Evaluation of ground-state entanglement in spin systems with the random phase approximation

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We discuss a general treatment based on the mean field plus random-phase approximation (RPA) for the evaluation of subsystem entropies and negativities in ground states of spin systems. The approach leads to a tractable general method that becomes straightforward in translationally invariant arrays. The method is examined in arrays of arbitrary spin with XYZ couplings of general range in a uniform transverse field, where the RPA around both the normal and parity-breaking mean-field state, together with parity-restoration effects, is discussed in detail. In the case of a uniformly connected XYZ array of arbitrary size, the method is shown to provide simple analytic expressions for the entanglement entropy of any global bipartition, as well as for the negativity between any two subsystems, which become exact for large spin. The limit case of a spin s pair is also discussed.

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I. INTRODUCTION

The study of entanglement constitutes one of the most active and challenging research areas, being of central interest in the fields of quantum information [1] and many-body physics [2]. The concept of entanglement has provided a new perspective for analyzing quantum correlations and quantum critical phenomena in many-particle systems and has led to fundamental results and new insights in the field [2–5]. Nonetheless, the evaluation of entanglement in general strongly interacting many-body systems remains a difficult task, particularly in systems with long-range interactions, high connectivity, and large dimensionality, where usual treatments such as the quantum Monte Carlo [6], density-matrix renormalization group (DMRG) [7], or matrix product states [8] become more involved or difficult to implement. In previous works [9,10] we have applied a general mean field plus random-phase approximation (RPA) treatment to the evaluation of pairwise entanglement (i.e., that between two elementary components) in spin systems at zero and finite temperature. The approach was able to capture the main features of the entanglement between two spins in arrays with XY and XYZ couplings of different ranges, including the prediction of full-range pairwise entanglement in the vicinity of the factorizing field [10–12]. The accuracy of the approach was shown to increase with the interaction range or connectivity.

The aim of the present work is to examine if the previous method is capable of predicting, in the ground state of spin systems, the entanglement properties of *general* subsystems. We will focus on the entanglement entropy of arbitrary bipartitions of the whole system, as well as on the negativity between *any* two subsystems, not necessarily complementary, where the rest of the spins play the role of an environment and entanglement can no longer be measured through the subsystem entropy. Other measures, like the negativity (an entanglement monotone computable for general mixed states [13,14]), have to be employed. This type of entanglement has recently received special attention [15–17] since its behavior can differ from that of global bipartitions. We will show that the present approximation provides a general tractable scheme for evaluating these quantities and becomes analytic in translationally invariant systems.

In Sec. II we present the general RPA formalism and describe the RPA spin state, the associated bosonic estimation of subsystem entropies and negativities, the implementation in translationally invariant systems, and the application to a general spin s array with XYZ couplings of arbitrary range in a transverse magnetic field. Symmetry-restoration effects in the case of parity-breaking mean fields are also discussed. As an illustration, we derive in Sec. III results for a spin s pair and for a fully connected finite spin s array, where RPA is able to provide simple full analytic expressions for subsystem entropies and negativities, which represent the exact large-spin limit at any fixed size. Conclusions are drawn in Sec. IV. Appendix A discusses the equivalence between the spin and the bosonic RPA treatments, and Appendix B contains details of the analytic results of Sec. III.

II. FORMALISM

A. RPA for spin systems at $T = 0$

We will consider a general finite system of spins $\boldsymbol{s}_i = (s_{ix}, s_{iy}, s_{iz})$, connected through general quadratic couplings and immersed in a magnetic field, not necessarily uniform. The corresponding Hamiltonian is

$$H = \sum_{i,\mu} B^{i\mu} s_{i\mu} - \frac{1}{2}\sum_{i\neq j,\mu,\nu} J^{i\mu j\nu} s_{i\mu} s_{j\nu}, \tag{1}$$

where $\mu = x,y,z,$ and $B^{i\mu}$ are the field components at site i. Ising, XY, XYZ ($J^{i\mu j\nu} = \delta^{\mu\nu} J^{ij}_{\mu}$), as well as Dzyaloshinskii-Moriya ($J^{i\mu,j\nu} = -J^{i\nu,j\mu}$) couplings of arbitrary range are particular cases of Eq. (1).

The first step in the RPA [18] is to determine the mean-field ground state, i.e., the separable state

$$|0\rangle \equiv \otimes_{i=1}^{n} |0_i\rangle = |0_1 \cdots 0_n\rangle,$$

with the lowest energy $\langle H\rangle_0 = \langle 0|H|0\rangle$, given by

$$\langle H\rangle_0 = \sum_{i,\mu} B^{i\mu}\langle s_{i\mu}\rangle_0 - \frac{1}{2}\sum_{i\neq j,\mu,\nu} J^{i\mu j\nu}\langle s_{i\mu}\rangle_0 \langle s_{j\nu}\rangle_0, \tag{2}$$

where $\langle \boldsymbol{s}_i\rangle_0 = \langle 0_i|\boldsymbol{s}_i|0_i\rangle$. Each local state $|0_i\rangle$ can be determined self-consistently as the lowest eigenstate of the local mean-field Hamiltonian

$$h_i = \sum_{\mu} \frac{\partial \langle H\rangle_0}{\partial \langle s_{i\mu}\rangle_0} s_{i\mu} = \boldsymbol{\lambda}^i \cdot \boldsymbol{s}_i, \tag{3}$$

being the state with maximum spin s_i directed along $-\boldsymbol{\lambda}^i$ (a local coherent state). This leads to the self-consistent equations

$$\lambda^{i\mu} = B^{i\mu} - \sum_{j\neq i,\nu} J^{i\mu j\nu}\langle s_{j\nu}\rangle_0, \quad \langle \boldsymbol{s}_i\rangle_0 = -s_i\boldsymbol{\lambda}^i/\lambda^i, \quad (4)$$

where $\lambda^i = |\boldsymbol{\lambda}^i|$. Equation (4) can be solved iteratively starting from an initial guess for $|0_i\rangle$ or $\boldsymbol{\lambda}_i$, although other procedures (such as the gradient method) can be employed. Equation (2) becomes $\langle H\rangle_0 = \frac{1}{2}\sum_i(\boldsymbol{\lambda}^i + \boldsymbol{B}^i)\cdot\langle \boldsymbol{s}_i\rangle_0$.

Since the form (1) is valid for any choice of the local axes, it is now convenient to choose z_i along $\boldsymbol{\lambda}^i$, such that $\langle s_{i\mu}\rangle_0 = -s_i\delta_{\mu z}$ and $\lambda^{i\mu} = \lambda^i\delta^{\mu z}$, with $\lambda^i > 0$. The second step in the RPA is the approximate bosonization

$$s_{i+} \to \sqrt{2s_i}b_i^\dagger, \quad s_{i-} \to \sqrt{2s_i}b_i, \quad s_{iz} \to -s_i + b_i^\dagger b_i, \quad (5)$$

where $s_{i\pm} = s_{ix} \pm i s_{iy}$ and b_i, $b_i^\dagger$ are considered standard boson operators ($[b_i,b_j^\dagger] = \delta_{ij}$, $[b_i,b_j] = [b_i^\dagger,b_j^\dagger] = 0$), with $|0\rangle \to |0_b\rangle$ as their vacuum. This bosonization is in agreement with that implied by the path integral formalism of Refs. [9,10] for $T \to 0$ and preserves two of the exact spin commutators exactly ($[s_i^z,s_j^\pm] = \pm\delta_{ij}s_i^\pm$); the remaining one is preserved as vacuum average ($\langle[s_i^-,s_j^+]\rangle_0 = 2s_i\delta_{ij}$). It coincides with the Holstein-Primakoff and other exact bosonizations [18–21] up to zeroth order in s_i^{-1}.

The third step is to replace Eq. (5) in the original Hamiltonian (1), neglecting all cubic and quartic terms in b_i, $b_i^\dagger$. This leads to the quadratic boson Hamiltonian:

$$H^b = \langle H\rangle_0 + \sum_i \lambda^i b_i^\dagger b_i - \sum_{i\neq j}\Delta_+^{ij} b_i^\dagger b_j + \frac{1}{2}(\Delta_-^{ij} b_i^\dagger b_j^\dagger + \text{H.c.})$$

$$= \langle H\rangle_0 - \frac{1}{2}\sum_i \lambda^i + \frac{1}{2}\mathcal{Z}^\dagger\mathcal{H}\mathcal{Z}, \quad (6)$$

$$\mathcal{Z} = \begin{pmatrix} b \\ b^\dagger \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} \Lambda - \Delta_+ & -\Delta_- \\ -\bar{\Delta}_- & \Lambda - \bar{\Delta}_+ \end{pmatrix}, \quad (7)$$

$$\Delta_\pm^{ij} = \frac{1}{2}\sqrt{s_i s_j}[J^{ixjx} \pm J^{iyjy} - i(J^{iyjx} \mp J^{ixjy})], \quad (8)$$

where $\mathcal{Z}^\dagger = (b^\dagger, b)$ and $\Lambda^{ij} = \lambda^i\delta^{ij}$. The choice of the mean-field axes for the bosonization (5) ensures that no linear terms in b_i, $b_i^\dagger$ appear in H^b; this reflects the stability of the mean-field state $|0\rangle$ with respect to one-site excitations.

The last step is the diagonalization of the bosonic quadratic form (6), which is always possible when the Hermitian matrix $\mathcal{H}$ in Eq. (7) *is positive definite*, i.e., when $|0\rangle$ is a stable vacuum [18]. H^b can then be rewritten as

$$H^b = \langle H\rangle_0 + \sum_\alpha \omega^\alpha b'^\dagger_\alpha b'_\alpha + \frac{1}{2}(\omega^\alpha - \lambda^\alpha), \quad (9)$$

where λ^α stands for λ^i, ω^α are the symplectic eigenvalues of $\mathcal{H}$, i.e., the positive eigenvalues of the matrix

$$\mathcal{M}\mathcal{H} = \begin{pmatrix} \Lambda - \Delta_+ & -\Delta_- \\ \bar{\Delta}_- & -\Lambda + \bar{\Delta}_+ \end{pmatrix}, \quad \mathcal{M} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (10)$$

whose eigenvalues come in pairs of opposite sign (and which is diagonalizable with real nonzero eigenvalues when $\mathcal{H}$ is positive definite), and b'_α, $b'^\dagger_\alpha$ are "collective" boson operators related to the local ones by a Bogoliubov transformation $\mathcal{Z} = \mathcal{W}\mathcal{Z}'$, i.e.,

$$\begin{pmatrix} b \\ b^\dagger \end{pmatrix} = \mathcal{W}\begin{pmatrix} b' \\ b'^\dagger \end{pmatrix}, \quad \mathcal{W} = \begin{pmatrix} U & V \\ \bar{V} & \bar{U} \end{pmatrix}, \quad (11)$$

with $\binom{U}{\bar{V}}_\alpha$ and $\binom{V}{\bar{U}}_\alpha$ being the eigenvectors of $\mathcal{M}\mathcal{H}$ associated with the eigenvalues ω_α and $-\omega_\alpha$, respectively (such that $\mathcal{W}^{-1}\mathcal{M}\mathcal{H}\mathcal{W} = \mathcal{M}\Omega$, with $\Omega_{\alpha\alpha'} = |\omega_\alpha|\delta_{\alpha\alpha'}$). In order to preserve the boson commutation relations, which can be cast as $\mathcal{Z}\mathcal{Z}^\dagger - [(\mathcal{Z}^\dagger)^{\text{tr}}\mathcal{Z}^{\text{tr}}]^{\text{tr}} = \mathcal{M}$, $\mathcal{W}$ should satisfy

$$\mathcal{W}\mathcal{M}\mathcal{W}^\dagger = \mathcal{M}, \quad (12)$$

which also implies $\mathcal{W}^\dagger\mathcal{M}\mathcal{W} = \mathcal{M}$ and hence $\mathcal{W}^\dagger\mathcal{H}\mathcal{W} = \Omega$. This means that $U^\dagger V - V^{\text{tr}}\bar{U} = 0$, $U^\dagger U - V^{\text{tr}}\bar{V} = I$, which are the natural orthogonality relations fulfilled by the eigenvectors of Eq. (10) with normalization $\binom{U}{\bar{V}}^\dagger_\alpha\mathcal{M}\binom{U}{\bar{V}}_\alpha = 1$.

The RPA matrix (7) is of dimension $2n \times 2n$, with n being the number of spins. The RPA then involves an exponential reduction in the dimension [from $(2s+1)^n$ to $2n$ for n identical spins]. Moreover, in a translationally invariant system (see Sec. II D), it can be further reduced to n 2×2 matrices and become *fully analytic*.

B. The RPA ground state

The vacuum of the new bosons b' ($b'_\alpha|0'_b\rangle = 0$) is [18]

$$|0'_b\rangle = C_b \exp\left(\frac{1}{2}\sum_{i,j} Z^{ij} b_i^\dagger b_j^\dagger\right)|0_b\rangle, \quad Z = V\bar{U}^{-1}, \quad (13)$$

where $C_b = \langle 0_b|0'_b\rangle = \det[(\bar{U})]^{-\frac{1}{2}}$ is a normalization factor, and Z is a symmetric matrix. The associated RPA spin state can then be defined as

$$|0_{\text{RPA}}\rangle = C_s \exp\left(\frac{1}{2}\sum_{i\neq j}\frac{Z^{ij}}{2\sqrt{s_i s_j}} s_{i+}s_{j+}\right)|0\rangle. \quad (14)$$

The expectation values generated by Eq. (14) will be close to those obtained with the mapping (5), coinciding exactly up to second order in V (Appendix A). In contrast with $|0\rangle$, the state (14) is *entangled* (unless $V = 0$).

Let us note the following for the quadratic Hamiltonian (1):

(i) $|0_{\text{RPA}}\rangle = |0\rangle$ *if and only if* $|0\rangle$ is an exact eigenstate of H, since H^b contains the *exact* matrix elements connecting $|0\rangle$ with the rest of the Hilbert space:

$$H|0\rangle = \langle H\rangle_0|0\rangle - \frac{1}{2}\sum_{i,j}\Delta_-^{ij}|1_i 1_j\rangle, \quad (15)$$

where $|1_i 1_j\rangle = \frac{s_{i+}s_{j+}}{2\sqrt{s_i s_j}}|0\rangle$, and we have used the mean-field condition $\langle 1_i|H|0\rangle = \langle 1_i|h_i|0_i\rangle = 0$ [Eqs. (3) and (4)]. Thus, if $|0_{\text{RPA}}\rangle = |0\rangle$, $Z = 0$ and hence $V = 0$ in $\mathcal{W}$, which implies that $\Delta_- = 0$. Hence, $|0\rangle$ is an exact eigenstate by Eq. (15). Conversely, if $|0\rangle$ is an exact eigenstate, it is a solution of the mean-field equations leading to $\Delta_- = 0$, which implies that $|0_{\text{RPA}}\rangle = |0\rangle$ (although Δ_+ may be nonzero and $\omega^\alpha \neq \lambda^\alpha$). In particular, when H has an exactly separable ground state $|0\rangle$ (i.e., at the factorizing field [12,22,23]), $|0_{\text{RPA}}\rangle = |0\rangle$.

(ii) $|0_{\rm RPA}\rangle$ is always exact for sufficiently strong fields ($|\boldsymbol{B}| \gg J$). In this limit $|0\rangle$ is the state with all spins $\boldsymbol{s}_i$ fully aligned along $-\boldsymbol{B}^i$ plus small corrections ($\boldsymbol{\lambda}^i \approx \boldsymbol{B}^i + sJ\cdot \boldsymbol{B}^i/|\boldsymbol{B}|^i$). Up to first order in $\Delta_\pm/\lambda$, Eqs. (10)–(13) lead to $Z^{ij} \approx V_{ij} \approx \frac{\Delta_-^{ij}}{\lambda_i+\lambda_j}$, which means that

$$|0_{\rm RPA}\rangle \approx |0\rangle + \sum_{i<j} \frac{\Delta_-^{ij}}{\lambda_i+\lambda_j}|1_i 1_j\rangle, \qquad (16)$$

which, by Eq. (15), is just the first-order expansion (in Δ_-/Λ) of the exact ground state.

In the case of a symmetry-breaking mean field, the RPA spin state allows us to implement the necessary rotations for symmetry restoration: The exact ground state will actually be close to the superposition with the correct symmetry of the degenerate RPA ground states (rather than to a particular RPA state), as will be discussed in Sec. II E in the context of parity breaking. This restoration enlarges considerably the capabilities of the RPA.

C. Bosonic evaluation of subsystem entropy and negativity

The direct evaluation of many-body correlations and entanglement measures from the RPA spin state (14) is, in general, difficult. However, the values of these quantities in the associated bosonic vacuum (13), which will be close to those obtained from Eq. (14), can be straightforwardly evaluated using the general Gaussian state formalism [24,25]. The reduced density matrix of any subsystem is just a Gaussian state, i.e., a canonical thermal state of an effective quadratic bosonic Hamiltonian, since Wick's theorem holds for the evaluation of the mean value of any observable and in particular those of the subsystem. We may then evaluate its entropy and other invariants through standard expressions for independent boson systems.

Let us formalize the previous scheme. We will use a generalized contraction matrix formalism, equivalent to that based on covariance matrices [24,25], which is more natural for the present RPA formulation. In the new vacuum $|0'_b\rangle$, $\langle b'^\dagger_\alpha b'_{\alpha'}\rangle_{0'} = \langle b'_\alpha b'_{\alpha'}\rangle_{0'} = 0$, which implies that

$$F_{ij} \equiv \langle b_j^\dagger b_i\rangle_{0'} = (VV^\dagger)_{ij}, \qquad (17a)$$

$$G_{ij} \equiv \langle b_j b_i\rangle_{0'} = (VU^{\rm tr})_{ij}. \qquad (17b)$$

Equations (5)–(17) determine the basic RPA spin averages and correlations, i.e., $\langle s_{i\mu}\rangle_{0'} = \delta_{\mu z}(F_{ii} - s_i)$ and, for $i \neq j$,

$$\langle s_{i+}s_{j-}\rangle_{0'} = 2\sqrt{s_i s_j}F_{ji}, \quad \langle s_{i-}s_{j-}\rangle_{0'} = 2\sqrt{s_i s_j}G_{ji}, \qquad (18)$$

with $\langle s_{i\pm}s_{jz}\rangle_{0'} = 0$, which coincide exactly with the averages derived from Eq. (14) up to second order in V, i.e., first order in the average occupation $VV^\dagger$ (which is normally very small outside critical regions). Through the use of Wick's theorem, we also obtain $\langle s_{iz}s_{jz}\rangle_{0'} = \langle s_{iz}\rangle_{0'}\langle s_{jz}\rangle_{0'} + |F_{ij}|^2 + |G_{ij}|^2$ for $i \neq j$.

We may now define the generalized contraction matrix

$$\mathcal{D} \equiv \langle \mathcal{Z}\mathcal{Z}^\dagger\rangle_{0'} - \mathcal{M} = \begin{pmatrix} F & G \\ \bar{G} & I+\bar{F}\end{pmatrix}, \qquad (19)$$

which exhibits the correct transformation rule under Bogoliubov transformations: If $\mathcal{Z} = \mathcal{W}\mathcal{Z}'$, then

$$\mathcal{D} = \mathcal{W}\mathcal{D}'\mathcal{W}^\dagger, \qquad (20)$$

with $\mathcal{D}' = \langle \mathcal{Z}'\mathcal{Z}'^\dagger\rangle_{0'} - \mathcal{M}$. Equation (17) can in fact be written in the form (20) if $\mathcal{W}$ is the diagonalizing Bogoliubov matrix (11) and $\mathcal{D}'$ is the vacuum density ($F' = G' = 0$). We may also obtain $\mathcal{W}$ and $\mathcal{D}'$ through the symplectic diagonalization of $\mathcal{D}$, i.e., through the diagonalization of

$$\mathcal{D}\mathcal{M} = \begin{pmatrix} F & -G \\ \bar{G} & -I-\bar{F}\end{pmatrix} \qquad (21)$$

such that $\mathcal{W}^{-1}\mathcal{D}\mathcal{M}\mathcal{W} = \mathcal{D}'\mathcal{M}$, with $\mathcal{D}'$ diagonal.

Let us consider now a subsystem A of $m < n$ sites. It will be characterized by a truncated contraction matrix

$$\mathcal{D}_A = \langle \mathcal{Z}_A\mathcal{Z}_A^\dagger\rangle_{0'} - \mathcal{M}_A = \begin{pmatrix} F_A & G_A \\ \bar{G}_A & I+\bar{F}_A\end{pmatrix}, \qquad (22)$$

where $\mathcal{Z}_A$ contains just the bosons of sites in A. A symplectic diagonalization of $\mathcal{D}_A$ will lead to

$$\mathcal{D}_A = \mathcal{W}_A\mathcal{D}'_A\mathcal{W}_A^\dagger, \quad \mathcal{D}'_A = \begin{pmatrix} f_A & 0 \\ 0 & I+f_A\end{pmatrix}, \qquad (23)$$

where $f_A^{\alpha\alpha'} = f_A^\alpha\delta^{\alpha\alpha'}$ with $f_A^\alpha = \langle b'^\dagger_{\alpha_A}b'_{\alpha_A}\rangle_{0'} \geqslant 0$ (where $\mathcal{D}_A\mathcal{M}_A$ has eigenvalues f_A^α and $-1-f_A^\alpha$) and $\mathcal{W}_A\mathcal{M}_A\mathcal{W}_A^\dagger = \mathcal{M}_A$, with $\mathcal{Z}_A = \mathcal{W}_A\mathcal{Z}'_A$. The entanglement between A and its complement $\bar{A}$ is then given by the associated bosonic entropy:

$$S(\rho_A^b) = -{\rm Tr}\rho_A^b\log_2\rho_A^b \qquad (24)$$

$$= -\sum_\alpha f_A^\alpha\log_2 f_A^\alpha - \left(1+f_A^\alpha\right)\log_2\left(1+f_A^\alpha\right). \qquad (25)$$

Here $\rho_A^b \equiv {\rm Tr}_{\bar{A}}|0'_b\rangle\langle 0'_b|$ is the bosonic reduced density of subsystem A, which can be explicitly written as

$$\rho_A^b = C\exp\left(-\frac{1}{2}\mathcal{Z}_A^\dagger\mathcal{H}_A\mathcal{Z}_A\right) = C'\exp\left(-\sum_\alpha \omega_A^\alpha b'^\dagger_{\alpha_A}b'_{\alpha_A}\right), \qquad (26)$$

where $C' = Ce^{-\sum_\alpha\omega_\alpha/2} = \prod_\alpha(1+f_\alpha^A)^{-1}$, and $\mathcal{H}_A$, $\mathcal{D}_A$ are related by

$$\mathcal{D}_A\mathcal{M}_A = [\exp(\mathcal{M}_A\mathcal{H}_A) - I]^{-1}. \qquad (27)$$

Here $\mathcal{H}_A$ represents an effective "Hamiltonian" matrix for subsystem A with symplectic eigenvalues ω_A^α such that $f_A^\alpha = (e^{\omega_A^\alpha}-1)^{-1}$ [and hence $-1-f_A^\alpha = (e^{-\omega_A^\alpha}-1)^{-1}$]. Equation (26) leads to the contraction matrix (22) and hence to the same expectation values as the full vacuum $|0'_b\rangle\langle 0'_b|$ for any operator of subsystem A.

Equation (25) provides a tractable RPA estimation of the entanglement entropy of any subsystem. It is shown in Appendix A that a direct spin evaluation of the subsystem entropy based on the RPA state (14) coincides with Eq. (25) up to second order in V.

On the other hand, the internal entanglement of subsystem A with respect to a partition (B,C) of A (where the complement $\bar{A}$ plays the role of an environment) can be measured through the corresponding negativity [13], defined as minus the sum of the negative eigenvalues of the partial transpose $\rho_A^{t_C}$ of ρ_A:

$$N_{BC} = \tfrac{1}{2}\left(\mathrm{Tr}\left|\rho_A^{t_C}\right| - 1\right). \tag{28}$$

Expectation values with respect to $(\rho_A^b)^{t_C}$ of an observable O_A^b correspond to those of the partial transpose $(O_A^b)^{t_C}$ with respect to ρ_A^b. This implies the replacements $F_{ij} \leftrightarrow G_{ij}$, $F_{j'j} \leftrightarrow F_{jj'}$, and $G_{j'j} \leftrightarrow \bar{G}_{j'j}$, in the contraction matrix for $j,j' \in C$, $i \in B$, leading to a matrix $\tilde{\mathcal{D}}_A$ with symplectic eigenvalues $\tilde{f}_A^\alpha$. The latter can now be negative. We may still write $(\rho_A^b)^{t_C}$ as in Eq. (26) in terms of an effective matrix $\tilde{\mathcal{H}}_A$ with symplectic eigenvalues $\tilde{\omega}_A^\alpha$ such that $\tilde{f}_A^\alpha = (e^{\tilde{\omega}_A^\alpha} - 1)^{-1}$.

Since the trace remains unchanged [$\mathrm{Tr}(\rho_A^b)^{t_C} = 1$], $|e^{-\tilde{\omega}_A^\alpha}| < 1$, which implies that $\tilde{f}_A^\alpha > -\frac{1}{2}$. A negative $\tilde{f}_A^\alpha > -\frac{1}{2}$ corresponds to $e^{-\tilde{\omega}_A^\alpha} < 0$ and hence to a nonpositive $(\rho_A^b)^{t_C}$, which indicates an entangled ρ_A^b with respect to this bipartition. Noting that $(1 + e^{-\tilde{\omega}_A^\alpha})^{-1} = (1 + \tilde{f}_A^\alpha)/(1 + 2\tilde{f}_A^\alpha)$, we obtain the final result [13,24,25]:

$$\mathrm{Tr}\left|\left(\rho_A^b\right)^{t_c}\right| = \prod_{\tilde{f}_A^\alpha < 0} \frac{1}{1 + 2\tilde{f}_A^\alpha}, \tag{29}$$

which allows the evaluation of the negativity (28). Negativities obtained from the spin density matrices coincide with this result up to first order in V (Appendix A).

In the case of a global bipartition $(A,\bar{A})$, $N_{A\bar{A}}$ becomes a function of the reduced density ρ_A, namely [17],

$$N_{A\bar{A}} = \tfrac{1}{2}(\mathrm{Tr}||0\rangle\langle 0|^{t_{\bar{A}}}| - 1) = \tfrac{1}{2}[(\mathrm{Tr}\sqrt{\rho_A})^2 - 1]. \tag{30}$$

In a boson system, this implies that $N_{A\bar{A}}$, a limit case of Eqs. (28) and (29), can also be expressed just in terms of the symplectic eigenvalues f_A^α of the contraction matrix $\mathcal{D}_A$:

$$N_{A\bar{A}} = \frac{1}{2}\left[\prod_\alpha \left(\sqrt{f_A^\alpha} + \sqrt{1 + f_A^\alpha}\right)^2 - 1\right]. \tag{31}$$

D. Translationally invariant systems

The only quantities required in the bosonic RPA scheme are, therefore, the basic contractions (17). Their evaluation becomes remarkably simple in translationally invariant systems, in either one or d dimensions, i.e., systems with a common spin $s_i = s$ in a uniform field $\mathbf{B}^i = \mathbf{B}$ with couplings dependent just on separation:

$$J^{i\mu j\nu} = J^{\mu\nu}(i - j), \tag{32}$$

where $J^{\mu\nu}(l) = J^{\nu\mu}(-l)$, and $J^{\mu\nu}(-l) = J^{\mu\nu}(n - l)$ in a finite cyclic chain or system (in d dimensions, i,j,l,n stand for d-dimensional vectors). We will also assume a uniform mean field $\boldsymbol{\lambda}^i = \boldsymbol{\lambda}$, which should then satisfy

$$\lambda^\mu = B^\mu - \sum_\nu J_0^{\mu\nu}\langle s_\nu\rangle_0, \quad J_0^{\mu\nu} \equiv \sum_l J^{\mu\nu}(l), \tag{33}$$

with $\langle \boldsymbol{s}\rangle_0 = -s\boldsymbol{\lambda}/\lambda$ [Eq. (4)]. The uniform mean field is thus determined just by the total strengths $J_0^{\mu\nu}$.

By choosing again the z axis in the direction of $\boldsymbol{\lambda}$, such that $\langle s_{i\mu}\rangle = -s\delta_{\mu z}$ and $B^\mu + sJ_0^{\mu z} = \lambda\delta^{\mu z}$, with $\lambda > 0$, the bosonized Hamiltonian will have the form (6) with couplings $\Delta_\pm^{ij} = \Delta_\pm(i - j)$. By means of a discrete Fourier transform of the boson operators, we can rewrite it as

$$H_b = \langle H\rangle_0 + \sum_k (\lambda - \Delta_+^k) b_k^\dagger b_k - \frac{1}{2}(\Delta_-^k b_k^\dagger b_{-k}^\dagger + \mathrm{H.c.}), \tag{34}$$

$$\Delta_\pm^k = \sum_{l=0}^{n-1} e^{i2\pi kl/n}\Delta_\pm(l), \tag{35}$$

where $k = 0,\ldots,n-1$ and $b_k = \frac{1}{\sqrt{n}}\sum_{j=1}^n e^{i2\pi kj/n} b_j$ are boson operators in momentum space, with $b_{-k} = b_{n-k}$. Diagonalization of (34) is straightforward and leads to

$$H^b = \langle H\rangle_0 + \sum_k \omega^k b'^\dagger_k b'_k + \frac{1}{2}(\omega^k - \lambda + \Delta_+^k), \tag{36}$$

where $\omega^k = \tilde{\omega}^k - \frac{1}{2}(\Delta_+^k - \Delta_+^{-k})$, $b'^\dagger_k = u_k b_k^\dagger - \bar{v}_k b_{-k}$, and

$$\tilde{\omega}^k = \sqrt{(\lambda - \tilde{\Delta}_+^k)^2 - |\Delta_-^k|^2}, \tag{37}$$

$$u_k = \sqrt{\frac{\lambda - \tilde{\Delta}_+^k + \tilde{\omega}_k}{2\tilde{\omega}^k}}, \quad v_k = \frac{\Delta_-^k}{|\Delta_-^k|}\sqrt{\frac{\lambda - \tilde{\Delta}_+^k - \tilde{\omega}_k}{2\tilde{\omega}^k}}, \tag{38}$$

with $\tilde{\Delta}_+^k = \frac{1}{2}(\Delta_+^k + \Delta_+^{-k})$, $u_k^2 - |v_k|^2 = 1$, and $u_k = u_{-k}$, $v_k = v_{-k}$. All ω^k should be real and positive for a stable mean field, which implies the stability conditions $\Delta_+^k < \lambda$ and

$$|\Delta_-^k| < \sqrt{(\lambda - \Delta_+^k)(\lambda - \Delta_+^{-k})}, \quad k = 0,\ldots,n-1. \tag{39}$$

We can now obtain the basic contractions explicitly:

$$\langle b_k^\dagger b_{k'}\rangle_{0'} = \delta_{kk'}\left|v_k^2\right|, \quad \langle b_k b_{-k'}\rangle_{0'} = \delta_{kk'}u_k v_k = \frac{\Delta_-^k}{2\tilde{\omega}^k}, \tag{40}$$

which lead finally to [see Eq. (17)]:

$$F_{ij} = F(i - j) = \frac{1}{n}\sum_k e^{-i2\pi k(i-j)/n}\left|v_k^2\right|, \tag{41a}$$

$$G_{ij} = G(i - j) = \frac{1}{n}\sum_k e^{-i2\pi k(i-j)/n}u_k v_k. \tag{41b}$$

For strong fields $|B|$ such that $\lambda \gg |\Delta_\pm|$, $u_k v_k \approx \frac{1}{2}\Delta_-^k/\lambda$ and $|v_k^2| \approx \frac{1}{4}|\Delta_-^k|^2/\lambda^2$. The RPA vacuum (13) becomes

$$|0'_b\rangle = C_b \exp\left[\frac{1}{2}\sum_{i,j} Z(i - j) b_i^\dagger b_j^\dagger\right]|0_b\rangle, \tag{42}$$

where $C_b = \prod_k u_k^{-\frac{1}{2}}$ and $Z(l) = \frac{1}{n}\sum_k e^{-i2\pi lk/n}\frac{v_k}{u_k}$.

Thus, these systems allow an analytic evaluation of the contractions (17). Both the mean-field equations (33) and the RPA Hamiltonian (34) become independent of the common spin s after a rescaling $J^{\mu\nu}(l) \to J^{\mu\nu}(l)/s$, which we will adopt in what follows and which indicates that the RPA is describing the large-spin limit of the system, as is apparent from Eq. (5).

E. *XYZ* systems

Let us now examine in more detail the previous formalism in a translationally invariant spin s array with XYZ couplings of arbitrary range in a uniform transverse field:

$$H = B\sum_i s_{iz} - \frac{1}{2s}\sum_{i\neq j}\sum_{\mu=x,y,z} J_\mu(i-j)s_{i\mu}s_{j\mu}. \quad (43)$$

Equation (43) commutes with the S_z spin-parity,

$$[H,P_z]=0,\quad P_z=\exp\left[i\pi\sum_i(s_{iz}+s)\right],$$

for any value of its parameters, such that the exact ground state in a finite array will always have a definite parity outside degeneracy points. We will focus here on the ferromagnetic-type case where $J_x(l)\geqslant 0\ \forall\, l$ with

$$|J_y(l)|\leqslant J_x(l), \quad (44)$$

which exhibits a normal and a parity-breaking phase at the mean-field level.

1. RPA around the normal state

For the Hamiltonian (43), the state $|0\rangle$ with all spins fully aligned along the $-z$ axis is always a solution of the mean-field equation (33), being the lowest solution for a sufficiently strong field B. It leads to $\lambda^i=\lambda\delta^{\mu z}$, with

$$\lambda=|B|+J_z^0>0,\quad J_z^0\equiv\sum_l J_z(l). \quad (45)$$

All previous equations can then be directly applied. Now $\Delta_\pm(l)=\frac{J_x(l)\pm J_y(l)}{2}=\Delta_\pm(-l)$, which implies that $\Delta_\pm^k=\Delta_\pm^{-k}$ and

$$\omega^k=\sqrt{\left(\lambda-J_x^k\right)\left(\lambda-J_y^k\right)}, \quad (46)$$

where $J_\mu^k=\sum_l e^{i2\pi kl/n}J_\mu(l)$ ($\Delta_\pm^k=\frac{J_x^k\pm J_y^k}{2}$). This solution is therefore stable provided that $J_\mu^k\leqslant\lambda\ \forall\, k$ and $\mu=x,y$, i.e., for $|B|$ above a certain critical field B_c. In the case (44), the strongest condition is obtained for $k=0$, i.e.,

$$|B|>B_c\equiv J_x^0-J_z^0. \quad (47)$$

2. RPA around the parity-breaking state

For $|B|\leqslant B_c$, the normal state becomes unstable: The lowest normal RPA frequency ω^0 vanishes for $|B|\to B_c$ and becomes imaginary for $|B|<B_c$. The lowest mean field for $|B|<B_c$ corresponds instead to a parity-breaking state with all spins aligned along an axis in the xz plane forming an angle θ with the z axis:

$$|0\rangle\to|\Theta\rangle\equiv|\theta_1\cdots\theta_n\rangle,\quad |\theta_j\rangle=\exp(-i\theta s_{jy})|0_j\rangle. \quad (48)$$

This leads to $\langle \boldsymbol{s}_j\rangle_0=-s(\sin\theta,0,\cos\theta)=-s\boldsymbol{\lambda}/\lambda$, with

$$\lambda=J_x^0,\quad \cos\theta=\frac{B}{B_c}, \quad (49)$$

as determined by Eq. (33). We should now express the original spin operators in terms of the rotated operators, i.e.,

$$s_{ix}=s_{ix'}\cos\theta+s_{iz'}\sin\theta,\quad s_{iz}=s_{iz'}\cos\theta-s_{ix'}\sin\theta, \quad (50)$$

with $s_{iy}=s_{iy'}$. The RPA around this state therefore amounts to the replacements

$$\lambda\to J_x^0,\quad J_x^k\to J'^k_x=J_x^k\cos^2\theta+J_z^k\sin^2\theta, \quad (51)$$

in Eq. (46), with J_y^k unchanged and $\Delta_\pm^k=\frac{1}{2}(J'^k_x\pm J_y^k)$.

Correlations $\langle s_{i\mu'}s_{j\mu'}\rangle_{\rm RPA}$ of rotated spin operators have the same previous expressions (17), whereas those of the original operators must be obtained using Eq. (50). It should be noted, however, that in a finite system, the associated RPA spin state will no longer be a good approximation to the actual ground state because of parity breaking. Parity restoration, at least approximately, must be implemented before obtaining final results. We will not discuss here the case of a continuous broken symmetry (arising, for instance, in the XXZ case), which can be treated through the RPA formalism of Ref. [9].

3. Definite parity RPA ground states

Since $[H,P_z]=0$, the parity-breaking mean-field state $|\Theta\rangle$ is degenerate: Both $|\Theta\rangle$ and $|-\Theta\rangle=P_z|\Theta\rangle$ are mean-field ground states. In order to describe the definite parity ground states, the correct RPA ground state should be taken as the definite parity combinations

$$|\Theta_{\rm RPA}^\pm\rangle=\frac{|\Theta_{\rm RPA}\rangle\pm|-\Theta_{\rm RPA}\rangle}{\sqrt{2(1\pm\langle-\Theta_{\rm RPA}|\Theta_{\rm RPA}\rangle)}}, \quad (52)$$

where $|\pm\Theta_{\rm RPA}\rangle$ are the RPA states around each mean field. The overlap $\langle-\Theta_{\rm RPA}|\Theta_{\rm RPA}\rangle=\langle\Theta_{\rm RPA}|P_z|\Theta_{\rm RPA}\rangle$ is proportional to the overlap between the two mean-field states,

$$\langle-\Theta|\Theta\rangle=\cos^{2ns}\theta=\left(\frac{B}{B_c}\right)^{2ns}, \quad (53)$$

which is small except for $B\to B_c$ or small ns.

By neglecting the previous overlap, Eq. (52) will lead to reduced densities:

$$\rho_A^\pm\approx\tfrac{1}{2}[\rho_A(\theta)+\rho_A(-\theta)] \quad (54)$$

provided that the complementary overlap $\langle-\Theta_{\rm RPA}^{\bar A}|\Theta_{\rm RPA}^{\bar A}\rangle\propto(B/B_c)^{2(n-n_A)s}$ can also be neglected. Here $\rho_A(\pm\Theta)$ are the reduced spin densities determined by each RPA state, given up to $O(V^2)$ by the expressions of Appendix A.

The restoration (54) is essential to achieving a good description of the actual subsystem entropy, although its main effect for a subsystem A that is not too small is actually quite simple: If the product $\rho_A(\Theta)\rho_A(-\Theta)\propto(B/B_c)^{2n_As}$ can be neglected, then Eq. (54) can be considered as the sum of two densities with orthogonal support and identical distributions, leading to

$$S(\rho_A^\pm)\approx S[\rho_A(\theta)]+1, \quad (55)$$

where $S[\rho_A(\Theta)]$ can be evaluated through the boson approximation (25). Under the same assumptions, the effect on the global negativity (30) is just

$$N_{A\bar{A}}(\rho_A^{\pm}) \approx 2N_{A\bar{A}}[\rho_A(\theta)] + \tfrac{1}{2}, \tag{56}$$

as $\mathrm{Tr}\sqrt{\rho_A^{\pm}} \approx \sqrt{2}\mathrm{Tr}\sqrt{\rho_A(\theta)}$, while the subsystem negativity N_{BC} of a bipartition (B,C) of A remains approximately unchanged: $N_{BC}(\rho_A^{\pm}) \approx N_{BC}[\rho_A(\theta)]$.

When the product $\rho_A(\Theta)\rho_A(-\Theta)$ cannot be neglected (as in a subsystem of two spins), we should in principle construct the spin density (54). This can be done by rotating $\rho_A(\theta)$ [Eq. (A2) in the mean-field frame] to the original z axis and removing all parity-breaking elements [which is the final effect of Eq. (54)]. For instance, the reduced two-spin density for $s=\frac{1}{2}$ has the blocked form (A2) in the standard basis of $s_{iz}s_{jz}$ eigenstates in the normal phase as well as in the parity-breaking phase after parity restoration [12]. The final effect on $S(\rho_A)$ is the replacement of the term $+1$ in Eq. (55) by the entropy of the reduced mean-field mixture $-\sum_{\nu=\pm} q_\nu \log_2 q_\nu$, with $q_\pm = \frac{1}{2}[1 \pm (B/B_c)^{2s_A}]$, plus smaller RPA corrections.

Although $\rho_A^{\pm}$ are both identical in the approximation (54), the actual $\rho_A^{\pm}$ derived from (52) will depend on parity. The correct parity in such a case should be chosen as that leading to the lowest energy $E_{\mathrm{RPA}}^{\pm} = \langle \Theta_{\mathrm{RPA}}^{\pm}|H|\Theta_{\mathrm{RPA}}^{\pm}\rangle$.

4. Factorizing field

The explicit value of the basic RPA couplings $\Delta_\pm^k$ in the parity-breaking phase are, using Eqs. (49)–(51),

$$\Delta_\pm^k = \tfrac{1}{2}\big[\big(J_x^k - J_z^k\big)(B/B_c)^2 + \big(J_z^k \pm J_y^k\big)\big]. \tag{57}$$

In the case of a common anisotropy, such that the ratio

$$\chi = \frac{J_y(l) - J_z(l)}{J_x(l) - J_z(l)} \tag{58}$$

is *independent* of the separation l, we have $J_y^k - J_z^k = \chi(J_x^k - J_z^k)$ and hence $\Delta_-^k = \frac{1}{2}(J_x^k - J_z^k)[(B/B_c)^2 - \chi]$. It is then seen that if $\chi \in [0,1]$, then $\Delta_-^k = 0 \;\forall\, k$ when

$$|B| = B_s \equiv B_c\sqrt{\chi}, \tag{59}$$

with all Δ_-^k changing sign at $|B| = B_s$. Here B_s is the *factorizing field* [2,12,22,23,26]: At $B = B_s$ the parity-breaking mean-field state becomes an *exact* ground state, since the RPA corrections vanish (see Sec. II B). This effect is independent of the number of spins n (as long as χ is constant) and spin s (with the present scaling). Nonetheless, the actual side limits at $B = B_s$ will be given by the definite parity states (52), which are still entangled. As a consequence, the subsystem entropy $S(\rho_A)$ and the negativity $N_{A\bar{A}}$ will actually approach a *finite* value for $B \to B_s$ [1 and $\frac{1}{2}$, respectively, in the approximations given by (55) and (56)], while the entanglement between two spins will reach an infinite range [10–12]. Note finally that at $B = B_s$, $\Delta_+^k = J_y^k$ and, hence,

$$\omega^k = J_x^0 - J_y^k. \tag{60}$$

III. APPLICATION

A. Spin *s* pair

As a first example, let us consider a system of two spins s coupled through the Hamiltonian (43). We can obviously always set $J_x \geqslant |J_y|$ (44), since the sign of J_x can be changed by a π rotation around the z axis of one of the spins (and we can always set $|J_x| \geqslant |J_y|$ by a proper choice of axes). The Fourier transform of $J_\mu(l) = \delta_{l1} J_\mu$ reduces here to $J_\mu^k = (-1)^k J_\mu, k = 0,1$, leading to an attractive and a repulsive normal mode:

$$\omega_0 = \sqrt{(\lambda - J_x)(\lambda - J_y)}, \quad \omega_1 = \sqrt{(\lambda + J_x)(\lambda + J_y)}.$$

The contractions (41) become $F_{ij} = \frac{\lambda-\Delta_+}{4\omega_0} - \frac{\lambda+\Delta_+}{4\omega_1}(1 - 2\delta_{ij}) - \frac{1}{2}\delta_{ij}$, $G_{ij} = \frac{\Delta_-}{4\omega_0} + \frac{\Delta_-}{4\omega_1}(1-2\delta_{ij})$, where $\Delta_\pm = \frac{1}{2}(J_x \pm J_y)$ and replacements (51) are to be applied for $|B| < B_c$. The ensuing entanglement entropy of the pair in the bosonic approximation (25) is just

$$S(\rho_1) = -f\log_2 f + (1+f)\log_2(1+f) + \delta, \tag{61}$$

$$f = \frac{1}{2}\left(\sqrt{1 + \frac{\lambda^2 - \overline{\omega}^2}{\omega_0\omega_1}} - 1\right), \quad \overline{\omega} = \frac{\omega_0 + \omega_1}{2}, \tag{62}$$

where $f = \sqrt{(F_{11} + \frac{1}{2})^2 - (G_{11})^2} - \frac{1}{2}$ is the positive symplectic eigenvalue of the 2×2 contraction matrix for one spin and $\delta = 0$ (1) for $|B| > B_c$ ($< B_c$) in the approximation (55), which is valid for $(B/B_c)^{2s} \ll 1$. For small f, we may just use $S(\rho_1) \approx f(\log_2 e - \log_2 f)$, with $f \approx F_{11}$, in agreement with the results of Appendix A.

Thus, at the RPA level entanglement is determined by the average local occupation f and driven by the ratio $\frac{\lambda^2 - \overline{\omega}^2}{\omega_0\omega_1}$, which is small away from B_c and vanishes at $B = B_s$ [where $\overline{\omega} = \lambda = J_x^0$ by Eq. (60), and hence $f = 0$]. For $|B| \gg B_c$, $f \approx (\frac{J_x - J_y}{4B})^2$, while in the vicinity of B_s, $f \propto (B - B_s)^2$. For $B \to B_c$, $f \approx \frac{1}{2}\sqrt{\frac{\lambda^2 - \overline{\omega}^2}{\omega_0\omega_1}} \propto |B - B_c|^{-1/4}$, with $S(\rho_1) \approx \log_2 fe$.

The bosonic RPA negativity [Eqs. (28), (29), and (31)] becomes

$$N_{12} = \frac{-\tilde{f}}{1 + 2\tilde{f}} = f + \sqrt{f(f+1)}, \tag{63}$$

where $\tilde{f} = f - \sqrt{f(f+1)}$ is the negative symplectic eigenvalue of the 4×4 contraction matrix. The correction of Eq. (56) ($N_{21} \to 2N_{21} + \frac{1}{2}$) should be applied for $|B| < B_c$. For small f, we have simply $N_{12} \approx -\tilde{f} \approx \sqrt{f}$. This will lead to a slope discontinuity of N_{12} at the factorizing field B_s (see Fig. 1), as f vanishes there quadratically ($N_{12} - \frac{1}{2} \propto |B - B_s|$ for $B \approx B_s$). On the other hand, for $f \to \infty$ ($|B| \to B_c$), $\tilde{f} \to -\frac{1}{2}$, with $\tilde{f} \approx -\frac{1}{2} + \frac{1}{8f}$ and $N_{12} \approx 2f$. Both $S(\rho_1)$ and N_{12} are concave increasing functions of f and measure the entanglement of the pair.

Comparison with exact numerical results, obtained through the diagonalization of H [a $(2s+1)^2 \times (2s+1)^2$ matrix], is shown in Fig. 1 for the XY case ($J_z = 0$) with anisotropy $\chi = J_y/J_x = 0.5$. Exact results are seen to rapidly approach the RPA values [Eqs. (61)–(63)] as the spin s increases, the discrepancy for finite s arising just in the vicinity of B_c or for very small s, i.e., where tunneling effects arising from the

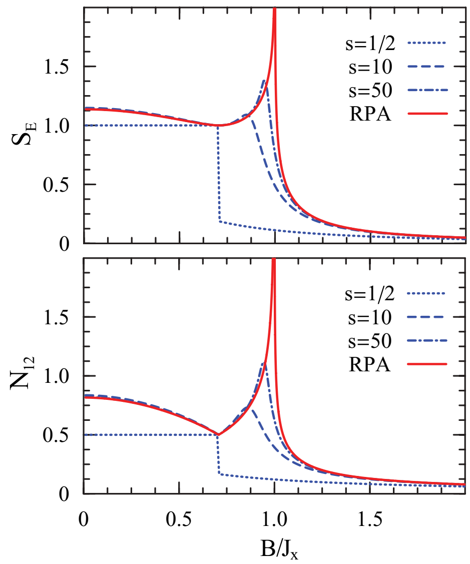

FIG. 1. (Color online) Entanglement between two spins s as a function of the transverse field B for an XY coupling with $J_y/J_x = 0.5$. The exact entanglement entropy $S_E = S(\rho_1)$ (top) and negativity (bottom) for different values of the spin s and the bosonic RPA results [(61) and (63)] are depicted. The exact results approach those of RPA as s increases, with differences for not-too-small s arising just for B close to $B_c = J_x$. At the factorizing field $B_s \approx B_c/\sqrt{2}$, $S_E = 1$ while $N_{12} = \frac{1}{2}$.

nonzero overlap (53) between the degenerate parity-breaking states become appreciable.

Nonetheless, this overlap can be taken into account using the full definite parity RPA spin state (52) with lowest energy, which for finite s improves results for B close to B_c (but otherwise yields results almost coincident with those of the corrected bosonic RPA), as seen in Fig. 2. Equation (52) also yields the *exact* side limits at the factorizing field [12] for *any* s, although for $\chi = 0.5$ these limits rapidly approach the high spin values $S(\rho_1) = 1$ and $N_{12} = \frac{1}{2}$ predicted by the approximations of Eqs. (55) and (56).

Figure 2 also depicts the behavior of the average occupations f and $\tilde{f}$. The former is seen to be quite small ($f \lesssim 0.05$) except in the vicinity of B_c, which implies that, away from B_c, all bosonic RPA results can be reproduced by the spin densities of Appendix A, with $\tilde{f} \approx \sqrt{f}$. In the bottom panels we depict the RPA energies ω_0,ω_1 and the RPA state coefficients $Z_k \equiv v_k/u_k$ used in Eq. (42). Although ω_0 vanishes at B_c, the difference $\lambda - \overline{\omega}$, which is responsible for entanglement, remains quite small everywhere. Both Z_k vanish and change sign at the factorizing field B_s, which indicates a qualitative change in the type of correlations at this point: It is well known that entanglement between two spins $\frac{1}{2}$ changes from antiparallel to parallel (in the original frame) at B_s [11,12], an effect that arises within the RPA from this sign change.

B. Fully connected spin system

Let us now consider a fully and uniformly connected XYZ array of n spins, where

$$J_\mu(l) = (1 - \delta_{l0})J_\mu/(n-1), \tag{64}$$

in Eq. (43). This scaling ensures a finite intensive energy $\langle H\rangle/n$ for large n and finite J_μ. Entanglement properties of this well-known model [18,27] for $s = \frac{1}{2}$ in the large-n limit have been previously analyzed [28], including recently

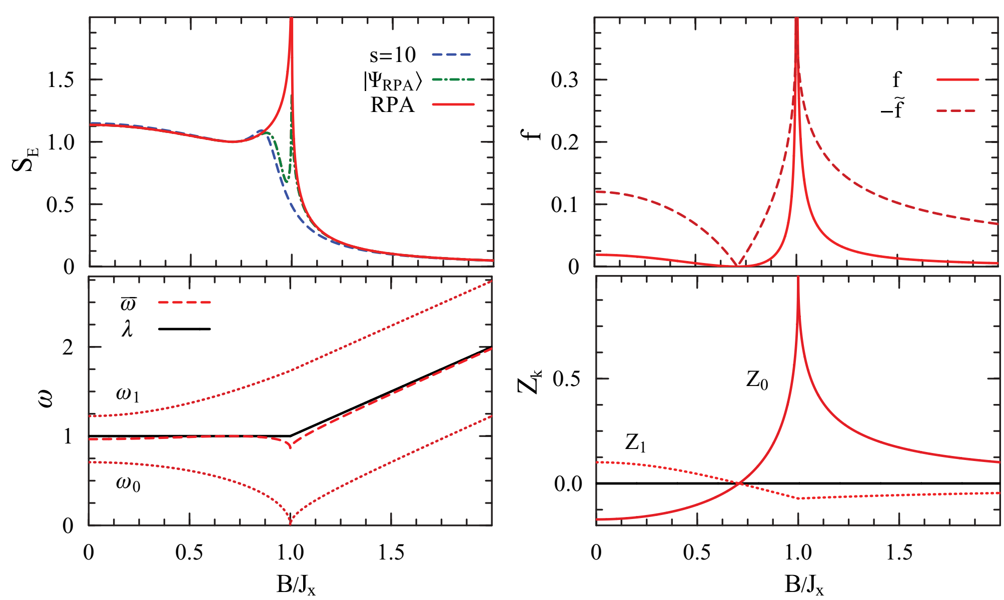

FIG. 2. (Color online) Top left: The entanglement entropy obtained from the definite parity RPA spin state (52) (dashed-dotted line), compared with the bosonic RPA result (61) and the exact value, for $s = 10$ at the same parameters as in Fig. 1. The result from the RPA spin state improves the bosonic RPA for B just below B_c. Top right: The average local boson occupation f (62), which is small away from B_c, and the negative eigenvalue $\tilde{f}$ of the partial transpose of the contraction matrix ($\tilde{f} \approx \sqrt{f}$ for small f). Bottom left: RPA energies ω_0, ω_1, together with the mean-field energy λ and the mean RPA energy $\overline{\omega}$ in Eq. (62). Bottom right: The quantities $Z_k = v_k/u_k$ for $k = 0,1$, which determine the RPA state (42) and vanish at the factorizing field B_s.

Holstein-Primakoff-based bosonization [16,21,29,30]. Direct application of the present RPA formalism will be shown to yield full analytic expressions for any size n and spin s. The Fourier transform of Eq. (64) is $J^0_\mu = J_\mu$ and $J^k_\mu = -J_\mu/(n-1)$ for $k = 1,\ldots,n-1$, which leads again to two distinct RPA energies: one associated with a fundamental attractive mode (ω_0) and $n-1$ degenerate weak repulsive modes $\omega_k = \omega_1, k \neq 0$, which add a small repulsive correction, nonzero for finite n, accounting for the absence of self-energy terms $\propto s^2_{i\mu}$ in H:

$$\omega_0 = \sqrt{(\lambda - J_x)(\lambda - J_y)},$$
$$\omega_1 = \sqrt{\left(\lambda + \frac{J_x}{n-1}\right)\left(\lambda + \frac{J_y}{n-1}\right)},$$

where the replacements (51) are to be used for $B < B_c$. The ensuing contractions (41) here become obviously independent of separation for $i \neq j$:

$$F_{ij} = \frac{1}{2n}\left[\frac{\lambda - \Delta^0_+}{\omega_0} - \frac{\lambda - \Delta^1_+}{\omega_1}(1 - n\delta_{ij})\right] - \frac{1}{2}\delta_{ij}, \quad (65a)$$
$$G_{ij} = \frac{1}{2n}\left[\frac{\Delta^0_-}{\omega_0} - \frac{\Delta^1_-}{\omega_1}(1 - n\delta_{ij})\right], \quad (65b)$$

and imply that, for any bipartition $(L, n-L)$, the entanglement entropy $S(\rho_L)$ will depend just on L. Moreover, there is again a *single* nonzero eigenvalue f_L of the reduced matrix $\mathcal{D}_L$ of L spins for *any* L (see Appendix B), such that, in the bosonic approximation (25)–(55),

$$S(\rho_L) = -f_L \log_2 f_L + (1 + f_L)\log_2(1 + f_L) + \delta,$$
$$f_L = \tfrac{1}{2}[\sqrt{1 + 2\alpha_L\Delta} - 1], \quad \alpha_L = L(n-L)/n^2, \quad (66)$$

where $\delta = 0$ (1) for $|B| < B_c$ $[(B/B_c)^{2Ls} \ll 1]$ and

$$\Delta = \frac{n^2(\lambda^2 - \varpi^2)}{2(n-1)\omega_0\omega_1}, \quad \varpi = \frac{\omega_0 + (n-1)\omega_1}{n}. \quad (67)$$

For $n = 2$ we recover Eqs. (61) and (62), while for large n, $\Delta \approx \frac{\lambda - \Delta^0_+}{\omega_0} - 1$. Entanglement is then driven again by the ratio $\frac{\lambda^2 - \varpi^2}{\omega_0\omega_1}$, which is small away from B_c and vanishes at B_s. For small Δ, $f_L \approx \frac{1}{2}\alpha_L\Delta$, with $\Delta \approx \frac{1}{2}[\frac{n}{(n-1)}\frac{J_x - J_y}{2B}]^2$ for $|B| \gg B_c$ and $\Delta \propto (B - B_s)^2$ in the vicinity of B_s. For $B \to B_c$, $f_L \propto \sqrt{\alpha_L}(B - B_c)^{-1/4}$ and $S(\rho_L) \approx \log_2 f_L e$.

The bosonic negativity of a bipartition $(m, L-m)$ of a subsystem of $L \leqslant n$ spins can again be explicitly obtained, since there is also *a single* negative eigenvalue $\tilde{f}_{Lm}$ of the partial transpose of the contraction matrix (see Appendix B):

$$N_{m,L-m} = \frac{-\tilde{f}_{Lm}}{1 + 2\tilde{f}_{Lm}}, \quad (68)$$

$$\tilde{f}_{Lm} = \frac{1}{2}\sqrt{1 + \gamma_{Lm}\Delta - \sqrt{8\beta_{Lm}\Delta + \gamma^2_{Lm}\Delta^2}} - \frac{1}{2}, \quad (69)$$
$$\gamma_{Lm} = \alpha_L + 4\beta_{Lm}, \quad \beta_{Lm} = m(L-m)/n^2. \quad (70)$$

For a global partition ($L = n$), $\alpha_n = 0$ while $\beta_{nm} = \alpha_m$, and $\tilde{f}_{nL} = f_L - \sqrt{f_L(f_L + 1)}$, with $N_{nL} = f_L + \sqrt{f_L(f_L + 1)}$, as in Eq. (63). In general, for small Δ,

$$\tilde{f}_{Lm} \approx -\sqrt{\tfrac{1}{2}\beta_{Lm}\Delta} \approx -\sqrt{(\beta_{Lm}/\alpha_L)f_L}, \quad (71)$$

such that for strong fields, $\tilde{f}_{Lm} \approx -\sqrt{\beta_{Lm}}\frac{n}{n-1}\frac{J_x - J_y}{4B}$, while for B close to B_s, $\tilde{f}_{Lm} \propto \sqrt{\beta_{Lm}}|B - B_s|$. On the other hand, for $B \to B_c$, $\tilde{f}_{Lm} \to -\frac{1}{2}(1 - \sqrt{\frac{\alpha_l}{\alpha_L + 4\beta_{Lm}}}) + O(|B - B_c|^{\frac{1}{2}})$ if $\alpha_L \neq 0$, which implies that subsystem negativities $N_{m,L-m}$ with $L < n$ *remain finite* at B_c (in agreement with the results of Ref. [16]), as $\tilde{f}_{Lm}$ remains *above* $-\frac{1}{2}$.

In the parity-breaking phase, the replacement (56) ($N \to 2N + \frac{1}{2}$) should be used for global negativities $N_{n,L-n}$, whereas subsystem negativities $N_{m,L-m}$ remain unchanged after parity restoration if $(B/B_c)^{2s(n-L)}$ and $(B/B_c)^{2sL}$ can both be neglected.

Equations (66)–(69) represent essentially the exact expressions for the subsystem entropy and negativity for large spin at finite n, as well as for large n at finite spin, as verified by exact numerical calculations. For instance, exact (obtained through diagonalization of H) and RPA results for a spin $\frac{1}{2}$ XY array of $n = 100$ spins are shown in Figs. 3 and 4. RPA results for the entanglement entropy are quite accurate except in the vicinity of B_c, where differences decrease as n or s increases. For large L they were obtained with the previous expression (66), whereas for small L (like the $L = 2$ case), we have used the proper spin state (54), whose main effect is to take into account the correct overlap for B below but close to B_c (roughly, δ replaced by the entropy of the reduced mean-field superposition).

The variation of $S(\rho_L)$ with L at fixed field (bottom left panel in Fig. 3) is also correctly predicted, being quite accurate in both the normal and parity-breaking phase for fields not too close to B_c. The bottom right panel shows that f_L remains small except for B around B_c, while $\tilde{f}_{Lm}$ also becomes small as L decreases, in full agreement with Eq. (71). RPA results for global ($N_{n,L-n}$) and in particular subsystem negativities ($N_{m,L-m}$ for $L < n$), which are much smaller and vanish at B_s, are also very accurate, as seen in Fig. 4. Subsystem negativities were directly obtained with Eq. (68), whereas global negativities were corrected with Eq. (56) for $B < B_c$ and large L and using Eq. (54) for $L = 2$.

IV. DISCUSSION

We have shown that the mean field plus RPA method is able to provide, through the bosonic representation, a general tractable method for estimating, in the ground state of general spin arrays, the entanglement entropy of any bipartition of the whole system as well as the negativity associated with any bipartition of any subsystem. The approach becomes fully analytic in systems with translational invariance, where no numerical diagonalization is required for obtaining the basic contraction matrices.

The bosonic treatment provides essentially the exact behavior of the system in the large-spin limit. Finite spin corrections can be taken into account through the corresponding RPA spin state, which allows us in particular to implement the

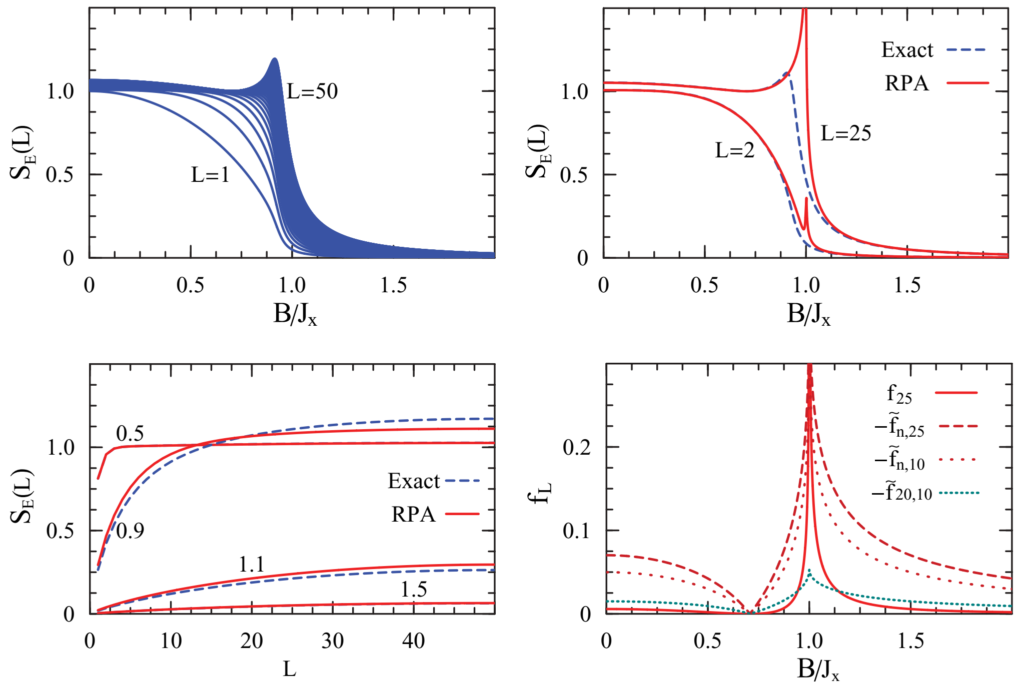

FIG. 3. (Color online) Results for a fully connected spin $\frac{1}{2}$ XY array of $n = 100$ spins with $J_y/J_x = 0.5$. Top left: Exact entanglement entropies $S_E(L) = S(\rho_L)$ of subsystems with $L \leqslant n/2$ spins as a function of the magnetic field. Top right: Comparison between exact and RPA results for $S(\rho_L)$. Bottom left: Exact and RPA results for $S(\rho_L)$ as a function of the subsystem size L at four different field ratios B/B_c. Bottom right: Magnetic behavior of the average boson occupation number (66) for $L = 25$ and the negative symplectic eigenvalue (69) of the partial transposed contraction matrix for different L, m.

nonnegligible symmetry-restoration effects in the case of the parity-breaking mean field, but which otherwise yields results that are in full agreement with the bosonic treatment at first order in the average local boson occupation. The latter is normally very low away from critical regions.

Through direct application of the present method, simple analytic expressions for the entanglement entropy and negativities for a spin s pair and for a fully connected array of n spins s in a uniform field have been straightforwardly obtained, and these depend explicitly on the RPA energies. The agreement with exact numerical results is confirmed to improve as the spin s increases at fixed size and in the fully connected case as well as when n increases at fixed s. Differences in fact are negligible away from the critical region if the spin s or the size n are not too small.

An important general prediction that arises from the present treatment is that entanglement from elementary excitations approaches a nonvanishing spin-independent limit as the spin

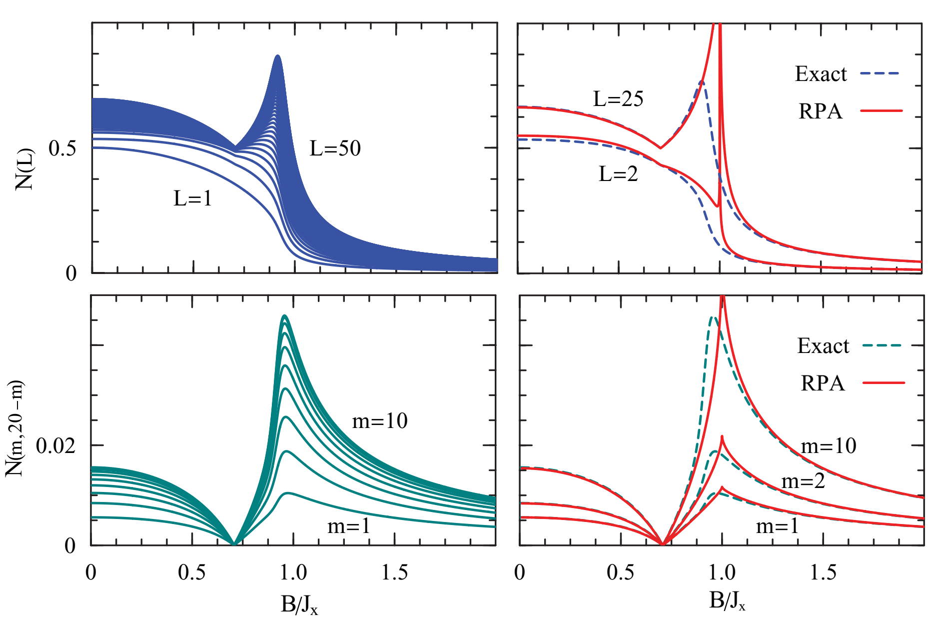

FIG. 4. (Color online) Top left: Exact global negativities $N(L) = N_{L,n-L}$ between L and $n - L$ spins in the fully connected array of Fig. 3 ($n = 100$ spins). Top right: Comparison between exact and RPA results for $N(L)$ for two values of L. Bottom left: Exact subsystem negativities $N_{m,L-m}$ between m and $L - m$ spins in a subsystem of $L = 20$ spins. Bottom right: Comparison between exact and RPA results for $N_{m,L-m}$.

increases. An RPA quantum regime, characterized by weak entanglement, then emerges between strictly classical and strongly quantum regimes.

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APPENDIX A: RPA SPIN DENSITIES

Here we will construct the spin density matrices compatible with the RPA spin state (14) and the contractions (17) up to second order in V, i.e., first order in the average occupation $VV^\dagger$ (implying zero or one boson per site). At this order, $F \approx GG^\dagger$ [Eqs. (17)], and the support of $\rho = |0_{\rm RPA}\rangle\langle 0_{\rm RPA}|$ is just the subspace spanned by the mean-field state $|0\rangle$ plus the two-site excitations $|1_i 1_j\rangle$ [Eq. (15)], leading to

$$\rho \approx \begin{pmatrix} \boldsymbol{G}\boldsymbol{G}^\dagger & \boldsymbol{G} \\ \boldsymbol{G}^\dagger & 1-\boldsymbol{G}^\dagger\boldsymbol{G} \end{pmatrix}, \quad \text{(A1)}$$

where $\boldsymbol{G}$ denotes a column matrix of elements G_{ij}, $i<j$. At this order, $\rho^2=\rho$. The ensuing reduced density matrix $\rho_A = {\rm Tr}_{\bar{A}}\rho$ of a subsystem A of L spins becomes

$$\rho_A \approx \begin{pmatrix} \boldsymbol{G}_A\boldsymbol{G}_A^\dagger & 0 & \boldsymbol{G}_A \\ 0 & F_A - G_A G_A^\dagger & 0 \\ \boldsymbol{G}_A^\dagger & 0 & 1-{\rm Tr}F_A + \boldsymbol{G}_A^\dagger\boldsymbol{G}_A \end{pmatrix}, \quad \text{(A2)}$$

where F_A, G_A are the $L\times L$ contraction matrices of subsystem A, and $\boldsymbol{G}_A$ is the concomitant column vector [of length $L(L-1)/2$]. The central block contains the one-site elements $|1_i\rangle\langle 1_j|$ arising from the partial trace of $\boldsymbol{G}\boldsymbol{G}^\dagger$. Here we have used the approximate identity $\sum_{k\in\bar{A}} G_{ik}G^\dagger_{kj} \approx F_{ij} - \sum_{k\in A} G_{ik}G^\dagger_{kj}$ for $i,j\in A$ (and neglected diagonal elements G_{ii}, of higher order due to the absence of self-energy terms), which allows us to write ρ_A entirely in terms of local contractions. Equation (A2) is then in agreement with direct state tomography at this order [for $i,j,k,l \in A$, $\langle b_j^\dagger b_i \prod_{k\neq i,j}(1-b_k^\dagger b_k)\rangle_{0'} \approx (F_A - G_A G_A^\dagger)_{ij}$, $\langle b_i^\dagger b_j^\dagger b_k b_l\rangle_{0'} \approx G_{kl}\bar{G}_{ij}$]. Up to $O(V^2)$, ρ_A is a positive matrix with ${\rm Tr}\rho_A = 1$ but is no longer pure.

Its entropy $S(\rho_A) = -{\rm Tr}\rho_A \log_2\rho_A$ is determined, at this order, by the central block $\rho_A^1 = F_A - G_A G_A^\dagger$,

$$S(\rho_A) \approx {\rm Tr}\rho_A^1\left(\log_2 e - \log_2 \rho_A^1\right), \quad \text{(A3)}$$

which coincides with Eq. (25) up to second order in V [at this order f_A^α coincides with the eigenvalues of ρ_A^1, and Eq. (25) becomes $\approx \sum_\alpha f_A^\alpha(\log_2 e - \log_2 f_A^\alpha)$].

On the other hand, the leading term in the negativity arising from a bipartition (B,C) of A is of first order in V and is just the sum of the singular values of the submatrix G_{BC} (of elements G_{ij}, $i\in B$, $j\in C$), whence $N_{BC} \approx {\rm Tr}[G_{BC}G^\dagger_{BC}]^{\frac{1}{2}}$. At this order, the negative symplectic eigenvalues $\tilde{f}_A^\alpha$ in Eq. (29) are again minus the singular values of G_{BC}, while Eq. (28) becomes $N_{BC} \approx -\sum_\alpha \tilde{f}_A^{\tilde{\alpha}}$, leading again to the previous result.

Let us finally note that Eq. (A2) always commutes with the S_z parity (along the mean-field axis) of subsystem A, i.e., $[\rho_A, P_{zA}] = 0$, $P_{zA} = \exp[i\pi\sum_{i\in A}(s_{iz}+s_i)]$. In the case of two spins i,j, $\boldsymbol{G}_A$ has length 1 and Eq. (A2) is just a 4×4 blocked matrix, while in the case of a single spin i, $\boldsymbol{G}_A$ has length 0 and Eq. (A2) becomes just $\rho_i \approx F_{ii}|1_i\rangle\langle 1_i| + (1-F_{ii})|0_i\rangle\langle 0_i|$.

APPENDIX B: FULLY CONNECTED SYSTEM

In the fully connected XYZ spin system, the contractions (65) are of the form $F_{ij} = F_0\delta_{ij} + F_1$, $G_{ij} = G_0\delta_{ij} + G_1$, with F_0, F_1, G_0, G_1 real. The ensuing contraction matrix $\mathcal{D}_L$ for a subsystem of L spins will then have symplectic eigenvalues (see also Ref. [25])

$$f_L = \sqrt{\left(F_0 + LF_1 + \tfrac{1}{2}\right)^2 - (G_0 + LG_1)^2} - \tfrac{1}{2}, \quad \text{(B1)}$$

$$f_0 = \sqrt{\left(F_0 + \tfrac{1}{2}\right)^2 - G_0^2} - \tfrac{1}{2}, \quad \text{(B2)}$$

plus their partners $1+f_L$, $1+f_0$, where f_L is nondegenerate while f_0 has $L-1$ degeneracy. Equations (B1) and (B2) can be obtained either by a Fourier transform of the local operators or by noticing that the $L\times L$ contraction matrix F_L can be written as $F_L = F_0 I_L + F_1 \mathbf{1}_L\mathbf{1}_L^t$ (and similarly for G_L), with I_L the $L\times L$ identity and $\mathbf{1}_L$ a column $L\times 1$ vector with unit elements. F_L and G_L will then be diagonal in the same local basis with eigenvalues $F_0 + LF_1$ and F_0 ($L-1$ degenerate) and similarly for G_L, which leads to Eqs. (B1) and (B2). In the case of a global vacuum, $f_0 = 0$ (since for $L=n$, we should have $f_{L=n} = f_0 = 0$), which implies a single positive eigenvalue f_L for any $L<n$. Equation (B1) leads then to Eq. (66).

For evaluating the negativity N_{mp} of a bipartition (m,p) of a subsystem of L spins ($m+p=L$), we may first note that F_L will be composed of blocks $F_{mm} = F_0 I_m + F_1 \mathbf{1}_m\mathbf{1}_m^t$, $F_{mp} = F_1\mathbf{1}_m\mathbf{1}_p^t = F_{pm}^t$, and $F_{pp} = F_0 I_p + F_1\mathbf{1}_p\mathbf{1}_p^t$, and similarly for G_L. A local transformation allows us to write F_L as a direct sum of a $(L-2)\times(L-2)$ diagonal block $F_0 I_{L-2}$ plus the block $F_0 I_2 + F_1\left(\begin{smallmatrix} m & \sqrt{mp} \\ \sqrt{mp} & p\end{smallmatrix}\right)$, and similarly for G_L. The ensuing partially transposed contraction matrix will then have symplectic eigenvalues $\tilde{f}_0 = f_0$ [Eq. (B2)], $L-2$ degenerate (with $\tilde{f}_0 = 0$ for a global vacuum), and

$$\tilde{f}_{Lm}^\pm = \tfrac{1}{2}\sqrt{{\rm Tr}\mathcal{A}^2 \pm \sqrt{({\rm Tr}\mathcal{A}^2)^2 - 16\det\mathcal{A}}} - \tfrac{1}{2}, \quad \text{(B3)}$$

together with their partners $1+\tilde{f}_0$, $1+\tilde{f}_{Lm}^\pm$, where $\mathcal{A} = \left(\begin{smallmatrix} A_{FG} & -A_{GF} \\ A_{GF} & -A_{FG}\end{smallmatrix}\right)$ is a 4×4 matrix with blocks $A_{FG} = (\frac{1}{2}+F_0)I_2 + \left(\begin{smallmatrix} mF_1 & \sqrt{mp}G_1 \\ \sqrt{mp}G_1 & pF_1\end{smallmatrix}\right)$ and similarly for $\mathcal{A}_{GF}$. Here $\tilde{f}_{Lm}^+ > 0$ but $\tilde{f}_{Lm}^- < 0$. The latter is the single negative symplectic eigenvalue given in Eq. (69).

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