach, also known as BPW (Bethe-Peierls-Weiss) approximation\(^\text{12}\). The essential point in these schemes is the consideration of composite sites containing more than one spin as the basic independent units. Their application to specific spin systems\(^\text{10,11}\) has shown their capability for predicting phase diagrams and critical temperatures, as well as for describing observables such as the magnetization and susceptibility.

The aim of this work is, first, to discuss a general self-consistent MF approach, suitable for an arbitrary system at zero or finite temperature, based on the selection of a subset of operators\(^\text{13}\). It contains as particular cases both the conventional and the cluster-type MF approaches. We then consider its capability for describing entanglement, both within the defined components as well as between them, the latter emerging through symmetry restoration or perturbative corrections. As a specific example, we examine a pair MF approach for the ground state (GS) of a dimer-type spin 1/2 XY chain immersed in a transverse field, a system which received considerable attention in recent years\(^\text{14–17}\). While conserving the conceptual simplicity of the conventional MF, we will show that in contrast with the latter, the pair MF approach is able to provide a reliable (and still analytic) description of this system. Its phase diagram differs significantly from that of the conventional MF, and clearly identifies a fully dimerized phase for weak fields, together with an \( S_z \) parity breaking degenerate phase which is now confined to a transition region between the former and the partially aligned strong field regime. The approach also leads to an accurate 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 chain, which shows a prominent peak precisely in the parity breaking sector of the approach. By means of simple perturbative corrections, the approach can also predict the entanglement between weakly coupled spins as well as the low lying energy spectrum. All predictions are contrasted with the exact results obtained through the Jordan-Wigner fermionization\(^\text{17,18}\). The present approach remains tractable, however, in more complex situations (like longer range couplings and finite temperatures), where exact solutions are no longer available.

II. GENERAL SELF-CONSISTENT APPROXIMATION

The canonical thermal state \( \rho \propto \exp[-\beta H] \) of a system at temperature \( T = 1/k\beta \) described by a Hamiltonian \( H \), minimizes the free energy functional

\[ F(\rho) = \langle H \rangle_\rho - TS(\rho) \ , \quad (1) \]
where \( \langle H \rangle_\rho = \text{Tr} \rho H \) is the mean energy and \( S(\rho) = -k \text{Tr} \rho \ln \rho \) the entropy. One can then formulate a general variational approximation\(^1\) based on the trial state
\[
\rho_h = \exp[-\beta h]/Z_h, \quad h = \sum \lambda_i O_i, \tag{2}
\]
where \( Z_h = \text{Tr} \exp[-\beta h] \) and \( \{O_i, \; i = 1, \ldots, m\} \) is an arbitrary set of linearly independent operators, with \( \lambda_i \) optimizable parameters determined through the minimization of \( \langle H \rangle_\rho \). Considering the averages \( \langle O_i \rangle \equiv \text{Tr} \rho_h O_i \), functions of the \( \lambda_i \)'s, as the independent parameters, it is seen that the equations \( \frac{\partial}{\partial \lambda_i} \langle H \rangle = 0 \) lead at once to the self-consistent conditions \( \lambda_i = \frac{\partial \langle H \rangle}{\partial \langle O_i \rangle} \), i.e.,
\[
h = \sum \frac{\partial \langle H \rangle}{\partial \langle O_i \rangle} O_i, \quad \langle H \rangle = \text{Tr} \rho_h H. \tag{3}
\]
Eq. (3) defines a self-consistent approximate hamiltonian \( h \) which depends on the averages it determines.

If the \( O_i \)'s form a complete set, \( H \) is a linear function of them and Eq. (3) leads to \( h = H \). For a restricted set, Eq. (3) becomes in general non-linear and may lead to different solutions, from which that leading to the lowest \( F(\rho_h) \) should be selected. The well-known MF approximations such as thermal Hartree-Fock (HF) or HF-Bogoliubov (HFB) are obtained when the \( O_i \)'s are restricted to general one-body operators and traces are taken in the grand canonical ensemble, with \( H \rightarrow H - \mu N \).

Here we are interested in applying the previous 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 \( \otimes_{i=1}^N S_i \), with \( S_i \) that of subsystem \( i \). We will consider Hamiltonians containing just local terms and two-body couplings,
\[
H = \sum \mu_i O_i^{\mu} - \frac{1}{2} \sum_{i \neq j} J_{ij}^{\mu\nu} O_i^{\mu} O_j^{\nu}, \tag{4}
\]
where \( O_i^{\mu} \) are local operators pertaining to subsystem \( i \) \( \{\langle O_i^{\mu} \rangle = 0 \; \text{if} \; i \neq j \) and \( J_{ij}^{\mu\nu} = J_{ij}^{\mu\nu} \) coupling strengths (sum over repeated labels \( \mu, \nu \) is implied). The standard MF approach arises when the \( O_i \)'s in \( \otimes (2) - (3) \) are restricted to local operators \( O_i^{\mu} \), i.e., when a "site" is identified with a single subsystem \( i \). The present scheme allows, however, to also consider composite sites \( C_i \) such as pairs or clusters of spins in a spin system, where products \( O_i^{\mu} O_i^{\nu} \) for sites \( i, j \) within the same cluster are also included in the operators \( O_i \) of \( \otimes (2) - (3) \). 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 \( h_k \) an operator local in \( C_k \), such that
\[
\rho_h = \otimes_k \rho_k, \quad \rho_k = \exp[-\beta h_k]/Z_{h_k}, \quad \langle H \rangle = \sum_{k,i \in C_k} \left[ B_{\mu_i} \langle O_i^{\mu} \rangle - \frac{1}{2} \sum_{j \in C_k} J_{ij}^{\mu\nu} \langle O_i^{\mu} O_j^{\nu} \rangle \right. \nonumber \\
- \left. \frac{1}{2} \sum_{j \notin C_k} J_{ij}^{\mu\nu} \langle O_i^{\mu} \rangle \langle O_j^{\nu} \rangle \right]. \tag{5}
\]
Eq. (6) leads then to
\[
h_k = \sum_{i \in C_k} \left[ B_{\mu_i} \langle O_i^{\mu} \rangle - \frac{1}{2} \sum_{j \in C_k} J_{ij}^{\mu\nu} \langle O_i^{\mu} O_j^{\nu} \rangle \right. \nonumber \\
- \left. \frac{1}{2} \sum_{j \notin C_k} J_{ij}^{\mu\nu} \langle O_i^{\mu} \rangle \langle O_j^{\nu} \rangle \right], \tag{6}
\]
entailing the self-consistent conditions
\[
\langle O_i^{\mu} \rangle = \text{Tr} \rho_k O_i^{\mu}, \quad i \in C_k. \tag{7}
\]
We will denote this approach as generalized MF (GMF). The Hamiltonian \( H \) can now be rewritten as
\[
H = h + \langle H - h \rangle - \frac{1}{2} \sum_{i \in C_k, j \notin C_k} J_{ij}^{\mu\nu} \langle O_i^{\mu} \rangle \langle O_j^{\nu} \rangle - \langle O_i^{\mu} \rangle \langle O_j^{\nu} \rangle, \tag{8}
\]
where the last term is the residual interaction.

In the zero temperature limit, \( \rho_k \rightarrow |0_k\rangle \langle 0_k| \), with \( |0_k\rangle \) the GS of \( h_k \) (Eq. (7)). The previous scheme will then lead to the product state
\[
|0_h \rangle = \otimes_k |0_k \rangle, \tag{9}
\]
which minimizes \( \langle H \rangle \) among cluster product states \( \otimes_k |\psi_k\rangle \). It follows from Eq. (9) that \( H \) will connect \(|0_k\rangle \) just with two-cluster excitations \(|n_k n_k'\rangle \), \( k \neq k', n_k \neq 0 \), 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
\[
|0_H^1 \rangle \propto |0_h \rangle + \sum_{k<k',n,n'>0} \alpha_{kn,k'n'} |n_k n_k'\rangle, \tag{10}
\]
\[
\alpha_{kn,k'n'} = \sum_{i \in C_k, j \in C_{k'}} J_{ij}^{\mu\nu} \frac{\langle n_k O_i^{\mu} |0_k\rangle \langle n_{k'} O_i^{\nu} |0_k\rangle}{\varepsilon_{n_k} - \varepsilon_{n_{k'}} + \varepsilon_{n_{k'}} - \varepsilon_{n_k}}, \tag{11}
\]
which contains just two-cluster excitations. While in-cluster correlations are already described by \( |0_k\rangle \), those between clusters can be estimated with the state \( |11\rangle \).

For instance, the reduced state of cluster \( k \) derived from \( |11\rangle \) is \( \langle k | \) (denotes the complementary system)
\[
\rho_k = \text{Tr}_{k \neq k'} |0_H^1\rangle \langle 0_H^1| \propto |0_k\rangle \langle 0_k| + \sum_{n,m} \langle \alpha_{kn,kn'm} \rangle |n_k\rangle \langle n_k|, \tag{12}
\]
which is a mixed state. Its entropy \( S(\rho_k) \) represents the entanglement entropy with the rest of the chain.

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 \( h_{-} = P_z h_{+} P_z \). We can then construct from the parity breaking GS \( |0_{h_{\pm}}\rangle = \otimes_k |0_{+}\rangle + |0_{-}\rangle \) and \( |0_{-}\rangle = P_z |0_{+}\rangle \), the definite parity states (symmetry restoration)
\[
|0_{\pm}\rangle = \frac{|0_{h_{+}}\rangle \pm |0_{h_{-}}\rangle}{\sqrt{2[1 + \text{Re}(|0_{h_{+}}\rangle |0_{h_{-}}\rangle)]}}, \tag{13}
\]
III. APPLICATION TO A DIMERIZED SPIN CHAIN

A. Model and conventional mean field

We now consider a spin 1/2 cyclic chain in a transverse uniform field $B$, coupled through alternating first neighbor $XY$ couplings, such that the system can be viewed, at least for sufficiently weak fields, as strongly coupled pairs weakly interacting with their neighboring pairs (Fig. 1). The Hamiltonian can be written as

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

(16)

where $s_{2i}^\mu$, $\mu = x, y, z$, denotes the spin component at site $i$. Without loss of generality we can suppose $|\alpha| \leq 1$ and, moreover, $\alpha > 0$, both in a cyclic chain ($s_{2n+1}^\mu = s_1^\mu$) with an even number $n$ of pairs or in an open chain with $n$ pairs, as its sign can be changed by a local rotation of angle $\pi$ around the $z$ axis at even pairs (sites $2i - 1$, $2i$, $i$ even)\textsuperscript{12}. A similar rotation at all even sites changes the sign of $J_\mu$, so that we can also assume $J_x \geq 0$, with $|J_y| \leq J_x$. We will set here $0 < J_y < J_x$. Finally, the sign of $B$ can be changed by a similar rotation around the $x$ axis at all sites, so that we will set $B \geq 0$.

Eq. (16) commutes with the total $S_z$ parity

$$ P_z = \exp[-i\pi(S_z + n)] = \otimes_{i=1}^{2n} (2s_i^z), $$

(17)

where $S_z = \sum_{i=1}^{2n} s_i^z$. This implies $(s_i^\mu) = 0$ for $\mu = x, y$ in any non-degenerate eigenstate. The breaking of this symmetry $(s_i^\mu) \neq 0$ for $\mu = x$ or $y$) can be, however, essential in MF descriptions for some field intervals.

In the conventional single spin MF, the trial GS for the present system will be of the form

$$ |0_{mf}\rangle = \otimes_{i=1}^{2n} |0_i\rangle, \quad |0_i\rangle = \cos \frac{\theta}{2} |\downarrow\rangle \pm \sin \frac{\theta}{2} |\uparrow\rangle, $$

(18)

where $\theta$ (assumed uniform) can be obtained from the minimization of $\langle 0_{mf}|H|0_{mf}\rangle = -n(B(\hat{s}_z^2) - \sum_\mu J_\mu (1 + \alpha)\langle \hat{s}_\mu^\mu \rangle^{2})$ or by solving Eq. (3). The result is (Fig. 2 top)

$$ \theta = \frac{B_{c}}{B_s}, \quad 0 \leq B_c \leq B_s^{\alpha} = J_x(1 + \alpha)/2, \quad B < B_{c}^{\alpha}. $$

(19)

For $B < B_{c}$, parity is broken $(s_i^\mu) = \frac{1}{2} \sin \theta$ and the MF solution is degenerate $(\theta = \pm \theta)$. The ensuing energy is

$$ \langle 0_{mf}|H|0_{mf}\rangle = -n \left\{ \frac{B}{2} \left( B_{c}^{\alpha} + B_c \right) \right. B \geq B_{c}^{\alpha} \left. \right\} \quad B < B_{c}^{\alpha}. $$

(20)

This simple approach ignores the dimerized structure of the chain (it is the same as that for a chain with uniform coupling $J_x(1 + \alpha)/2$, and is also blind to the weaker $J_y$ coupling. Yet, it is remarkable that it does become an exact GS at the separability field\textsuperscript{15,17,20,21}

$$ B_{s}^{\alpha} \equiv \sqrt{J_y/J_x}(1 + \alpha)/2, $$

(21)

where $\cos \theta = \sqrt{J_y/J_x}$. At this field the system exhibits a degenerate GS, with the GS subspace spanned by the pair of degenerate MF product states\textsuperscript{17,20}.

B. Pair Mean Field Approximation

In order to improve the conventional MF picture for $B \neq B_{s}^{\alpha}$, we now examine a generalized MF approach based on independent pairs, i.e., on the trial state

$$ |0^p_{mf}\rangle = \otimes_{i=1}^{n} |0_i^p\rangle, $$

(22)

where $|0_i^p\rangle$ are two-spin states. Eq. (22) is obviously exact in the dimerized limit $\alpha = 0$ (independent pairs), and can then be expected to provide a good approximation to the GS at least for weak coupling $|\alpha| \ll 1$.

In the cyclic case, and for the chosen signs of couplings, we may assume $|\psi_i^p\rangle$ site independent and real in the standard product basis of eigenstates of $s_i^x s_i^y$. The most general state of this form can be written as

$$ |0_i^p\rangle = \cos \frac{\beta}{2} |\psi_{\phi}\rangle + \sin \frac{\beta}{2} |\uparrow\uparrow\rangle, $$

(23)

$$ |\psi_{\phi}\rangle = \cos \frac{\theta}{2} (|\downarrow\downarrow\rangle \pm \sin \frac{\phi}{2} |\uparrow\uparrow\rangle) + \sin \frac{\theta}{2} |\uparrow\downarrow\rangle \pm \sin \frac{\phi}{2} |\downarrow\uparrow\rangle. $$

FIG. 1. (Color online) Schematic plot of the dimerized cyclic chain.

which will normally be non-degenerate in finite systems and which lead to a non-perturbative entanglement between composite sites: Neglecting the complementary overlap $\prod_{k \neq k} \langle 0_{k+} | 0_{k-} \rangle$, typically small, the ensuing reduced state of the cluster $k$ will be

$$ \rho_k = \text{Tr}_n |0_{k+} \rangle \langle 0_{k+}| \approx \frac{1}{2} (|0_{k+}\rangle \langle 0_{k+}| + |0_{k-}\rangle \langle 0_{k-}|), $$

(15)

which is a rank 2 mixed state with eigenvalues $p_\pm = \frac{1}{2}(1 \pm \prod_{k \in G} |0_{k+}\rangle \langle 0_{k-}|))$ 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 chain 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 $p_\pm = \frac{1}{2}(1 \pm \prod_{k \in G} |0_{k+}\rangle \langle 0_{k-}|)$. For a large group $p_\pm \rightarrow 1/2$, and $S(\rho_G) \rightarrow \ln 2$. Such contribution is analogous to a topological entropy\textsuperscript{12}.
Nonetheless, in the GS the singlet state will not be occupied \((\beta = 0)\) for the present couplings. We then obtain
\[
\langle 0^p_{\text{mf}} | H | 0^p_{\text{mf}} \rangle = n [B \langle s_1^x + s_2^x \rangle - \sum_{\mu=x,y} J_{\mu} (\langle s_1^\mu s_2^\mu \rangle + \alpha (\langle s_1^\mu \rangle \langle s_2^\mu \rangle)]
\]
\[= -n \left[ (B \cos \phi + J_+ \sin \phi) \cos^2 \frac{\theta}{2} + J_+ \sin^2 \frac{\theta}{2} + \frac{1}{2} \alpha J_x \sin^2 \theta (1 + \sin \phi) \right], \tag{24}
\]
where \(J_\pm = J_x \pm J_y\). The values of \(\theta, \phi\) can be determined by minimizing this expression, or alternatively, by Eqs. (23), i.e., imposing that \(|0^p_{\text{mf}}\rangle\) be the lowest eigenstate of
\[
h^p = B(s_1^x + s_2^x) - \sum_{\mu=x,y} J_{\mu} [s_{1\mu} s_{2\mu} + \alpha (\langle s_1^\mu \rangle s_{2\mu} + \langle s_2^\mu \rangle s_1^\mu)]. \tag{25}
\]
The resulting values of \(\theta \) and \(\phi \) are
\[
\begin{align*}
\theta &= 0, \tan \phi = J_- / B, \quad B \geq B_{c2}^\alpha, \tag{26a} \\
\cos \theta &= \frac{2 B \cos \phi + J_+ \sin \phi - J_+}{J_+ \cos \phi + \frac{1}{2} J_+ \sin^2 \phi}, \quad B_{c1}^\alpha < B < B_{c2}^\alpha \tag{26b} \\
\tan \phi &= \frac{J_+ \cos \theta + \frac{1}{2} J_+ \sin^2 \theta}{J_+ \cos \phi + \frac{1}{2} J_+ \sin^2 \phi}, \quad B = B_{c1}^\alpha \tag{26c}
\end{align*}
\]
where the critical fields are given by
\[
B_{c1}^\alpha = \frac{1}{2} \sqrt{J_x (J_y - 2 \alpha J_x)}, \tag{27}
\]
\[
B_{c2}^\alpha = \frac{1}{2} \sqrt{(J_+ + \frac{3}{2} J_x)^2 + 2 \alpha J_x J_-)^2 - 4 J_-^2}, \tag{28}
\]
as obtained from (26b) for \(\theta \to 0 \) and \(\pi \). The solution of system (26b) for \(\theta \) and \(\phi \) can in fact be determined analytically (it leads to a quartic equation for \(\cos \phi \)).

In contrast with the standard MF, it is first seen that a parity breaking solution \((\theta \in (0, \pi/2))\) will now arise just within a field window \(B_{c1}^\alpha < B < B_{c2}^\alpha \) if \(\alpha \) is sufficiently small, as depicted in Fig. 2 (bottom panel). For \(B < B_{c1}^\alpha\), the pair MF leads to a fully dimerized phase, where the strongly coupled pairs are in a \(P_z = -1\) Bell state \(\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}\) and hence maximally entangled. On the other hand, for \(B > B_{c2}^\alpha\) the approach leads to a partially entangled \(P_z = 1\) pair state \(\cos \frac{\theta}{2} |\downarrow\downarrow\rangle + \sin \frac{\theta}{2} |\uparrow\uparrow\rangle\), which is only partially aligned. The intermediate parity breaking phase (26b) 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 \((\theta = \pm \theta_0)\). It is verified that the actual exact GS obtained from the Jordan-Wigner fermionization becomes in a finite chain nearly two-fold degenerate within this interval, leading as well to almost maximally entangled pairs for lower fields (see appendix and next section).

In the parity preserving phases, the pair MF GS energy obtained from (24) is just
\[
\langle 0^p_{\text{mf}} | H | 0^p_{\text{mf}} \rangle = -n \left\{ \begin{array}{ll}
\sqrt{B^2 + J_-^2}, & B \geq B_{c2}^\alpha \\
J_+ , & B \leq B_{c1}^\alpha
\end{array} \right., \tag{29}
\]

which is verified to be lower than the conventional MF energy (20) in these intervals.

![Fig. 2](image-url)  
FIG. 2. (Color online) Phase diagram of the dimerized spin 1/2 chain according to the conventional (top panel) and pair (bottom panel) mean field approaches, for \(J_y/J_x = 1/2\). The corresponding states for the unit cell are indicated. While in the conventional MF the \(S_z\) parity breaking phase arises below a critical field \(B_{c1}^\alpha\), in the pair MF it occurs within a field window \(B_{c1}^\alpha < B < B_{c2}^\alpha\). At \(B < B_{c1}^\alpha\), the dimerized state with maximally entangled pairs is preferred. The dashed lines denote the factorizing field \(B_{c2}^\alpha\) where both MF approaches coincide and are exact.

The factorizing field $B_{c2}^\alpha$ lies within the parity breaking phase \(\forall \alpha > 0: B_{c1}^\alpha < B_{c2}^\alpha < B_{c2}^\alpha\). It is verified that at $B = B_{c2}^\alpha$, Eq. (26b) leads to $\cos \theta = J_y/J_x$ and $\tan \phi = 2 J_y/\sqrt{J_+ J_-}$, implying
\[
\tan^2 \theta/2 = \sin \phi, \tag{30}
\]
which is precisely the condition ensuring that the pair state (23) reduces to a product of single spin states.

On the other hand, for $\alpha \to 0$ (where the pair MF becomes exact), $B_{c2}^\alpha$ and $B_{c2}^\alpha$ merge (Fig. 2), approaching both the $\alpha = 0$ factorizing field $B_{0}^\alpha = \sqrt{J_y J_+/2} (B_{c1,2}^\alpha \approx B_{0}^\alpha (1 + \alpha J_x) / \sqrt{2} J_-)$ for small $\alpha$. The exact GS of an isolated pair undergoes (for $J_y > 0$) a sharp parity transition at $B = B_{0}^\alpha$, from the Bell state $\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}$ for $B < B_{0}^\alpha$, with energy $-J_+$, to the state $\cos \frac{\theta}{2} |\downarrow\downarrow\rangle + \sin \frac{\theta}{2} |\uparrow\uparrow\rangle$ for $B > B_{0}^\alpha$, with energy $-\sqrt{B^2 + J_-^2}$. At $B = B_{0}^\alpha$, these states become degenerate and coincide with the definite
parity combinations (14) of the MF product states (18).
It is also seen from Eq. (27) that $B_{c1}^0$ vanishes for 
\[ \alpha = \alpha_c \equiv \frac{J_y}{2J_x}. \] (31)
If $\alpha > \alpha_c$ (or $J_y < 0$) parity is broken for all $B < B_{c2}^0$, as in the standard MF. Nonetheless, important differences between the conventional and pair MF persist: $B_{c2}^0$ remains lower than the std. MF critical field $B_c^0$, even for $\alpha = 1$, and strongly coupled pair remains partially entangled even for strong fields $B > B_{c2}^0$. Full alignment occurs only for $B \to \infty$, 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 $\theta$ and $\phi$. We should add that if $J_y < 0$ (with $|J_y| \leq J_x$), $B_{c2}^0$ vanishes at $\alpha = -\frac{J_y}{2J_x}$, entailing no parity breaking phase in the pair MF for $\alpha$ below this value.

Let us remark that the pair MF approach remains applicable in more complex situations where exact analytic results are no longer feasible. For instance, if adjacent pairs are further connected by second and third neighboring couplings $\alpha_2 J_\mu$ (for spins like 1-3 and 2-4 in Fig. 1) and $\alpha_3 J_\mu$ (for spins like 1-4), all previous MF phases and expressions remain valid with the replacement 
\[ \alpha \to \alpha + 2\alpha_2 + \alpha_3, \] (32)
provided $\alpha_{2,3}$ are positive or sufficiently small. However, the Jordan-Wigner fermionization will no longer lead here to a quadratic fermionic Hamiltonian. Similar considerations hold for longer range couplings or the addition of $s_i^z s_j^z$ terms. The pair MF approach can also be directly applied for $T > 0$ (Eq. (31)), leading to a critical temperature $T_c(B, \alpha, J_\mu)$ for the parity-breaking phase.

C. Entanglement predictions and comparison with exact results

We plot in Figs. 3-4 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 (22) leads, after the symmetry restoration (14)-(15), to the reduced state 
\[ \rho_{12}^{\text{GMP}} = \left( \begin{array}{cccc}
\cos^2 \frac{\theta}{2} \sin^2 \frac{\phi}{2} & 0 & 0 & \frac{1}{2} \cos^2 \frac{\theta}{2} \sin \phi \\
0 & \frac{1}{2} \sin^2 \frac{\theta}{2} \sin^2 \frac{\phi}{2} & 0 & 0 \\
0 & 0 & \frac{1}{2} \sin^2 \frac{\theta}{2} \sin^2 \frac{\phi}{2} & 0 \\
\frac{1}{2} \cos^2 \frac{\theta}{2} \sin \phi & 0 & 0 & \cos^2 \frac{\theta}{2} \cos^2 \frac{\phi}{2} \end{array} \right) \] (33)
(expressed in the std. basis) after neglecting the overlap $\langle \psi_{\theta_0} | \psi_{-\theta_0} \rangle$ in the parity breaking phase. In this phase it is a rank 2 mixed state (and is pure otherwise), with eigenvalues $(\sin^2 \frac{\theta}{2}, \cos^2 \frac{\theta}{2})$. 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 remaining 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 (13).
Note that the entropy \( S(\rho_{12}) \) does not vanish as \( B \) approaches the factorizing field \( B_{c1}^d \) in Fig. 3, since the exact GS remains with a definite parity (and hence entangled) in its immediate vicinity. In fact, for \( B \to B_{c1}^d \) the result obtained from (33) becomes exact (except for the small neglected overlap), as the parity restored pair MF GS is exact in this limit. Actually, at \( B = B_{c1}^d \) the exact GS is degenerate (see appendix), so that GS entanglement will depend at this point on the choice of GS. The result obtained from (33) corresponds to the definite parity GS’s \( |\downarrow\downarrow\rangle \) which are the actual side limits of the exact GS for \( B \to B_{c1}^d \).

The single spin state derived from (33) is just

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

which is of the form \( \frac{1}{2}(\rho_1^+ + \rho_1^-) \) in the parity breaking phase, with \( \rho_1^\pm \) the single spin reduced states derived from the pair state \( |\downarrow\downarrow\rangle \) 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 maximum in the dimerized phase \( B < B_{c1}^d \), but decreases sharply in the parity breaking phase (when the pair becomes entangled with the rest of the chain) and smoothly in the partially aligned phase \( B > B_{c2}^d \). The result derived from (34) is again fully exact for \( B \to B_{c1}^d \).

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

In contrast, it is verified in all panels that the conventional MF [13] 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,

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

which is a rank 2 state for \( \theta \in (0, \pi) \) with eigenvalues \( \frac{1 \pm \cos^2 \theta}{2} \). Nonetheless, 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 (34) but with \( p_{\pm} = (1 \mp \cos \theta)/2 \), 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 \( B_{c1}^a \). Here the reduced states (33) and (34) become identical and, moreover, exact.

Fig. 3 depicts the concurrence, a measure of the entanglement between the spins of pair, for both strongly (1-2) and weakly (2-3) coupled pairs. In the first case, the pair MF state (33) leads to the concurrence

\[
C(\rho_{12}^{\text{GMF}}) = |\cos^2 \frac{\theta}{2}(1 + \sin \phi) - 1|,
\]

which is parallel (as that in a state \(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\) if the term within the bars is positive, i.e., \( B > B_{c1}^a \), and antiparallel (as that in \(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\) if this term is negative, i.e., \( B < B_{c1}^a \), vanishing at the factorizing field \( B_{c1}^a \) (see below). As seen in the top panel, the pair MF result shows again a very good agreement with the exact result for all fields, correctly predicting a maximally entangled pair for low fields \( B < B_{c1}^a \). Note that for \( B < B_{c3}^a \) and \( B > B_{c2}^a \), the state (33) is pure, implying that the pair MF concurrence
is just a function of $S(\rho_1^{\text{GMF}})$, and given by

$$C_{12}^{\text{GMF}} = \begin{cases} \frac{1}{B_{c1}^\alpha}, & B < B_{c1}^\alpha, \\ \frac{1}{B_{c2}^\alpha}, & B > B_{c2}^\alpha, \end{cases}$$

(37)
decreasing as $J_-/B$ for strong fields $B \gg J_-$. However, in the parity breaking phase the state (53) is mixed and the concurrence (56) is no longer a function of $S(\rho_1^{\text{GMF}})$.

In fact, and as opposed to the previous entropies, it vanishes at the factorizing field $B_{c1}^\alpha$, as can be verified from Eq. (30), since the state (53) becomes separable (a convex combination of product states) 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 ($S(\rho_1^{\text{GMF}}) \neq 0$), indicating that no traces of dimerization remain.

We also mention that the fidelity $\rho_{23}$ of the state (53) with the exact $\rho_{12}$, $F = \text{Tr} \sqrt{\rho_{12}^{\text{GMF}} \rho_{12}}$, is very high ($\gtrsim 0.99$ for $\alpha = 0.1$ in all phases). In contrast, the conventional MF state (35) has a low fidelity, especially for $B < B_{c2}^\alpha$, and leads to a zero concurrence $\forall B$, since it is a separable state ($\rho_{12}^{\alpha} = \frac{1}{2} (\rho_1^x \otimes \rho_1^y + \rho_1^y \otimes \rho_1^x)$, with $\rho_1^x$ 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 $\tilde{\rho}_{23}^{\text{GMF}+P}$ derived from the perturbed pair MF state (11). This concurrence is small and starts to be non-zero just before the factorizing field $B_{c1}^\alpha$, having peaks at both sides of $B_{c1}^\alpha$. We should actually recall that at the immediate vicinity of $B_{c1}^\alpha$ (i.e., $B \to B_{c1}^\alpha$) 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 $|\langle \psi_{0\alpha} | \psi_{-\alpha} \rangle|^{-1}$ is conserved$^{17,20}$.

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 $\forall \alpha$.

Finally, we plot in Fig. 5 some basic energy level predictions, in order to provide a general view of the approach. As seen in the top panel, the pair MF GS energy significantly improves the conventional MF result, especially for $B < B_{c1}^\alpha$. In the bottom panel, we depict for 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 $E_{0}^{\text{ex}} = \varepsilon_m - \varepsilon_0$ (using the notation of Eq. (11)), 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 MF, this leads to the perturbed pair excitation energies

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

(38)
where $\varepsilon_m$ are the eigenvalues of the single pair Hamiltonian (25) $(h^p|m\rangle = \varepsilon_m |m\rangle)$, with $\varepsilon_0$ its GS energy, and $k = 1, \ldots, n$. These energies are those of the (discrete) Fourier transformed states $|\hat{m}_k\rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} e^{i2\pi kj/n} |m_j\rangle$, where $|m_j\rangle$ denotes the state with pair $j$ at excited level $m$. As seen in the bottom panel, the result obtained from (38) 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 (38) become

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

(39)
with $+$ for $B < B_{c1}^\alpha$ and $-$ for $B > B_{c2}^\alpha$. For $n = 4$, $E_4 = E_{13}^{\text{ex}} = E_1^{\text{ex}}$, so that just three levels are seen.

In contrast, the conventional MF leads to a single spin excitation energy $E_{\text{ex}}^{\text{GMF}} = B$ for $B > B_{c2}^\alpha$ and $J_+ (1 + \alpha)/2$ if $B < B_{c2}^\alpha$, which lies well above the previous levels.

The parity breaking phase of the pair MF approach is also seen (bottom panel) to coincide approximately with
the region where the exact GS of the finite chain becomes nearly degenerate. The exact lowest energy levels of each parity sector become 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 $B^0$. This interval is enclosed by the fields $B^e_1$ and $B^e_2$ where the lowest quasiparticle energy of the Jordan-Wigner fermionized Hamiltonian vanishes (see appendix).

IV. CONCLUSIONS

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

In the dimer-type chain considered, the approach naturally leads to a pair MF approximation which is still analytic and simple, but which considerably improves the plain single spin MF. It produces a proper phase diagram which clearly identifies a dimerized phase for weak fields, together with a reduced parity breaking phase which represents a transitional region to the strong field regime. With the pair MF plus parity restoration, it is possible to directly describe the GS internal concurrence of strongly coupled pairs as well its entanglement (together with that of a single spin and that of a weakly coupled pair) with the rest of the chain. Parity breaking was shown to be a signature of a non-negligible entanglement of the strongly coupled pair with the remaining chain in the exact GS. With the addition of simple perturbative corrections, it is also possible to describe the concurrence of weakly coupled pairs and to improve the previous entanglement predictions, as well as to describe the main features of the energy spectrum.

The generalized MF can be used as starting point for implementing more sophisticated techniques. It is also directly applicable at finite temperatures. Besides, the extended formalism also allows to devise mixed self-consistent schemes in which just the main internal couplings of the cell are exactly taken into account, leaving the others for the MF. These aspects and their application to more complex systems are currently under investigation.

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Appendix: Exact solution of the dimer chain

By means of the Jordan-Wigner transformation, and for a fixed value $P = \pm$ of the global $S_z$-parity $P_z$ (Eq. (14)), we may exactly rewrite the dimerized Hamiltonian (16) as a quadratic form in standard fermion creation and annihilation operators $c_1^\dagger, c_j$, which in terms of the spin operators read

$$c_j^\dagger = s_j^+ \exp[-i\pi \sum_{k=1}^{j-1} s_k^+ s_k^-], \quad (A.1)$$

where $s_j^\pm = s_j^x \pm is_j^y$. These operators fulfill the fermionic anticommutation relations $[c_j, c_k^\dagger]_+ = \delta_{jk}, [c_j, c_k]_+ = 0$. The corresponding inverse transformation is

$$s_j^+ = c_j^\dagger \exp[i\pi \sum_{k=1}^{j-1} c_k^\dagger c_k]. \quad (A.2)$$

We then obtain, setting $J_{\pm} = \frac{J_{+} + J_{-}}{4}$,

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

where $r_j = \begin{cases} 1 & (j \text{ odd}) \\ 0 & (j \text{ even}) \end{cases}$ and $\eta_j^P = 1 - 2\delta_{j,2n}$, $\eta_j^P = 1$ in the cyclic case. Through separate parity dependent discrete Fourier transforms for even and odd sites,

$$\left( \begin{array}{c} c_{2j-1}^\dagger \\ c_{2j}^\dagger \\ \vdots \\ c_{2n}^\dagger \end{array} \right) = \frac{1}{\sqrt{n}} \sum_{k \in K_0} e^{-i2\pi kj/n} \left( \begin{array}{c} c_{k-1}^\dagger \\ c_k^\dagger \\ \vdots \\ c_{k+n-1}^\dagger \end{array} \right),$$

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

$$H^P = \sum_{k \in K_0} \sum_{\sigma = \pm} B(c_{k,\sigma}^\dagger c_{k,\sigma} - \frac{1}{2})$$

$$- (J_{\sigma}^k c_{k-\sigma}^\dagger c_{k+\sigma} + J_{\sigma}^k c_{k-\sigma} c_{k+\sigma} + h.c.)$$

$$= \sum_{k \in K_0} \sum_{\nu = \pm} \lambda_k^\nu (a_{k\nu}^\dagger a_{k\nu} - \frac{1}{2}), \quad (A.4)$$

where $J_{\pm}^k = J_{\pm} (1 + \alpha e^{-i2\pi k/n})$ and $-k \equiv n - k$. The final diagonal form (A.4) is obtained by means of a Bogoliubov transformation $c_{k,\sigma}^\dagger = \sum_{\nu = \pm} U_{k,\sigma\nu}^\dagger a_{k\nu} + V_{k,\sigma\nu}^\dagger a_{-k\nu}$ determined through the diagonalization of $4 \times 4$ blocks

$$\mathcal{H}_k = \left( \begin{array}{cccc} B & -J_0^- & 0 & -J_0^+ \\ -J_0^+ & B & J_0^- & 0 \\ 0 & J_0^- & -B & J_0^+ \\ -J_0^+ & 0 & J_0^- & -B \end{array} \right), \quad (A.5)$$

whose eigenvalues are $\pm \lambda_k^+, \pm \lambda_k^-$, with

$$|\lambda_k^\pm| = \sqrt{\Delta \pm \sqrt{\Delta^2 - (B^2 - (J_0^+ + J_0^-)(J_0^- - J_0^+))^2}} \quad (A.6)$$
\[ \Delta = B^2 + |J^x_k|^2 + |J^y_k|^2. \]

Care should be taken to select the correct signs of \( \lambda_k^z \) in order that the vacuum of the operators \( a_k \) 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 \( f_{ij} = \langle c_i^\dagger c_j \rangle - \frac{1}{2} \delta_{ij} \), \( g_{ij} = \langle c_i^\dagger_1 c_j^\dagger_1 \rangle \), which can be directly obtained from the inverse Fourier transform of \( \langle c^\dagger_1 k_\alpha c^\dagger_{-k_\alpha} \rangle = \sum_{\nu} V^\dagger_{k\nu} V_{k\nu} \), \( \langle c^\dagger_{k_\alpha} c^\dagger_{-k_\alpha} \rangle = \sum_{\nu} V^\dagger_{k\nu} V_{k\nu} \).

We then obtain, through the use of Wick’s theorem, matrices of elements \( f_{ij} \) and \( \Delta = \sum_{\nu} V^\dagger_{k\nu} V_{k\nu} \), \( \sum_{\nu} c_{k\nu}^\dagger c_{-k\nu} \).

The fields (A.7)–(A.8) enclose the interval where the pair MF critical fields \( B_{c1} \) and \( B_{c2} \), and satisfy

\[ B_{c1} \leq B_{c1}^{ex} \leq B_s^0 \leq B_{c2}^{ex} \leq B_{c2}, \quad (A.9) \]

for \( J_y \geq 0 \), all approaching the factorizing field \( B_{c2}^0 = \sqrt{J_x J_y} \) for \( \alpha \to 0 \) (where \( B_{c2}^{ex} \approx B_{c2}^0 [1 \mp \frac{B_{c2}^0}{J_y} (J_x + J_y)] \)).

The fields [A.7–A.8] 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 \( B = B_{c2}^{ex} \), the exact GS of the finite chain will experience \( n \) parity transitions in the interval \( (B_{c1}^{ex}, B_{c2}^{ex}) \), with the last one taking place exactly at the factorizing field \( B_s^0 \).

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