Even-odd entanglement in boson and spin systems

R. Rossignoli, N. Canosa, J.M. Matera
Departamento de Física-IFLP, Universidad Nacional de La Plata, C.C. 67, La Plata (1900), Argentina
(Dated: June 7, 2018)

We examine the entanglement entropy of the even half of a translationally invariant finite chain or lattice in its ground state. This entropy measures the entanglement between the even and odd halves (each forming a "comb" of $n/2$ sites) and can be expected to be extensive for short range couplings away from criticality. We first consider bosonic systems with quadratic couplings, where analytic expressions for arbitrary dimensions can be provided. The bosonic treatment is then applied to finite spin chains and arrays by means of the random phase approximation. Results for first neighbor anisotropic XY couplings indicate that while at strong magnetic fields this entropy is strictly extensive, at weak fields important deviations arise, stemming from parity-breaking effects and the presence of a factorizing field (in which vicinity it becomes size-independent and identical to the entropy of a contiguous half). Exact numerical results for small spin s chains are shown to be in agreement with the bosonic RPA prediction.

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

arXiv:1104.4005v1 [quant-ph] 20 Apr 2011

I. INTRODUCTION

The entanglement properties of many-body systems are of great interest for both quantum information theory [1] and condensed matter physics [2–4]. Their knowledge enables, on the one hand, to assess the potential of a given many-body system for quantum information processing tasks such as quantum teleportation [5] and quantum computation [1, 6, 7]. On the other hand, it provides a deep understanding of quantum correlations and their relation with criticality [2–4, 8, 9]. In non-critical systems with short range couplings, i.e., local couplings in boson or spin lattices, ground state entanglement is believed to satisfy a general area law by which the entropy of the reduced state of a given region, which measures its entanglement with the rest of the system, scales as the area of its boundary as the system size increases [4, 10]. This behavior is quite different from that of standard thermodynamic entropy which scales as the volume. In one dimensional systems this statement has been quite generally and rigorously proved [4, 11] and simply means that the entropy of a contiguous section saturates, i.e., approaches a size independent constant, as the size increases. Violation of this scaling is therefore an indication of criticality [8, 9, 12]. The exact expression of the entropy of a contiguous block in a one-dimensional XY spin 1/2 chain in the thermodynamic limit has been obtained [13–15] and confirms the previous behavior.

The conventional area law holds for contiguous subsystems. For non-contiguous regions it actually implies that the entropy is proportional to the number of couplings broken by the partition. For instance, for *comb*-like regions like the subset of all even sites in a chain, the entropy should scale as the total number n of sites for first neighbor or short range couplings. This was in fact verified in [11] for the harmonic cyclic chain, where the corresponding logarithmic negativity was calculated, and also verified numerically in [16] for some spin arrays and a 1-d half-filled Hubbard model, where the even entanglement entropy was computed. An exact treatment of general comb entropies for a large one-dimensional critical XX spin 1/2 chain with first neighbor couplings was given in [17], showing that they are indeed proportional to the size L plus a logarithmic correction.

The aim of this work is to analyze in detail the entanglement entropy of all even sites in *finite* boson and spin arrays, both in one dimension as well as in general d-dimensions. Such bipartition can be normally expected to be the maximally entangled bipartition at least for uniform nearest neighbor couplings, as it will there break all coupling links. We first analyze the bosonic case with general quadratic couplings, where a fully analytic treatment of this entropy is shown to be feasible and allows to derive simple general expressions in the weak coupling limit. Comparison with single site and block entropies is also made. The bosonic treatment is then applied to finite spin s arrays with anisotropic ferromagnetic-type XY couplings in a uniform transverse field through the RPA approach [18]. This allows to predict in a simple way the main properties of the total even entropy in these systems. Comparison with exact numerical results indicate that the RPA prediction, while qualitatively correct, is also quite accurate outside the critical region already for low spin $s \gtrsim 2$, representing the high spin limit. Results corroborate that for strong fields, the total even entropy in these systems is extensive, i.e., directly proportional to the total number n of sites. However, for low fields $B < B_c$, this entropy has an additive constant, which arises in the RPA from parity restoration [18]. Moreover, in the immediate vicinity of the factorizing field $B_s < B_c$ [19–22], extensivity is fully lost and the total even entropy reduces to this constant, which is the same as that for the block entropy and is exactly evaluated. The exact bosonic treatment is described in sec. II, whereas its application to spin systems is discussed in sec. III. Conclusions are finally drawn in IV.

II. ENTANGLEMENT ENTROPY IN BOSONIC SYSTEMS

We start by considering a system of n bosonic modes defined by boson creation operators $b_i^\dagger$ ($[b_i, b_j^\dagger] = \delta_{ij}$), interacting through a general quadratic coupling. The Hamiltonian can be written as

$$H = \sum_{i,j}(\lambda_i\delta_{ij} - \Delta_{ij}^+)(b_i^\dagger b_j + \tfrac{1}{2}\delta_{ij}) - \tfrac{1}{2}(\Delta_{ij}^- b_i^\dagger b_j^\dagger + \bar{\Delta}_{ij}^- b_j b_i) \quad (1)$$
$$= \tfrac{1}{2}\mathcal{Z}^\dagger\mathcal{H}\mathcal{Z}\,,\ \mathcal{Z} = \begin{pmatrix} b \\ b^\dagger \end{pmatrix},\ \mathcal{H} = \begin{pmatrix} \Lambda - \Delta^+ & -\Delta^- \\ -\bar{\Delta}^- & \Lambda - \bar{\Delta}^+ \end{pmatrix},$$

where $\mathcal{Z}^\dagger = (b^\dagger, b)$, $\Lambda_{ij} = \lambda_i\delta_{ij}$ and the $2n \times 2n$ matrix $\mathcal{H}$ is hermitian. The system is assumed stable, such that the matrix $\mathcal{H}$ is *positive definite*. We may then also write (1) in the standard diagonal form

$$H = \sum_k \omega_k (b'^\dagger_k b'_k + \tfrac{1}{2})\,, \quad (2)$$

where ω_k are the symplectic eigenvalues of $\mathcal{H}$, i.e., the positive eigenvalues of the matrix $\mathcal{M}\mathcal{H}$, with $\mathcal{M} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$, which come in pairs of opposite sign and are all real nonzero when $\mathcal{H}$ is positive definite [23], and $b'^\dagger_k$ are the normal boson operators determined by the diagonalizing Bogoliubov transformation [23] $\mathcal{Z} = \mathcal{W}\mathcal{Z}'$ satisfying $\mathcal{W}^\dagger\mathcal{M}\mathcal{W} = \mathcal{M}$ and $(\mathcal{W}^\dagger\mathcal{H}\mathcal{W})_{kk'} = \omega_k\delta_{kk'}$. The ground state is the vacuum $|0'\rangle$ of the operators b'_k and is non-degenerate.

Ground state entanglement properties can be evaluated through the general Gaussian state formalism [11, 24, 25], which we here recast in terms of the contraction matrix [18, 23]

$$\mathcal{D} = \langle \mathcal{Z}\mathcal{Z}^\dagger\rangle_{0'} - \mathcal{M} = \mathcal{W}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\mathcal{W}^\dagger \quad (3)$$
$$= \begin{pmatrix} F^+ & F^- \\ \bar{F}^- & I + \bar{F}^+ \end{pmatrix},\ \begin{matrix} F^+_{ij} = \langle b_j^\dagger b_i\rangle_{0'} \\ F^-_{ij} = \langle b_j b_i\rangle_{0'} = \langle b_i^\dagger b_j^\dagger\rangle^*_{0'} \end{matrix}. \quad (4)$$

This hermitian matrix determines, through application of Wick's theorem [23], the average of any many-body operator. In particular, the reduced state $\rho_A = \mathrm{Tr}_{\bar{A}}|0'\rangle\langle 0'|$ of a subsystem A of n_A modes ($\bar{A}$ denoting the complementary subsystem and $\mathrm{Tr}_{\bar{A}}$ the partial trace) is fully determined by the corresponding sub-matrix $\mathcal{D}_A = \langle Z_A Z_A^\dagger\rangle - \mathcal{M}_A$ (Eq. (4) with $i, j \in A$) and can be written as [18]

$$\rho_A = \exp[-\tfrac{1}{2}Z_A^\dagger\tilde{\mathcal{H}}_A Z_A]/\mathrm{Tr}\exp[-\tfrac{1}{2}Z_A^\dagger\mathcal{H}_A Z_A]\,, \quad (5)$$

where $\tilde{\mathcal{H}}_A = \mathcal{M}_A \ln[I + \mathcal{M}_A\mathcal{D}_A^{-1}]$. Eq. (5) represents a thermal-like state of suitable n_A independent modes determined by the effective Hamiltonian $\tilde{\mathcal{H}}_A$. The entanglement entropy of the $(A, \bar{A})$ partition, $S(\rho_A) = S(\rho_{\bar{A}})$, is then determined by the symplectic eigenvalues f_k^A of $\mathcal{D}_A$ (i.e., the positive eigenvalues of the matrix $\mathcal{D}_A\mathcal{M}_A$, which has eigenvalues f_k^A and $-1 - f_k^A$), and given by

$$S(\rho_A) = -\mathrm{Tr}\,\rho_A \ln\rho_A = \sum_{k=1}^{n_A} h(f_k^A)\,, \quad (6)$$
$$h(f) = -f\ln f + (1+f)\ln(1+f)\,. \quad (7)$$

For instance, the entanglement of a *single mode* i with the rest of the system is just

$$S(\rho_i) = h(f_i)\,,\ f_i = \sqrt{(F^+_{ii} + \tfrac{1}{2})^2 - |F^-_{ii}|^2} - \tfrac{1}{2}\,, \quad (8)$$

where f_i, the symplectic eigenvalue of the single mode contraction matrix $\mathcal{D}_i$, represents the deviation from minimum uncertainty of the mode: $(F^+_{ii} + \frac{1}{2})^2 - |F^-_{ii}|^2 = \langle q_i^2\rangle_{0'}\langle p_i^2\rangle_{0'} - [\mathrm{Re}(\langle q_i p_i\rangle_{0'})]^2 \geq 0$ for $q_i = \frac{b_i + b_i^\dagger}{\sqrt{2}}$, $p_i = \frac{b_i - b_i^\dagger}{\sqrt{2}i}$.

A. Finite translationally invariant systems

Let us now associate each bosonic mode with a given site in a cyclic chain and consider a translationally invariant system of n sites, such that $\lambda_i = \lambda$ and $\Delta^\pm_{ij} = \Delta^\pm(i-j)$, with $\Delta^\pm(-l) = \Delta^\pm(n-l)$. We first consider for simplicity the one-dimensional case. Through a discrete Fourier transform $b_i^\dagger = \frac{1}{\sqrt{n}}\sum_{k=0}^{n-1} e^{i2\pi ki/n} b_k^\dagger$, we can diagonalize $\mathcal{H}$ analytically and obtain an explicit expression for the contractions $F^\pm_{ij}$. We will assume $\Delta^\pm(l) = \Delta^\pm(-l)\ \forall\ l$, in which case the energies ω_k in (2) adopt the simple form [18]

$$\omega_k = \sqrt{(\lambda - \Delta_k^+)^2 - (\Delta_k^-)^2}\,, \quad (9)$$

where $\Delta_k^\pm$ are the Fourier transforms of the couplings:

$$\Delta_k^\pm = \sum_{l=0}^{n-1} e^{i2\pi kl/n}\Delta^\pm(l)\,. \quad (10)$$

The contractions $F^\pm_{ij}$ depend just on the separation $l \equiv |i-j|$ and are given by

$$F_l^\pm \equiv F^\pm_{j+l,j} = \frac{1}{n}\sum_{k=0}^{n-1} e^{-i2\pi kl/n} f_k^\pm\,, \quad (11)$$
$$f_k^+ = \langle b_k^\dagger b_k\rangle_{0'} = \frac{\lambda - \Delta_k^+}{2\omega_k} - \tfrac{1}{2},\ f_k^- = \langle b_k b_{-k}\rangle_{0'} = \frac{\Delta_k^-}{2\omega_k}\,. \quad (12)$$

The symplectic eigenvalues of the full contraction matrix (4) are of course $f_k = \sqrt{(\frac{1}{2} + f_k^+)^2 - (f_k^-)^2} - \frac{1}{2} = 0\ \forall\ k$.

In the *weak coupling limit* $|\Delta_k^\pm| \ll \lambda\ \forall\ k$, $f_k^\pm$ become small and up to lowest non-zero order we obtain

$$f_k^- \approx \frac{\Delta_k^-}{2\lambda},\ \ f_k^+ \approx \frac{(\Delta_k^-)^2}{4\lambda^2} \approx (f_k^-)^2\,, \quad (13)$$

which leads to

$$F_l^- \approx \frac{\Delta^-(l)}{2\lambda},\ F_l^+ \approx \frac{\sum_{l'}\Delta^-(l')\Delta^-(l-l')}{4\lambda^2}\,. \quad (14)$$

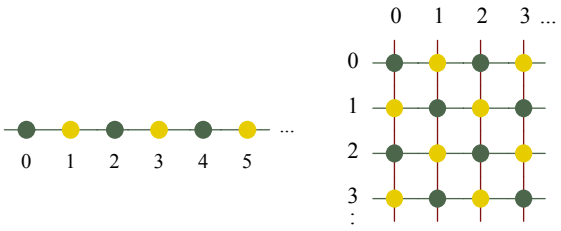

FIG. 1. (Color online) Even-odd partitions of one- and two-dimensional arrays

At this order just sites linked by $\Delta^-(l)$ or its convolution are correlated. The eigenvalues f_k^A of subsystem contraction matrices will depend up to lowest non-zero order on F_l^+ and $(F_l^-)^2$, being then $O(\Delta_-^2/\lambda^2)$ for $\Delta^-(l) \propto \Delta_-$. We can then use in (6) the approximation

$$h(f) \approx -f(\ln f - 1) + O(f^2)\,, \tag{15}$$

such that $S(\rho_A) = O(\frac{\Delta^2}{\lambda^2} \ln \frac{\Delta^2}{\lambda^2})$.

On the other hand, it is seen from Eq. (9) that the present system is stable provided $\lambda \geq \Delta_k^+ + |\Delta_k^-| \;\forall\; k$. For *attractive* couplings $\Delta^+(l) \geq 0 \;\forall\; l$, with all $\Delta^-(l)$ of the *same* sign, the strongest condition is obtained for $k = 0$, so that stability occurs for

$$\lambda > \lambda_c = \Delta_0^+ + |\Delta_0^-| = \sum_l \Delta^+(l) + |\Delta^-(l)|\,. \tag{16}$$

For $\lambda \to \lambda_c$, $\omega_0 \to 0$ (while all other ω_k remain finite in a finite system), implying a divergence of $f_0^\pm$ (Eq. (12)):

$$|f_0^-| \approx \sqrt{\frac{|\Delta_0^-|}{8(\lambda - \lambda_c)}}\,, \quad f_0^+ \approx |f_0^-| - 1/2\,, \tag{17}$$

plus terms $O(\lambda/\lambda_c - 1)^{1/2}$. This entails in turn a divergence $f_0^A \propto (\lambda/\lambda_c - 1)^{-1/4}$ of the largest eigenvalue of a subsystem contraction matrix $\mathcal{D}_A$, with $S(\rho_A) \approx \ln f_0^A + 1 \approx -\frac{1}{4}\ln(\lambda/\lambda_c - 1)$ plus constant terms.

For example, the single site entropy (8) becomes

$$S(\rho_i) = h(f), \quad f = \sqrt{(\tfrac{1}{2} + F_0^+)^2 - (F_0^-)^2} - \tfrac{1}{2}\,, \tag{18}$$

with $F_0^\pm = \frac{1}{n}\sum_k f_k^\pm$ (Eq. (11)). For weak coupling,

$$f \approx F_0^+ - (F_0^-)^2 \approx \frac{\sum_{l\neq 0}(\Delta^-(l))^2}{4\lambda^2}\,, \tag{19}$$

which involves just the couplings $\Delta^-(l)$ connecting the site with the rest of the system. On the other hand, for $\lambda \to \lambda_c$, $f \propto \sqrt{\frac{f_0^-}{n}} \propto (\lambda/\lambda_c - 1)^{-1/4}$.

B. Even-odd entanglement entropy

We now evaluate the entropy of the reduced state of all even sites, $S(\rho_E) = S(\rho_O)$, which measures their entanglement with the complementary set of odd sites (Fig. 1 left). We will assume n even, such that the even subsystem, defined by $(-1)^i = +1$, is again translationally invariant. The ensuing contraction matrix $\mathcal{D}_E$ can be obtained by removing contractions between even and odd sites in the full matrix (4) and extracting then the even part. This leads to elements

$$\tilde{F}_{ij}^\pm = \tfrac{1}{2}F_{ij}^\pm(1 + e^{i\pi(i-j)})\,, \tag{20}$$

whose Fourier transforms are, using Eq. (11),

$$\tilde{f}_k^\pm = \tfrac{1}{2}(f_k^\pm + f_{k+n/2}^\pm)\,. \tag{21}$$

The final symplectic eigenvalues of $\mathcal{D}_E$ then become

$$\tilde{f}_k = \sqrt{(\tfrac{1}{2} + \tilde{f}_k^+)^2 - (\tilde{f}_k^-)^2]} - \tfrac{1}{2}\,, \tag{22}$$

for $k = 0, \ldots, n/2 - 1$. We then obtain

$$S(\rho_E) = \sum_{k=0}^{n/2-1} h(\tilde{f}_k) = \tfrac{1}{2}\sum_{k=0}^{n-1} h(\tilde{f}_k)\,. \tag{23}$$

Whenever $\tilde{f}_k$ can be approximated by a smooth function $\tilde{f}(\tilde{k})$ of $\tilde{k} \equiv k/n$, we may replace (23) by the integral

$$S(\rho_E) \approx \frac{n}{2}\int_0^1 h[\tilde{f}(\tilde{k})]d\tilde{k}\,. \tag{24}$$

In these cases, we may then expect $S(\rho_E)$ *extensive*, i.e., proportional to the number $n/2$ of even sites. Let us remark, however, that this is not always the case: In a completely and uniformly connected system like the Lipkin model [23, 26, 27], the contraction matrix will have a *single* non-zero symplectic eigenvalue f_{n_A} for *any* subsystem [18], including the whole even set, and $S(\rho_E) = h(f_{n/2})$ is no longer proportional to n. A similar lack of extensivity holds in a finite system in the vicinity of the instability ($\lambda \to \lambda_c$, see below).

For *weak coupling*, Eqs. (13), (14) and (21) lead to

$$\tilde{f}_k \approx \frac{(\Delta_k^- - \Delta_{k+n/2}^-)^2}{16\lambda^2} = \frac{(\sum_{l\ \mathrm{odd}} e^{i2\pi kl/n}\Delta^-(l))^2}{4\lambda^2} \tag{25}$$

which involves again just the couplings $\Delta^-(l)$ connecting the even and odd subsystems. On the other hand, for $\lambda \to \lambda_c$ (Eq. (16)), $\tilde{f}_0 \approx \frac{1}{2}\sqrt{(1 + 2f_{n/2}^+)|f_0^-| - 2f_{n/2}^- f_0^-}$ diverges as $(\lambda/\lambda_c - 1)^{-1/4}$ whereas all other $\tilde{f}_k$ remain finite, and extensivity is lost.

C. First neighbor coupling

Let us now examine in detail the first neighbor case $\Delta^\pm(l) = \frac{1}{2}\Delta^\pm(\delta_{l1} + \delta_{l,-1})$, where Eq. (10) becomes

$$\Delta_k^\pm = \Delta^\pm \cos(2\pi k/n)\,. \tag{26}$$

The exact $S(\rho_E)$ can be obtained from Eqs. (21)–(23). In the weak coupling limit, Eqs. (19) and (25) lead to

$$f \approx \frac{(\Delta^-)^2}{8\lambda^2}\,, \tag{27}$$

$$\tilde{f}_k \approx \frac{(\Delta^-_k)^2}{4\lambda^2} \approx 2f\cos^2(2\pi k/n)\,. \tag{28}$$

Using Eqs. (15)–(24), the single site and the total even entropies can then be expressed just in terms of f:

$$S(\rho_i) \approx -f(\ln f - 1)\,, \tag{29}$$

$$\begin{aligned} S(\rho_E) &\approx -nf\int_0^1 \cos^2(2\pi\tilde{k})\{\ln[2f\cos^2(2\pi\tilde{k})]-1\}\,d\tilde{k} \\ &= -\frac{n}{2}f(\ln f - \ln 2)\,. \end{aligned} \tag{30}$$

Hence, in this limit $S(\rho_E)$ is *extensive*, becoming $n/2$ times the single site entropy (29) minus a $O(nf)$ correction accounting for the interaction between even sites:

$$S(\rho_E) \approx \frac{n}{2}S(\rho_i) - \frac{n}{2}f(1-\ln 2)\,. \tag{31}$$

The last term represents the *even mutual entropy* $\frac{n}{2}S(\rho_i) - S(\rho_E)$, which is always a positive quantity and becomes here also *extensive* in this limit.

In contrast, the block entropy $S(\rho_L)$, where ρ_L denotes a contiguous block of $L < n$ spins, rapidly saturates as L increases [11]. In the weak coupling limit, it is verified that the ensuing contraction matrix $\mathcal{D}_L$ possesses, up to lowest non-zero order, just *two* positive non-zero symplectic eigenvalues $f_L^\pm \approx \frac{1}{2}f$ for *any* $L \geq 2$, such that

$$S(\rho_L) \approx -f(\ln f/2 - 1) \approx S(\rho_i) + f\ln 2\ , \tag{32}$$

for $2 \leq L \leq n-2$, i.e., it saturates already for $L = 2$. Hence, in this limit,

$$S(\rho_E) \approx \frac{n}{2}S(\rho_L) - \frac{n}{2}f\,. \tag{33}$$

Assuming $\Delta^+ > 0$ (if $\Delta^+ < 0$ we can change its sign by a local change $b_i \to -b_i$ at odd sites) the present system is stable for $\lambda > \lambda_c = \Delta_+ + |\Delta_-|$ (Eq. (16)). For $\lambda \to \lambda_c$, $\omega_0 \to 0$ and all previous entropies diverge. In particular, Eq. (22) leads to

$$\tilde{f}_0 \approx \tfrac{1}{2}[\sqrt[4]{\frac{|\Delta^-|\lambda_c}{2^3\Delta^+(\lambda-\lambda_c)}} - 1]\,,$$

being then verified that $S(\rho_E) \approx -\frac{1}{4}\ln(\lambda/\lambda_c - 1)$ plus a constant term up to leading order. Hence, in this limit $S(\rho_E)/S(\rho_i) \to 1$.

As illustration, the left panels in Fig. 2 depict the single site, block and even-odd entanglement entropies for a ring of $n = 36$ sites with $\Delta^- = \Delta^+/3$, where $\lambda_c = 4\Delta^+/3$.

D. Even-Odd entropy in d-dimensions

The whole previous treatment can be directly extended to a translationally invariant cyclic array in d dimensions. We should just replace l, k, n by vectors $\boldsymbol{l} = (l_1, \ldots, l_d)$, $\boldsymbol{k} = (k_1, \ldots, k_d)$ and $\boldsymbol{n} = (n_1, \ldots, n_d)$, with $l_i, k_i = 0, \ldots, n_i - 1$. We will assume couplings satisfying $\Delta^\pm_{\boldsymbol{i},\boldsymbol{j}} = \Delta^\pm(\boldsymbol{i}-\boldsymbol{j})$, with $\Delta^\pm(-\boldsymbol{l}) = \Delta^\pm(\boldsymbol{n}-\boldsymbol{l}) = \Delta^\pm(\boldsymbol{l})$. The same previous expressions (9)–(12) then hold, with

$$\Delta^\pm_{\boldsymbol{k}} = \sum_{\boldsymbol{l}} e^{i2\pi\tilde{\boldsymbol{k}}\cdot\boldsymbol{l}}\Delta^\pm(\boldsymbol{l})\,, \tag{34}$$

$$F^\pm_{\boldsymbol{l}} = \frac{1}{n}\sum_{\boldsymbol{k}} e^{-i2\pi\tilde{\boldsymbol{k}}\cdot\boldsymbol{l}} f^\pm_{\boldsymbol{k}}\,, \tag{35}$$

where $\tilde{\boldsymbol{k}} = (k_1/n_1, \ldots, k_d/n_d)$ and $n = \prod_{i=1}^d n_i$ is the total number of sites. Eqs. (13)–(14) remain unchanged with $i, k, l \to \boldsymbol{i}, \boldsymbol{k}, \boldsymbol{l}$.

The subsystem of all even sites, like that formed by the blue sites in Fig. 1 right, is defined by

$$(-1)^{i_1+\ldots+i_d} = +1\,.$$

Its contraction matrix will then be the even block of

$$\tilde{F}^\pm_{\boldsymbol{i}\boldsymbol{j}} = \tfrac{1}{2}F^\pm_{\boldsymbol{i}\boldsymbol{j}}(1 + e^{i\pi(\boldsymbol{i}-\boldsymbol{j})\cdot\boldsymbol{1}}) \tag{36}$$

where $\boldsymbol{1} = (1, \ldots, 1)$. Assuming n_i even $\forall\ i$, its Fourier transform is then given again by

$$\tilde{f}^\pm_{\boldsymbol{k}} = \tfrac{1}{2}[f^\pm_{\boldsymbol{k}} + f^\pm_{\boldsymbol{k}+\boldsymbol{n}/2}]\,, \tag{37}$$

where $k_i + n_i/2 \to k_i - n_i/2$ if $k_i \geq n_i/2$. The symplectic eigenvalues of $\mathcal{D}_E$ are then given again by Eq. (22) with $k \to \boldsymbol{k}$, and the even-odd entanglement entropy reads

$$S(\rho_E) = \tfrac{1}{2}\sum_{\boldsymbol{k}} h(\tilde{f}_{\boldsymbol{k}}) \approx \frac{n}{2}\int h[\tilde{f}(\tilde{\boldsymbol{k}})]d^d\tilde{k}\,, \tag{38}$$

where $k_i = 0, \ldots, n_i - 1$ in the sum and the integral is restricted to the unit cube $0 \leq \tilde{k}_i \leq 1$ and valid if $\tilde{f}_{\boldsymbol{k}}$ is a smooth function $\tilde{f}(\tilde{\boldsymbol{k}})$ of $\tilde{\boldsymbol{k}}$.

In the case of first neighbor couplings

$$\Delta^\pm(\boldsymbol{l}) = \frac{1}{2}\sum_{i=1}^d \Delta^\pm_i(\delta_{\boldsymbol{l},\boldsymbol{e}_i} + \delta_{\boldsymbol{l},-\boldsymbol{e}_i})\,,$$

where $\boldsymbol{e}_i = (0, \ldots 1_i, \ldots 0)$, Eq. (34) leads to

$$\Delta^\pm_{\boldsymbol{k}} = \sum_{i=1}^d \Delta^\pm_i\cos(2\pi k_i/n_i)\,. \tag{39}$$

with $\Delta^\pm_{\boldsymbol{k}+\boldsymbol{n}/2} = -\Delta^\pm_{\boldsymbol{k}}$. In the weak coupling limit we then obtain

$$f \approx \frac{|\boldsymbol{\Delta}^-|^2}{8\lambda^2},\ \ |\boldsymbol{\Delta}^-|^2 = \sum_{i=1}^d (\Delta^-_i)^2\,, \tag{40}$$

$$\tilde{f}_{\boldsymbol{k}} \approx u(\tilde{\boldsymbol{k}})\,f\,,\ \ u(\tilde{\boldsymbol{k}}) = 2(\sum_i \frac{\Delta^-_i}{|\boldsymbol{\Delta}^-|}\cos\frac{2\pi k_i}{n_i})^2\,. \tag{41}$$

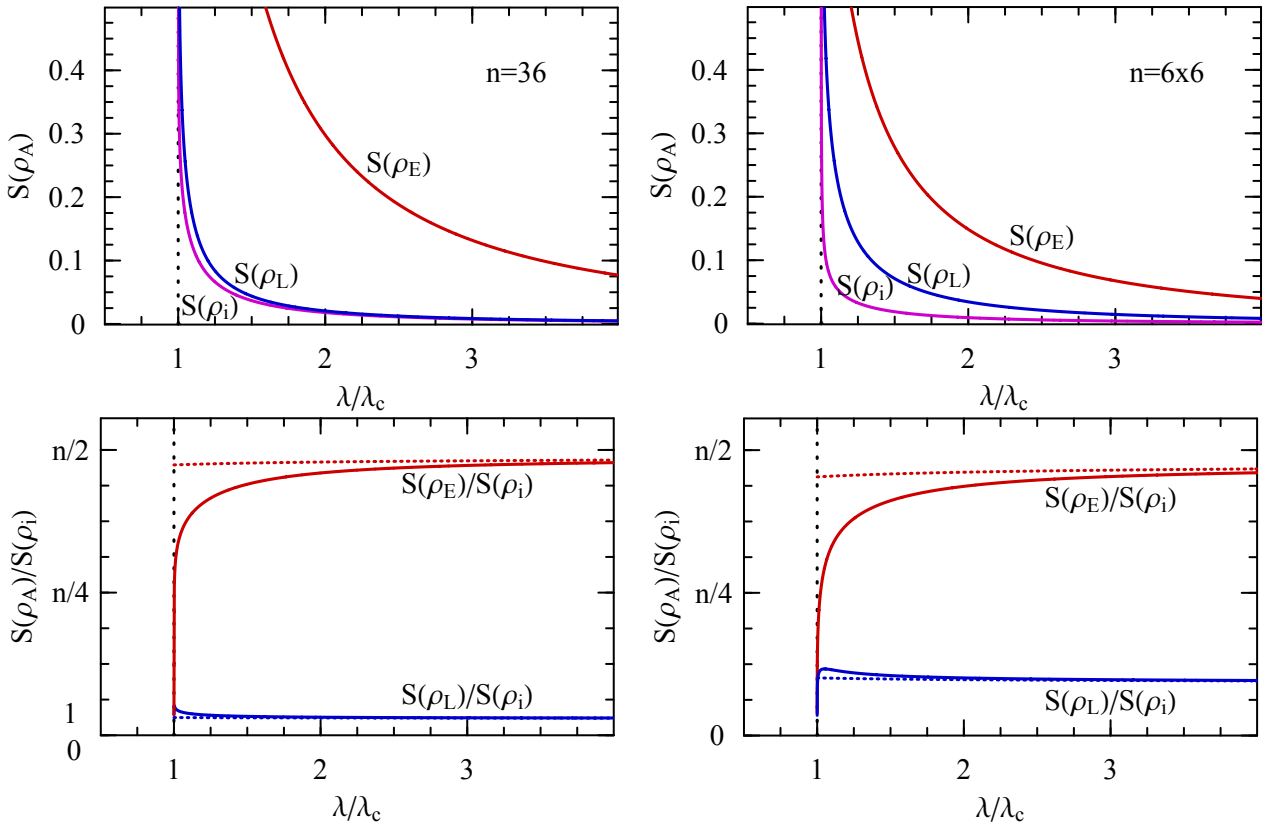

FIG. 2. (Color online) Top left: Entanglement entropies in the ground state of a one-dimensional bosonic chain of $n = 36$ sites described by the Hamiltonian (1) with first neighbor cyclic couplings and $\Delta^- = \Delta^+/3$. $S(\rho_i)$, $S(\rho_L)$ and $S(\rho_E)$ denote, respectively, the entropy of the reduced state of a single site, a block of $L = n/2$ contiguous sites and the set all even sites. Bottom left: The ratios $S(\rho_E)/S(\rho_i)$ and $S(\rho_L)/S(\rho_i)$. Dotted lines depict the ratios determined by the asymptotic expressions (29)–(32), For large λ these ratios are then close to $n/2$ and 1 respectively, while for $\lambda \to \lambda_c$ they all approach 1. The right panels depict the same quantities for a two-dimensional square array of $n = 6 \times 6$ sites with isotropic cyclic couplings and the same ratio Δ^-/Δ^+. $S(\rho_L)$ denotes the entropy of a contiguous half of 6×3 sites. Dotted lines correspond to the expressions (42)–(46). At fixed λ/λ_c, $S(\rho_E)$ and $S(\rho_i)$ are now roughly half the value of the left panel (Eq. (45)), while $S(\rho_L)/S(\rho_i)$ is proportional to $\sqrt{n}$ (Eq. (46)).

Hence, the single site entropy is again $S(\rho_{\boldsymbol{i}}) \approx -f(\ln f - 1)$ while Eq. (38) yields

$$S(\rho_E) \approx -\frac{n}{2} f(\ln f - 1 + \alpha) \tag{42}$$

$$\approx \frac{n}{2} S(\rho_{\boldsymbol{i}}) - \frac{n}{2} f\,\alpha\,, \tag{43}$$

where α is a *geometric* entropy factor:

$$\alpha = \int u(\tilde{\boldsymbol{k}}) \ln u(\tilde{\boldsymbol{k}})\, d^d\tilde{k}\,, \tag{44}$$

($u(\tilde{\boldsymbol{k}}) \geq 0$, $\int u(\tilde{\boldsymbol{k}}) d^d\tilde{k} = 1$). In the isotropic case $\Delta_i^- = \Delta^-\ \forall\ i$, we have $\alpha = \alpha_d$, with $\alpha_1 = 1 - \ln 2 \approx 0.307$ (Eq. 31), $\alpha_2 = 2\alpha_1 \approx 0.614$ and $\alpha_3 \approx 0.636$, approaching $\approx \ln 2$ for large d.

At fixed λ, and for $\Delta_i^\pm = \Delta^\pm$, $f = (\Delta^-)^2 d/(8\lambda^2)$ and hence both $S(\rho_{\boldsymbol{i}})$ and $S(\rho_E)$ increase as d increases, reflecting the larger number of links. However, and assuming again $\Delta^+ \geq 0$, $\lambda_c = d(\Delta^+ + |\Delta^-|)$ also increases, entailing that at fixed λ/λ_c, f (and so $S(\rho_{\boldsymbol{i}})$ and $S(\rho_E)$) decreases:

$$f \approx \frac{[\Delta^-/(\Delta^+ + |\Delta^-|)]^2}{8d(\lambda/\lambda_c)^2}\quad . \tag{45}$$

For example, the right panels in Fig. 2 depict $S(\rho_E)$ and $S(\rho_{\boldsymbol{i}})$ in an isotropic square lattice of 6×6 sites, with the same previous ratio $\Delta^-/\Delta^+ = 1/3$. At fixed λ/λ_c, their values are verified to be roughly half that of the similar one-dimensional case (Eq. (45)). Their ratio is also slightly smaller due to the increase in the parameter α in (43). On the other hand, for $\lambda \to \lambda_c$ there is again a single vanishing energy $\omega_{\boldsymbol{0}}$, so that all entropies behave as $-\frac{1}{4}\ln(\lambda/\lambda_c - 1)$ up to leading order, with all ratios approaching 1.

We also depict there the entropy $S(\rho_L)$ of a contiguous half-size block ($n_x \times n_y/2 = 6 \times 3$ sites), which is now proportional to its boundary $2n_x$. For $\lambda \gg \lambda_c$, it is verified that the number of non-zero positive eigenvalues of the corresponding contraction matrix $\mathcal{D}_L$ is just the number of couplings "broken" by the partition ($2n_x$), being all approximately equal to $f/4$ up to leading non-zero

order. We then obtain

$$S(\rho_L) \approx -\frac{n_x}{2} f(\ln f/4 - 1) \approx \frac{n_x}{2}[S(\rho_{\boldsymbol{i}}) + 2f \ln 2]\,, \quad (46)$$

whence $S(\rho_L)/S(\rho_i) \propto n_x/2$ in this limit, as verified in the right panels of Fig. 2.

III. APPLICATION TO SPIN SYSTEMS

The previous bosonic formalism can be directly applied to interacting spin s systems in an external magnetic field through the RPA approximation [18]. Denoting with $s_{i\mu}$ the dimensionless spins $S_{i\mu}/\hbar$ at site i, we will consider a cyclic translationally invariant finite array which can be described by an XY Hamiltonian of the form

$$H = B\sum_i s_{iz} - \frac{1}{2s}\sum_{i\neq j}(J^x_{ij} s_{ix}s_{jx} + J^y_{ij} s_{iy}s_{jy}) \quad (47a)$$

$$= B\sum_i s_{iz} - \frac{1}{2s}[\sum_{i\neq j} \Delta^+_{ij} s_{i+}s_{j-} + \tfrac{1}{2}\Delta^-_{ij}(s_{i+}s_{j+} + \text{H.c.})] \quad (47b)$$

where $s_{j\pm} = s_{jx} \pm i s_{jy}$, $J^{ij}_\mu = J_\mu(i-j)$ and

$$\Delta^\pm_{ij} = \tfrac{1}{2}(J^x_{ij} \pm J^y_{ij}) = \Delta^\pm(i-j)\,. \quad (48)$$

We note that x, y, z may in principle also denote local intrinsic axes at each site, in which case the field is assumed to be directed along the local z axis. The s^{-1} scaling of the couplings ensures a spin-independent mean field and effective RPA boson Hamiltonian (see below).

Normal RPA. For sufficiently strong field B, the lowest mean field state (i.e., the separable state with lowest energy) is the aligned state $|0\rangle = |0_1\rangle \otimes \ldots \otimes |0_n\rangle$, where $|0_i\rangle$ denotes the local state with maximum spin along the $-z$ axis ($s_{iz}|0_i\rangle = -s|0_i\rangle$). In such a case, RPA implies the approximate bosonization [18]

$$s_{i+} \to \sqrt{2s} b^\dagger_i\,, \;\; s_{i-} \to \sqrt{2s} b_i\,, \;\; s_{iz} \to b^\dagger_i b_i - \tfrac{1}{2}\,, \quad (49)$$

which is similar to the Holstein-Primakoff bosoniztion [23, 26] and leads to the quadratic boson Hamiltonian (1) with the parameters (48) and $\lambda = B$. We may then directly apply all previous expressions.

The bosonic RPA scheme becomes exact for strong fields $|B| \gg B_c$ for any size n, spin s, geometry or interaction range, since for weak coupling it corresponds to the exact first order perturbative expansion of the ground state wave function [18]. As a check, in the case of the spin 1/2 one-dimensional chain with first neighbor XY coupling, an analytic expression of the block entropy in the limit $n \to \infty$ has been obtained in [13–15]. For $\lambda = B > \Delta^+$, it is given in present notation by [13]

$$S(\rho_L) = \tfrac{1}{6}[\ln \tfrac{4}{\alpha\alpha'} + (\alpha^2 - \alpha'^2)\tfrac{2I(\alpha)I(\alpha')}{\pi}], \quad (50)$$

where $\alpha = \Delta^-/\sqrt{\lambda^2 + \Delta^{-2} - \Delta^{+2}}$, $\alpha' = \sqrt{1-\alpha^2}$ and $I(\alpha) = \int_0^1 dx/\sqrt{(1-x^2)(1-\alpha^2 x^2)}$ is the elliptic integral of the first kind. An expansion of (50) for $\lambda \gg \Delta^\pm$ leads exactly to present Eq. (32), with f given by (27). We can then expect the asymptotic expressions (30) and (43) for $S(\rho_E)$ to be exact in this limit also in spin systems.

Parity breaking RPA. Considering now the anisotropic ferromagnetic-type case $|J_y(l)| \leq J_x(l)\ \forall\ l$ in (47a), the previous normal RPA scheme will hold, according to Eq. (16), for $B \geq B_c = J^0_x \equiv \sum_l J_x(l)$, i.e., when the corresponding boson system is stable.

For $|B| < B_c$, the normal RPA becomes unstable (ω_0 becomes imaginary). The lowest mean field state corresponds here to degenerate states $|\pm\Theta\rangle$ fully aligned along an axis z' forming an angle $\pm\theta$ with the z axis in the x, z plane: $|\Theta\rangle = |\theta_1\rangle \otimes \ldots \otimes |\theta_n\rangle$, with $|\theta_i\rangle = \exp[-i\theta s_{iy}]|0_i\rangle$. We are assuming here an anisotropic XY coupling such that H commutes with the S_z parity $P_z = e^{i\pi(\sum_i s_{iz} + ns)}$, but not with an arbitrary rotation around the z axis (as in the XX case). Such states break then parity symmetry, satisfying $P_z|\Theta\rangle = |-\Theta\rangle$. The angle θ is to be determined from [18]

$$\cos\theta = B/B_c, \;\; B_c = \sum_l J_x(l)\,. \quad (51)$$

For $|B| < B_c$, the bosonization (49) is then to be applied in the RPA to the rotated spin operators $s_{iz'} = s_{iz}\cos\theta + s_{ix}\sin\theta$, $s_{i\pm'} = s_{ix'} \pm i s_{iy'}$, with $s_{ix'} = s_{ix}\cos\theta - s_{iz}\sin\theta$ and $s_{iy'} = s_{iy}$. This leads again to a *stable* Hamiltonian of the form (1) with [18]

$$\lambda = B_c\,, \;\; \Delta^\pm(l) = \tfrac{1}{2}[J^x(l)\cos^2\theta \pm J^y(l)]\,. \quad (52)$$

For $|B| < B_c$ we should also take into account the important effects from parity restoration for a proper RPA estimation of entanglement entropies [18]. The exact ground state in a finite array will have a definite parity P_z outside crossing points [21], implying that the actual RPA ground state should be taken as a definite parity superposition of the RPA spin states constructed around $|\pm\Theta\rangle$ [18]. This leads to reduced RPA spin densities of the form $\rho_A \approx \frac{1}{2}[\rho_A(\theta) + \rho_A(-\theta)]$ if the complementary overlap $O_{\bar{A}} = \langle -\Theta_{\bar{A}}|\Theta_{\bar{A}}\rangle$ can be neglected. If the subsystem overlap $O_A = \langle -\Theta_A|\Theta_A\rangle = \cos^{2n_A s}\theta$ is also negligible, such that $\rho_A(\theta)\rho_A(-\theta) \approx 0$, then [18]

$$S(\rho_A) \approx S(\rho_A(\theta)) + \delta\,, \quad (53)$$

where $\delta = \ln 2$. The final effect is then the addition of a constant shift to the bosonic subsystem entropy for $|B| < B_c$. This is applicable to both $S(\rho_E)$ and $S(\rho_L)$ if θ, n and the block size L are not too small.

For first neighbor couplings with anisotropy $\chi = J_y/J_x \in (0,1)$ (if $\chi > 1$ we just redefine the x, y axes) as well as for arbitrary range couplings with a common anisotropy $\chi = J_y(l)/J_x(l) \in (0,1)$, another fundamental feature for $|B| < B_c$ is the existence of a transverse factorizing field $B_s = B_c\sqrt{\chi}$ where the mean field states $|\pm\Theta\rangle$ become exact ground states [19–22]. As seen from (52), at this field $\Delta^-(l) = 0\ \forall\ l$, so that the RPA vacuum remains the same as the mean field vacuum [18] and

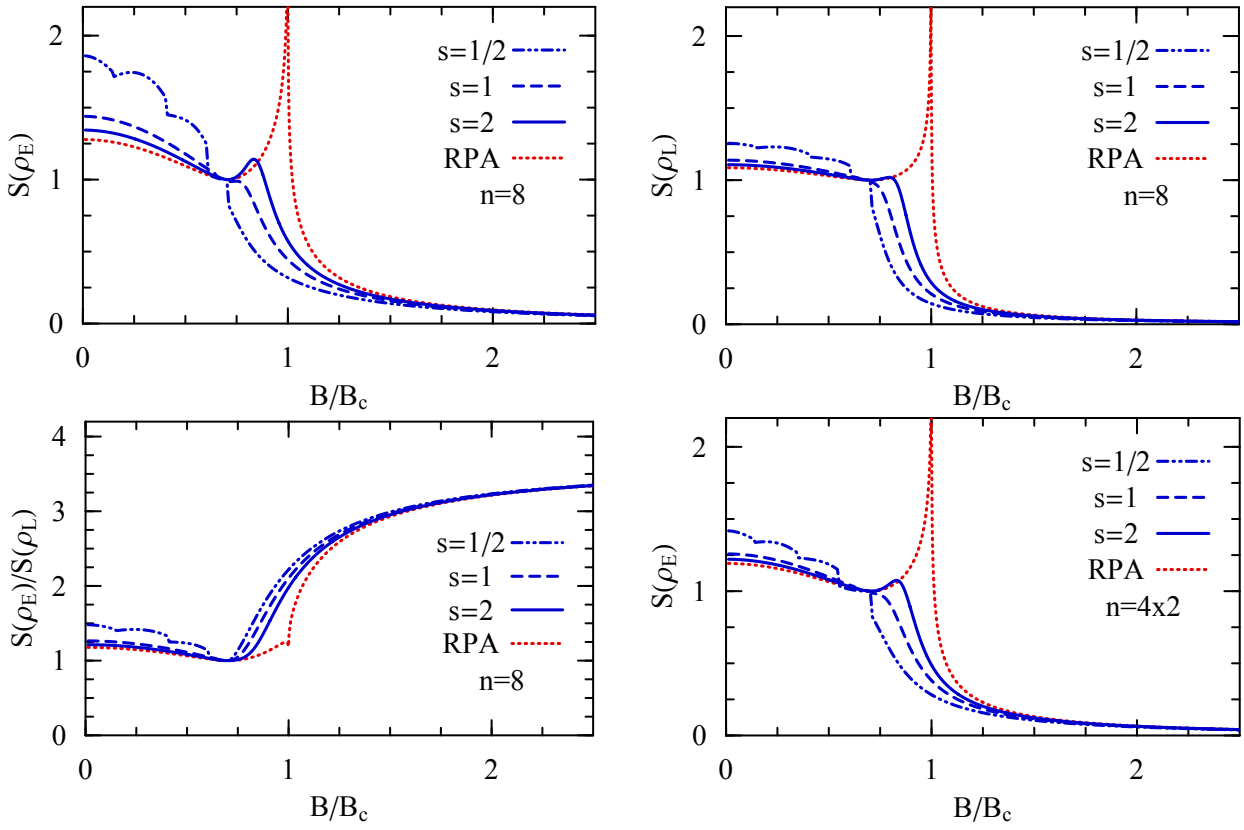

FIG. 3. (Color online) Top: Exact entanglement entropy of all even sites (left) and of a contiguous block of $n/2$ sites (right) in the ground state of a one dimensional cyclic chain of $n = 8$ spins with anisotropic XY first neighbor couplings ($J_y/J_x = \frac{1}{2}$) and spin $s = 1/2$, 1 and 2, as a function of the transverse magnetic field. The dotted line depicts the bosonic RPA result, with $B_c = J_x$ the mean field critical field. We have used base 2 logarithm in the entropy, such that all entropies approach 1 at the factorizing field $B_s \approx 0.71 B_c$. Bottom: Left: The corresponding ratio $S(\rho_E)/S(\rho_L)$. Right: The entanglement entropy of all even sites in a rectangular lattice of 4×2 spins. Remaining details as in the top panels.

all contractions $F^{\pm}_{ij}$ vanish, implying $S(\rho_A(\theta)) = 0$. All RPA entropies at B_s reduce then to the correction term δ arising from parity restoration [18].

This is essentially also the exact result at B_s: The transverse factorizing field corresponds to the last ground state parity transition as B increases from 0 [21] and the ground state side-limits for $B \to B_s$ are actually the definite parity combinations of the mean field states $|\pm\Theta\rangle$ [21, 28]. These definite parity states have Schmidt number 2 for any bipartition, implying that the side-limits of the *exact* entropy of the reduced state of any subsystem at B_s do not approach 0 but rather the values [28]

$$S(\rho^{\pm}_A(B_s)) = \sum_{\nu=\pm} q^{\pm}_{\nu} \ln q^{\pm}_{\nu} \,, \; q^{\pm}_{\nu} = \frac{(1+\nu O_A)(1 \pm \nu O_{\bar{A}})}{2(1 \pm O_A O_{\bar{A}})} \,, \tag{54}$$

where $+$ $(-)$ corresponds to positive (negative) parity, i.e. the right (left) side limit at B_s [28]. Eq. (54) is valid for any size or spin. For small complementary overlap $O_{\bar{A}}$, $q^{\pm}_{\nu} \approx \frac{1}{2}(1 + \nu O_A)$ and both side limits coincide, while if O_A is also small, $q_{\nu} \approx 1/2$ and Eq. (54) reduces to $+\ln 2$. This is also in agreement with the exact limit of the block entropy of the large one dimensional $s = 1/2$ XY chain at B_s [13].

Illustrative exact results for the even-odd entanglement entropy in a finite linear cyclic spin s chain with first neighbor couplings are plotted in the top left panel of Fig. 3 for spins $s = 1/2$, 1 and 2, together with the bosonic RPA estimation. The exact definite parity ground state was employed in all cases. We also depict for comparison the entropy of a contiguous half (top right), and the ratio $S(\rho_E)/S(\rho_L)$ (bottom left). The anisotropy of the coupling is the same as in Fig. 2 ($\Delta_-/\Delta_+ = 1/3$). The RPA result (independent of s for the scaling used in (47)), represents the large spin limit but is already quite close to the exact results for $s = 2$ except in the vicinity of B_c, where the exact entropies remain of course finite in a finite chain. The ratio $S(\rho_E)/S(\rho_L)$ is nonetheless quite accurately reproduced and shows the extensive character of $S(\rho_E)$ for $B > B_c$, in agreement with (33), where the entropies for all spin values rapidly approach the RPA result and become spin independent. For $|B| < B_c$ the shift δ in (53) ($\delta = +1$ in Figs 3–4 since base 2 logarithm was employed) is essential for the agreement and explains the lack of direct extensivity in this region. The collapse of all entropies to the value δ at B_s is also verified, and

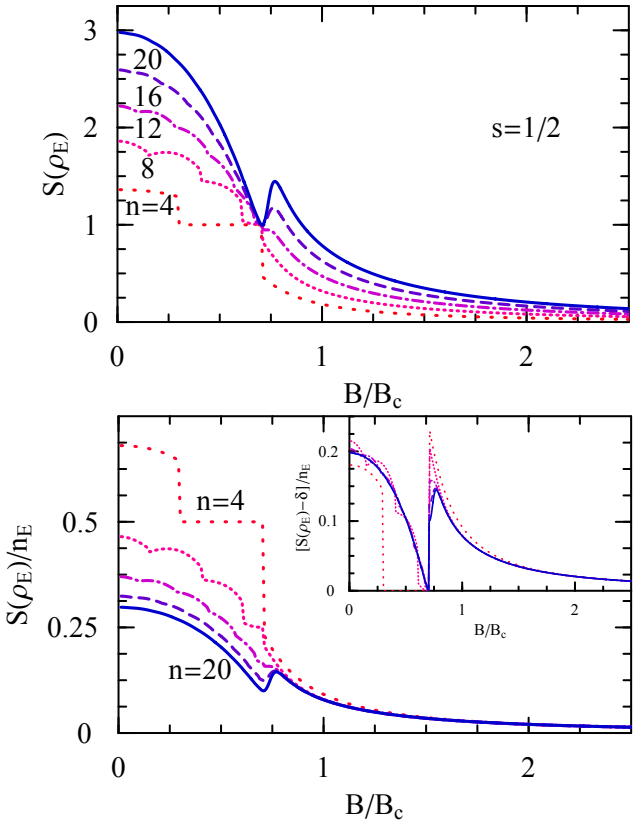

FIG. 4. (Color online) Top: Exact entanglement entropy of all $n/2$ even sites in the ground state of a spin 1/2 cyclic chain for different values of n. Couplings are the same as in Fig. 3. Bottom: The intensive entropy $S(\rho_E)/n_E$ ($n_E = n/2$). All curves coalesce for $B \gtrsim \Delta_+$. The inset depicts the intensive shifted entropy $(S(\rho_E) - \delta)/n_E$, where $\delta = 0$ for $B > B_s$ and $\delta = 1$ for $B < B_s$, which makes curves for $n \geq 8$ coalesce also for $B < B_s$.

for $s = 1/2$ even the small discontinuity at B_s predicted by Eq. (54) can be appreciated (together with the other parity transitions for $B < B_s$). The bottom right panel depicts $S(\rho_E)$ in a 4×2 square lattice with identical couplings in both directions and the same ratio Δ_-/Δ_+, where a similar behavior is obtained. Exact results for $s = 2$ are now even closer to the RPA prediction, indicating that the accuracy of the latter tends to improve, for stable mean fields, as the connectivity increases [29].

Exact results for a spin 1/2 chain for different sizes are depicted in Fig. 4. Even though RPA is not accurate for such low spin with a first neighbor coupling [29], the exact results are again in qualitative agreement with its predictions away from the critical region: Direct extensivity $S(\rho_E) \propto n$ is verified for strong fields $B \gtrsim \Delta_+$ (bottom panel), whereas for $B < B_s$ it holds for the shifted entanglement entropy $S(\rho_E) - \delta$, as seen in the inset. Complete lack of extensivity takes place at the factorizing field B_s, where the discontinuity implied by (54) is appreciable for $n = 8$ and becomes quite noticeable for $n = 4$.

IV. CONCLUSIONS

We have shown that the total even-odd entanglement entropy displays a strict extensive behavior in both bosonic and spin chains or lattices for weak first neighbor couplings (i.e., strong fields in a spin chain), providing explicit asymptotic expressions for the general d dimensional case. Extensivity of the associated mutual information is also implied by these expressions. Deviations from this behavior, however, were shown to arise for stronger couplings, i.e., proximity to the instability in the finite bosonic case or low fields in the spin case. In the latter, a constant shift is essential to understand the exact results for $|B| < B_c$, which has an evident meaning as a symmetry restoration effect in the RPA. Besides, full loss of extensivity occurs in the vicinity of the factorizing field. Present results confirm the validity of the RPA approach (with inclusion of symmetry-restoration effects) for obtaining a simple direct understanding of the main aspects of ground state entanglement in spin chains, at least in those regions where a well defined mean field minimum exists.

The authors acknowledge support from CIC (RR) and CONICET (NC,JMM) of Argentina.

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