Global entanglement in *XXZ* chains

N. Canosa and R. Rossignoli
Departamento de Física, Universidad Nacional de La Plata, Casilla de Correo 67, La Plata (1900) Argentina
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We examine the thermal entanglement of *XXZ*-type Heisenberg chains in the presence of a uniform magnetic field along the z axes through the evaluation of the negativity associated with bipartitions of the whole system and subsystems. Limit temperatures for nonzero global negativities are shown to depend on the asymmetry Δ, but not on the uniform field, and can be much higher than those limiting pairwise entanglement. It is also shown that global bipartite entanglement may exist for $T>0$ even for $\Delta \geqslant 1$, i.e., when the system is fully aligned (and hence separable) at $T=0$, and that the bipartition leading to the highest limit temperature depends on Δ.

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I. INTRODUCTION

Quantum entanglement is a fundamental trait of quantum mechanics, representing the nonlocal correlations with no classical analogue that can be exhibited by composite quantum systems. Interest on entanglement has been triggered in the last few years by the discovery of its potential for developing new forms of information transmission and processing [1–4], being a resource in quantum information science [5]. Entanglement has also provided a new perspective for the analysis of correlations and transitions in many-body quantum systems [6–10]. In systems at finite temperature T, two fundamental questions which immediately arise [11,12] are (a) the determination of the limit temperatures for the existence of different kinds of entanglement and (b) the possible emergence of entanglement for $T>0$ when the ground state is separable due to entangled excited states.

Let us first recall that a mixed state ρ of a bipartite quantum system $A+B$ is said to be *separable* or *classically correlated* if it can be expressed as a convex combination of product densities [13], i.e., $\rho=\Sigma_\alpha q_\alpha \rho_A^\alpha \otimes \rho_B^\alpha$, with $q_\alpha>0$, $\Sigma_\alpha q_\alpha=1$ and ρ_A^α, ρ_B^α density matrices for each component. Otherwise, ρ is *entangled* or *inseparable*. Separable states can be created by local operations and classical communication (LOCC) and satisfy Bell inequalities as well as other classical properties, such as being more disordered globally than locally [14,15]. Pure states ($\rho^2=\rho$) are separable if and only if $\rho=\rho_A\otimes\rho_B$, but this is not necessarily the case for mixed states, where the determination of separability is, in general, a NP hard problem [16,17]. Accordingly, while for pure states, bipartite entanglement can be measured in terms of the entropy of the reduced density of a subsystem [18], a rigorous computable measure of entanglement for mixed states has so far been obtained just for the case of two qubits, through the concurrence [19].

Nonetheless, bounds for entanglement in general mixed states can be obtained by means of the *negativity* [20–22], which is a measure of the degree of violation of the criterion of positive partial transpose (PPT) [23,24] in entangled states and is easily computable. Although the PPT criterion is a necessary separability condition, sufficient just for two-qubit or qubit+qutrit systems, the negativity fulfills some fundamental properties of an entanglement measure [20], being an entanglement monotone and providing bounds to the teleportation capacity and distillation rate. In n-qubit systems at finite temperature, it can then be employed [25] to detect the entanglement between the components of any bipartition $\{m\}-\{n-m\}$ of the *whole* system, as well as of *any* subsystem, beyond the level of pairwise two-qubit entanglement measured by the concurrence. Another fundamental result is that any state ρ is completely separable (convex combination of n-product densities) if it is sufficiently close to the fully mixed state I/d [21,26,27] (d is the system dimension). This ensures that any canonical thermal state $\rho(T)\propto\exp[-H/T]$ of a finite system described by a Hamiltonian H becomes *separable* above a *finite* limit temperature, since it will be as close as desired to I/d for sufficiently high T. In particular, no bipartite entanglement can arise if $\mathrm{Tr}(\rho-I/d)^2\leqslant[d(d-1)]^{-1}$ [27].

The aim of this work is then to examine, by means of the negativity, the *global* bipartite entanglement of thermal states $\rho(T)$ of n-spin chains interacting through a *XXZ*-type coupling placed in a transverse magnetic field. Heisenberg chains can be employed for solid state quantum computers [28] and *XXZ* chains have been used to describe quantum computers based on NMR [29] and on electrons on Helium [30,31]. Relevant studies of the *pairwise* thermal entanglement between two qubits in Heisenberg chains have been made [6,12,29,32–36], revealing rich phenomena. In small *XXZ* chains [29,34], it has been shown that there is no pairwise entanglement for $T\geqslant 0$ for anisotropies $\Delta>1$, i.e., when the ground state is fully aligned for any field, and that the corresponding limit temperature remains bounded for large negative Δ if n is odd (vanishing $\forall\Delta$ in the $n=3$ antiferromagnetic case at zero field [34]). In contrast, we will show here that global entanglement between m and $n-m$ qubits *may also exist for* $\Delta>1$ *if* $n\geqslant 4$ *and* $T>0$, implying a *thermal reentry*. Moreover, limit temperatures for nonzero global negativities *do not saturate* for $\Delta\to-\infty$ in odd systems, but diverge in *both* the ferromagnetic and antiferromagnetic cases, even for $n=3$. These temperatures are *independent* of the magnetic field, but dependent on Δ and the bipartition, displaying crossings as Δ is varied. Numerical results up to $n=10$ qubits will be provided, together with full analytical results for $n=3$.

II. FORMALISM

We will consider a *XXZ* Hamiltonian for n qubits or spins of the form

$$H = bS_z - \sum_{i<j} [v_x^{ij}(s_x^i s_x^j + s_y^i s_y^j) + v_z^{ij} s_z^i s_z^j], \tag{1}$$

where $\mathbf{s}_i$ denotes the spin operator at site i, $S_z=\Sigma_i s_z^i$ is the total spin z component, b accounts for the Zeeman coupling to a uniform magnetic field and $s_x^i s_x^j + s_y^i s_y^j = (s_+^i s_-^j + s_-^i s_+^j)/2$ is the hopping or entangling term. Our attention will be centered on a cyclic chain with nearest neighbor coupling ($v_\alpha^{ij} = v_\alpha \delta_{j,i+1}$ for $\alpha=x,z$, with $n+1\equiv 1$), although some results for the fully connected case ($v_\alpha^{ij}=v_\alpha \forall\, i<j$) will also be commented for comparison. In the first case, the spectrum of H and the entanglement of its eigenstates are independent of the sign of v_x for even n, as it can be changed by a rotation around the z axes at odd sites $[s_{x,y}^i \to (-1)^i s_{x,y}^i]$. In any case, $[H,S_z]=0$, so that the eigenstates of H have good quantum number M (eigenvalues of S_z).

We will consider the n-spin thermal state

$$\rho(T) = Z^{-1} \exp[-H/T], \tag{2}$$

where $Z=\mathrm{Tr}\exp[-H/T]$ is the partition function and $T>0$ the temperature (we set Boltzmann constant $k=1$). Global entanglement between m and $n-m$ selected qubits will be analyzed by means of the negativity [20]

$$N_p[\rho] = \tfrac{1}{2}(\mathrm{Tr}|\rho^{t_p}| - 1), \tag{3}$$

where $p \equiv \{m\}-\{n-m\}$ denotes the bipartition and ρ^{t_p} the ensuing partial transpose of ρ [23]. Equation (3) is just the absolute value of the sum of the negative eigenvalues of ρ^{t_p} (as $\mathrm{Tr}\,\rho^{t_p}=1$), so that according to the PPT criterion [23,24], $N_p[\rho]>0$ indicates entanglement between the m selected qubits and the rest. Equation (3) satisfies as well properties of an entanglement measure [20], being a *convex* function of ρ and an entanglement monotone (it does not increase under LOCC). Moreover, distillable entangled states satisfy $N_p[\rho]>0$ [22]. Although the present analysis leaves away bound PPT entangled states and does not capture all aspects of n-partite entanglement (separability of all bipartitions does not necessarily imply full separability), it goes beyond the standard analysis based on pairwise two-qubit entanglement (the latter may vanish even if $N_p[\rho]>0$ for all global bipartitions, as occurs in Greenberger-Horne-Zeilinger (GHZ) states [25]). For *pure* states $\rho=|\Psi\rangle\langle\Psi|$, it can be shown, by means of the Schmidt decomposition [5] $|\Psi\rangle = \Sigma_\alpha \sqrt{\lambda_\alpha^p}\,|\alpha_{\{m\}}\rangle|\alpha_{\{n-m\}}\rangle$ that

$$N_p[\rho] = \sum_{\alpha<\alpha'} \sqrt{\lambda_\alpha^p \lambda_{\alpha'}^p} = \frac{1}{2}\left[\left(\sum_\alpha \sqrt{\lambda_\alpha^p}\right)^2 - 1\right] \quad (\rho^2=\rho), \tag{4}$$

where λ_α^p represent the eigenvalues of the reduced density $\rho_{\{m\}} \equiv \mathrm{Tr}_{\{n-m\}}\rho$ of the m selected qubits (the same as those of $\rho_{\{n-m\}}$ when $\rho^2=\rho$). Equation (4) differs from the entanglement of formation [18] $E[\rho] \propto -\Sigma_\alpha \lambda_\alpha^p \log_2 \lambda_\alpha^p$, but is as well a measure of the disorder of the reduced system (see Appendix), satisfying $N_p[\rho] \geqslant N_p[\rho']$ if $\lambda^p \prec \lambda'^p$, where $\prec$ denotes "majorized by" (or "more mixed than") [5]: $\Sigma_{\alpha=1}^k \lambda_\alpha^p \leqslant \Sigma_{\alpha=1}^k \lambda_\alpha'^p$ for $k=1,\ldots,d_m$, where λ_α^p, $\lambda_\alpha'^p$ are sorted in decreasing order and $d_m=2^m$ is the subsystem dimension ($m \leqslant n/2$). The formal maximum is then obtained for a uniform distribution $\lambda_\alpha^p = 1/d_m$, in which case $N_p[\rho]=(d_m-1)/2$. Due to convexity, this is also the maximum for nonpure states.

In the nearest neighbor cyclic chain, global negativities $N_p[\rho]$ depend on the number m of selected qubits and on their spacings. For instance, in a three-qubit chain *abc* there is a single distinct global negativity N_{a-bc} ($=N_{b-ac}=N_{c-ba}$), whereas for $n=4$ qubits *abcd*, there are three distinct negativities N_{a-bcd}, N_{ab-cd}, and N_{ac-bd}, which measure respectively the entanglement between one qubit and the rest, adjacent pairs, and nonadjacent pairs. Each negativity $N_p[\rho(T)]$ will have its *own limit temperature* T_p above which it vanishes, although the behavior for $T<T_p$ may not be monotonous (even entanglement vanishing plus reentry may occur for $T<T_p$ [35,36]). A remarkable feature of these global limit temperatures is that for Hamiltonians of the form (1), they are strictly *independent* of the uniform field b [25] (see Appendix), even though $N_p[\rho(T)]$, as well as the entanglement of the ground state, depend of course on b.

The bipartite entanglement of subsystems of $m<n$ qubits can be analyzed in a similar way by evaluation of the reduced negativities $N_{p'}[\rho_{\{m\}}]$ determined by the reduced density $\rho_{\{m\}}$, with $p'=\{k\}-\{m-k\}$ a bipartition of the subsystem. These negativities will in general also depend on the relative location of the k qubits and satisfy inequalities of the form [20] $N_{\{k\}-\{m-k\}}[\rho_{\{m\}}] \leqslant N_{\{k\}-\{m+1-k\}}[\rho_{\{m+1\}}]$, as tracing out one qubit is a LOCC operation. The associated limit temperatures will then satisfy $T_{\{k\}-\{m-k\}} \leqslant T_{\{k\}-\{m+1-k\}}$, being thus higher for global bipartitions. In particular, the negativity of one qubit with the rest (N_{a-*}) is an upper bound to all pairwise negativities N_{a-b}, N_{a-c}, etc., so that T_{a-*} is an upper bound to all pairwise limit temperatures. Limit temperatures $T_{p'}$ of reduced negativities $N_{p'}[\rho_{\{m\}}(T)]$ *depend* in general on the field b.

For instance, for a three-qubit cyclic chain, there is a single reduced two-qubit density $\rho_{ab}=\mathrm{Tr}_c\,\rho$ (any other choice of pair is equivalent), with negativity $N_{a-b}[\rho_{ab}] \leqslant N_{a-bc}[\rho]$, while for a four-qubit chain, there is one distinct three-qubit density $\rho_{abc}=\mathrm{Tr}_d\,\rho$, with *two* different negativities $N_{a-bc}[\rho_{abc}]$, $N_{b-ac}[\rho_{abc}]$, satisfying $N_{a-bc} \leqslant (N_{a-bcd}, N_{ab-cd})$, $N_{b-ac} \leqslant (N_{a-bcd}, N_{ac-bd})$. There are also two different pair densities $\rho_{ab}=\mathrm{Tr}_{cd}\,\rho$, $\rho_{ac}=\mathrm{Tr}_{bd}\,\rho$, whose negativities N_{a-b}, N_{a-c}, measure the entanglement of contiguous and noncontiguous qubits and satisfy $N_{a-b} \leqslant (N_{a-bc}, N_{b-ac})$, $N_{a-c} \leqslant N_{a-bc}$.

III. RESULTS

We consider in what follows a cyclic chain with nearest neighbor coupling and define the anisotropy as $\Delta \equiv v_z/|v|$, with $v \equiv v_x$. At $T=0$ and fixed $b \neq 0$, the ground state of the Hamiltonian will experience a series of $[n/2]$ transitions $|M| \to |M|+1$ as Δ increases, starting from $|M|=0$ (1/2) for n even (odd) and large negative Δ, and ending in an *aligned*

state with maximum spin $|M|=n/2$ for $\Delta>\Delta_c(b)$. This state is completely separable, while all ground states with $|M|<n/2$ are entangled, so that $\Delta_c(b)$ indicates the entangled-separable border at $T=0$. The energy of the aligned state $|\Psi_0\rangle$ $(=|\downarrow\ldots\downarrow\rangle$ for $b>0)$ is $E_0=-n(2|b|+v_z)/4$, while for $v>0$, that of the lowest $|M|=1$ state, which is a *W*-type state $(|\Psi_1\rangle\propto\Sigma_{i=1}^n s_+^i|\Psi_0\rangle$ for $b>0)$, is $E_1=E_0+|b|+v_z-v$, so that the transition occurs at

$$\Delta_c(b)=1-|b/v| \quad (v>0 \text{ if } n \text{ odd}). \tag{5}$$

Equation (5) is, of course, also valid for $v<0$ if n is even.

The entanglement borders for $T>0$ are, however, quite different. As limit temperatures for nonzero global negativities are independent of the field b, so will be the concomitant borders $\Delta_c^p(T)$. Global bipartite entanglement for $T>0$ and $b\neq 0$ will then also arise for $\Delta_c(b)<\Delta<1$. Moreover, we will see that it may also arise for $\Delta\geqslant 1$ if $n\geqslant 4$.

A. Two and three qubit case

Let us first discuss the behavior for two and three qubits, where analytical expressions for $T>0$ can be found [for $n=2$, we consider just a single term v_α^{12} in (1)]. H can be rewritten in these cases in terms of the total spin components $S_\alpha=\Sigma_{i=1}^n s_\alpha^i$ as

$$H=bS_z-\tfrac{1}{2}[v(S_x^2+S_y^2)+v_zS_z^2]+E_0, \tag{6}$$

where $E_0=n(2v+v_z)/8$, so that its eigenstates have good total spin S with energies

$$E_M^S=bM-\tfrac{1}{2}[vS(S+1)+M^2(v_z-v)]+E_0, \tag{7}$$

where $S=0,1$, for $n=2$, and $S=1/2$ (twofold degenerate), $3/2$, for $n=3$, with $|M|\leqslant S$. In the fully connected case, Eqs. (6) and (7) are of course valid for all n, with $S=0(1/2),\ldots,n/2$ for n even (odd).

For $n=2$, the eigenstates of H are then either separable (the aligned states $|SM\rangle=|1,\pm 1\rangle$) or maximally entangled (the Bell states $|SM\rangle=|10\rangle$, $|00\rangle\propto|\uparrow\downarrow\rangle\pm|\downarrow\uparrow\rangle$), so that the ground state is maximally entangled for $\Delta<\Delta_c(b)$ (with $S=1$ if $v>0$ and $S=0$ if $v<0$). On the other hand, any two-qubit mixed state of the form $\rho=\Sigma_{S,M}p_M^S|SM\rangle\langle SM|$ is entangled whenever

$$|p_0^1-p_0^0|>2\sqrt{p_1^1p_{-1}^1}, \tag{8}$$

(see Appendix), which in the thermal case (2) $(p_M^S=e^{-E_M^S/T}/Z)$ leads to the b-independent border

$$\Delta<1-2t\ln[2/(1-e^{-1/t})], \quad t\equiv T/|v|. \tag{9}$$

Thermal entanglement arises then for $\Delta<1\ \forall\ b$, implying reentry for $T>0$ if $\Delta_c(b)<\Delta<1$. The limit temperature $T_{a-b}(\Delta)$ determined by (9) is a *decreasing* function of Δ (see Fig. 1), that vanishes for $\Delta\to 1$ and diverges for $\Delta\to-\infty$ $[\Delta<1-2t\ln(2t)$ for $t\gg 1]$.

For $n=3$ qubits, the behavior of *global* bipartite entanglement is qualitatively similar to that for $n=2$ (Fig. 1). For $v>0$, the ground state is a *W*-type entangled state if $\Delta<\Delta_c(b)$ [37] $(|SM\rangle=|\tfrac{3}{2},-\tfrac{1}{2}\rangle\propto|\uparrow\downarrow\downarrow\rangle+|\downarrow\uparrow\downarrow\rangle+|\downarrow\downarrow\uparrow\rangle$ for $b>0)$, with global negativity $N_{a-bc}=\sqrt{2}/3\approx 0.47$ and pair negativity $N_{a-b}=(1-\sqrt{5})/6\approx 0.21$, becoming the aligned state $|\tfrac{3}{2},\pm\tfrac{3}{2}\rangle$ for $\Delta>\Delta_c(b)$. Let us add that if $b=0$, the states $|\tfrac{3}{2},\pm\tfrac{1}{2}\rangle$ become degenerate but their mixture $\frac{1}{2}\Sigma_{M=\pm 1/2}|\frac{3}{2}M\rangle\langle\frac{3}{2}M|$ [the $T\to 0$ limit of $\rho(T)$ for $\Delta<\Delta_c(b)$] remains entangled, with lower values $N_{a-bc}=(\sqrt{3}-1)/3\approx 0.24$, $N_{a-b}=1/6$.

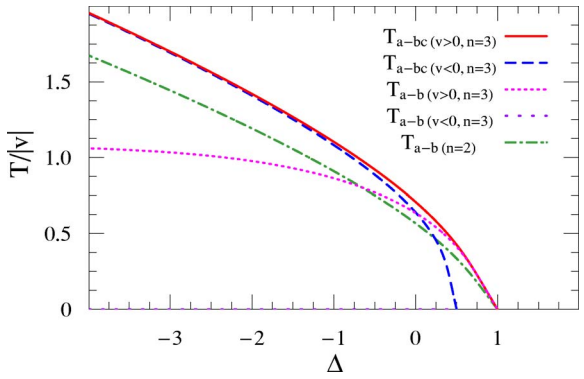

FIG. 1. (Color online) Limit temperatures T_{a-bc} for global bipartite entanglement for $n=3$ qubits as a function of the asymmetry $\Delta=v_z/|v|$, for both signs of v (they are independent of the uniform field b). Also depicted are the corresponding limit temperatures for pairwise entanglement T_{a-b} for $b=0$ (that for $v<0$ vanishes), and the concomitant result for $n=2$ qubits (the same for both signs of v and any b).

On the other hand, for any three-qubit mixed state $\rho=\Sigma_{S,M}p_M^SP_M^S$, where P_M^S denotes the projector onto the subspace with total spin S and z-component M, the global negativity N_{a-bc} will be nonzero if and only if (see Appendix)

$$|p_{\nu/2}^{3/2}-p_{\nu/2}^{1/2}|>\sqrt{3p_{3\nu/2}^{3/2}(p_{-\nu/2}^{3/2}+p_{-\nu/2}^{1/2}/2)}, \tag{10}$$

for $\nu=1$ *or* $\nu=-1$, which in the thermal case implies

$$\Delta<1-t\ln\left[\frac{3(2+e^{-3/2t})}{2(1-e^{-3/2t})^2}\right] \quad (v>0). \tag{11}$$

Global entanglement is then again feasible for $\Delta<1\ \forall\ b$ $(\Delta<1-t\ln 3$ for $t\ll 1)$ and the ensuing limit temperature T_{a-bc} is a decreasing function of Δ, that vanishes for $\Delta\to 1$ and *diverges* for $\Delta\to-\infty$ $(\Delta<1-2t\ln(\sqrt{2}t)$ if $t\gg 1)$ (see Fig. 1).

The behavior of the *pairwise* limit temperature T_{a-b} for $n=3$ is however quite different [29,34]. The reduced two-qubit density ρ_{a-b} is entangled in a smaller region which *depends* on the field b and is determined for $v>0$ by the equation (see Appendix)

$$\Delta<1-t\ln\frac{3}{\sqrt{\gamma^2(\eta^2-1)+2(1+\eta)(1-\alpha)^2}-\gamma\eta}, \tag{12}$$

where $\gamma=1+2\alpha$, $\alpha=e^{-3/2t}$, and $\eta=\cosh(b/T)$. For $t\ll 1$, $\Delta\lesssim 1-t\ln 3$ as before, so that for $T>0$, ρ_{a-b} is also entangled for $\Delta<1\ \forall\ b$. However, the denominator in (12) *vanishes* at a *finite* temperature $t_c(b)$, implying that T_{a-b}/v approaches a *finite* limit $t_c(b)$ for $\Delta\to-\infty$, in contrast with T_{a-bc}. Hence, for large negative Δ there is a large range of temperatures

where only *global* bipartite entanglement persists, with $T_{a-bc}/T_{a-b} \to \infty$ for $\Delta \to -\infty$. The limit $t_c(b)$ is an *increasing* function of $|b|$, with $t_c(0) = 3/(4 \ln 2) \approx 1.08$.

For $v < 0$, Eq. (11) is to be replaced by

$$\Delta < 1/2 - t \ln\left[\frac{3(1+2e^{-3/2t})}{2(1-e^{-3/2t})^2}\right] \quad (v<0), \tag{13}$$

so that global bipartite entanglement starts for $\Delta < 1/2$ ($\Delta < 1/2 - t \ln(3/2)$ for $t \ll 1$), although for $t \gg 1$, Eqs. (13) and (11) are almost coincident, implying that T_{a-bc} is almost the same as for $v > 0$ for large negative Δ (Fig. 1). This is not the case for T_{a-b}, which for $v < 0$ is determined by Eq. (12) with the first term 1 replaced by 1/2 and $\gamma = 2 + \alpha$, and is *lower* than the value for $v > 0$, *vanishing* for $b \to 0$ (no pairwise entanglement in the absence of field [29,34]). This effect is due to the larger degeneracy present for $v < 0$, where the ground state corresponds to $S = |M| = 1/2$ for $\Delta < \Delta_c^-(b) = 1/2 - |b/v|$, being then *twofold* degenerate for $b \neq 0$, and to an aligned state ($|M| = 3/2$) if $\Delta > \Delta_c^-(b)$. For $\Delta < \Delta_c^-(b)$ and $b \neq 0$, the mixture $\rho = \frac{1}{2} P_{1/2,\pm 1/2}$ [the $T \to 0$ limit of $\rho(T)$] is still fully entangled, with $N_{a-bc} = \sqrt{2}/6 \approx 0.23$ and $N_{a-b} = (\sqrt{2}-1)/6 \approx 0.07$. However, for $b = 0$, states $|S, \pm M\rangle$ become degenerate and the ensuing $T \to 0$ limit, $\rho = \frac{1}{4}(P_{1/2,1/2} + P_{1/2,-1/2})$, has still *global* entanglement ($N_{a-bc} = 1/6$), but *no pairwise entanglement* ($N_{a-b} = 0$), explaining the vanishing of T_{a-b} in this case.

B. Four qubit case

A surprise comes already for the $n = 4$ chain (Fig. 2), where for $T > 0$, *global bipartite entanglement is seen to arise also for* $\Delta > 1$. The ground state is entangled just for $\Delta < \Delta_c(b)$ [Eq. (5)], with the transitions $|M| \to |M| + 1$ occurring at $\Delta = (1 - 2\bar{b} - \bar{b}^2)/(1 + \bar{b})$, $\bar{b} = |b/v|$ $(0 \to 1)$, and $\Delta = \Delta_c(b)$ $(1 \to 2)$, collapsing both into a single $0 \to 2$ transition at $\Delta = 1$ for $b = 0$. The corresponding limit temperatures are depicted in the top panel, where it is seen that they all *vanish* for $\Delta \to 1$, but those corresponding to N_{ab-cd} (entanglement between *contiguous* pairs) and N_{a-bcd} (entanglement of one qubit with the rest) become again nonzero for $\Delta > 1$, indicating the reentry of the corresponding entanglement. The highest limit temperature for $\Delta \lesssim 1/2$ corresponds to N_{ac-bd} (entanglement between *noncontiguous* pairs), but changes to N_{ab-cd} for $\Delta \gtrsim 1/2$. The thermal behavior of N_{ab-cd} for $b = 0$ is depicted in the central panel, where it is seen that the reentry for $\Delta > 1$ is actually weak and vanishes smoothly for $T \to 0$. Let us remark that no entanglement reentry for $\Delta > 1$ takes place in the analogous fully connected four qubit case.

The $M = 0$ ground state in the four-qubit cyclic chain is an entangled state of the form

$$|\Psi\rangle = \alpha(|\uparrow\uparrow\downarrow\downarrow\rangle + \cdots) + \beta(|\uparrow\downarrow\uparrow\downarrow\rangle + \cdots), \tag{14}$$

where…denotes similar states obtained by translation and $\beta/\alpha = (\sqrt{8+\Delta^2} - \Delta)/2$, with $4\alpha^2 + 2\beta^2 = 1$ and $\beta > \alpha$ for $\Delta < 1$. Its energy is $-|v|\beta/\alpha$. This state exerts a strong influence on the entanglement of $\rho(T)$ even for $\Delta > 1$. It has maximum entanglement between one qubit with the rest,

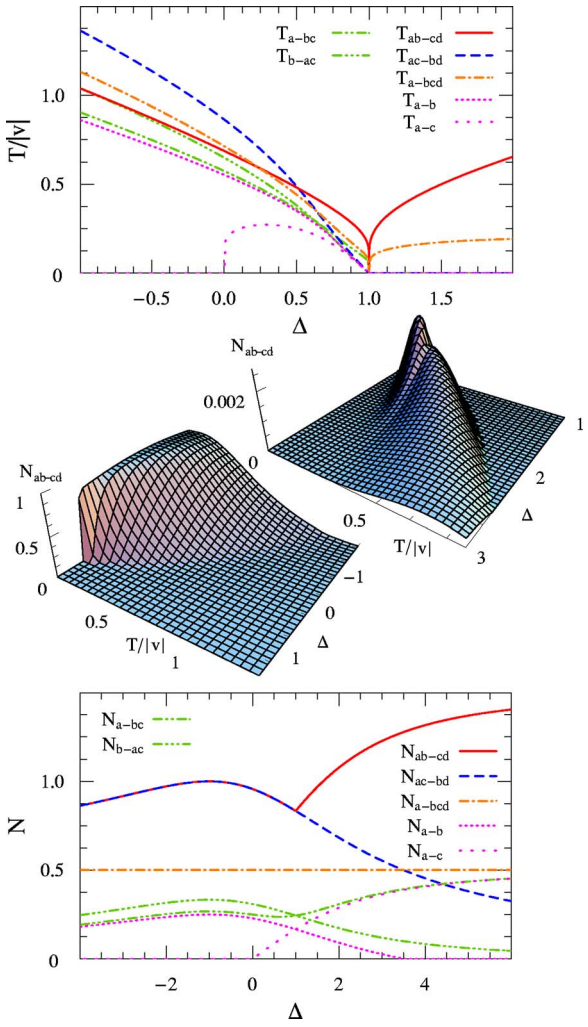

FIG. 2. (Color online) Top: Limit temperatures for global (T_{ab-cd}, T_{ac-bd}, T_{a-bcd}), pairwise (T_{a-b}, T_{a-c}), and three-qubit (T_{a-bc}, T_{b-ac}) negativities for $n = 4$ qubits in a nearest neighbor cyclic chain, as a function of the asymmetry Δ. There is global entanglement also for $\Delta > 1$. Results for reduced systems correspond to zero field. Center: The behavior of the global negativity N_{ab-cd} as a function of temperature and Δ (with different scales for $\Delta < 1$ and $\Delta > 1$) for $b = 0$. Bottom: Negativities of the state (14) as a function of Δ. For $b = 0$, they represent the ground state negativities for $\Delta < 1$.

$N_{a-bcd} = 1/2$ (the reduced one-qubit density ρ_a is maximally mixed), while $N_{ac-bd} = \beta(4\alpha + \beta)$, and $N_{ab-cd} = N_{ac-bd}$ if $\Delta < 1$ and $6\alpha^2 - \beta^2$ if $\Delta > 1$ (Fig. 2, lower panel), becoming N_{ab-cd} much larger than N_{ac-bd} for large Δ. This seems to affect the most persistent negativity of $\rho(T)$ for $\Delta > 1$, allowing a positive value of N_{ab-cd} and reducing N_{ac-bd} to 0. The $|M| = 1$ ground states are W states ($\propto |\uparrow\downarrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\downarrow\rangle + \ldots$ for $M = -1$), with lower values $N_{ab-cd} = N_{ac-bd} = 1/2$ and $N_{a-bcd} = \sqrt{3}/4$.

We also depict, in the upper panel, the limit temperatures for $b = 0$ of all reduced negativities, namely T_{a-bc}, T_{b-ac} for the three-qubit density ρ_{abc} and T_{a-b}, T_{a-c} for the reduced pair densities ρ_{ab} and ρ_{ac}. They all vanish for $\Delta > 1$, so that in this region just *global* bipartite entanglement persists (a result valid for any b). It is also seen that while T_{a-b} (adja-

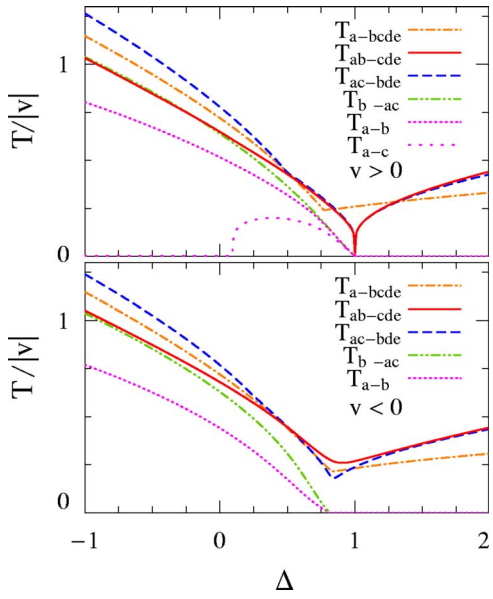

FIG. 3. (Color online) The set of limit temperatures for global negativities, T_{a-bcde}, T_{ab-cde}, T_{ac-bde}, for $n=5$ qubits in the cyclic chain as a function of Δ for $v>0$ (top) and $v<0$ (bottom). The concomitant limit temperatures for pairwise (T_{a-b}, T_{a-c}) and the most persistent three-qubit (T_{b-ac}) negativity for $b=0$ are also depicted. T_{a-c} vanishes for $v<0$ and $b=0$.

cent qubits) increases as Δ decreases, *diverging* for $\Delta\to-\infty$ (in contrast with the behavior for $n=3$), T_{a-c} (nonadjacent qubits) *vanishes* for $\Delta<0$. This is a consequence of the ground state behavior of N_{a-c}, which vanishes for $\Delta<0$ (see bottom panel). The state (14) leads to $N_{a-b}=\alpha(2\beta-\alpha)$ for $\Delta<7/2$ (and 0 for $\Delta>7/2$), and $N_{a-c}=2\alpha^2-\beta^2$ for $\Delta>0$ (and 0 for $\Delta<0$), with $N_{a-b}>N_{a-c}$ for $\Delta<1$. The ordering of negativities is, of course, in agreement with the discussion of Sec. II.

C. Five qubit case and beyond

The behavior of global negativities for $n=5$ qubits and $v>0$ (Fig. 3, upper panel) is quite similar, although there are some important changes: (a) for $T>0$, *all* global negativities exhibit a reentry for $\Delta>1$, including that of the noncontiguous 2-3 partition, N_{ac-bde}, with T_{ac-bde} lying close to T_{ab-cde} (contiguous 2-3 partition) for $\Delta\gtrsim 1/2$; (b) the negativity of one-qubit with the rest, N_{a-bcde}, remains nonzero $\forall\ \Delta$ if $T>0$, *including* the isotropic case $\Delta=1$, providing the highest limit temperature for $0.85\lesssim\Delta\lesssim 1.35$; (c) for $\Delta>1$ there is no pairwise nor three-qubit entanglement at any field, but there is four qubit entanglement (all reduced four-qubit negativities are small but nonzero). Besides, for $\Delta\to-\infty$ the limit temperature for adjacent pairwise entanglement T_{a-b} approaches a finite limit [29], as occurs for $n=3$, exhibiting a maximum at $\Delta\approx-5.6$ for $b=0$, but all those for three and four adjacent qubits ($T_{a-bc}, T_{b-ac}, T_{a-bcd}, \ldots$), diverge, as the global ones. Note also that T_{a-c} vanishes below a certain limit ($\Delta\lesssim 0.1$ for $b=0$), reflecting the vanishing of N_{a-c} at $T=0$ below this value. For $n=5$ and $v>0$, the ground state transitions

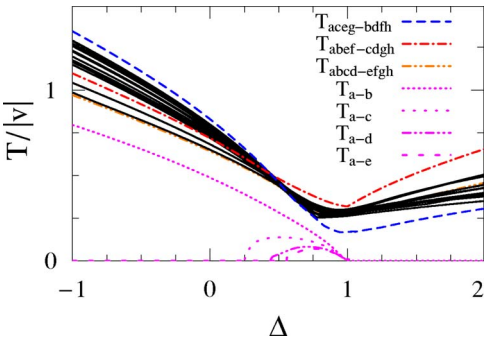

FIG. 4. (Color online) The limit temperatures of all 17 global negativities for $n=8$ qubits in a cyclic chain as a function of asymmetry. The highest and lowest temperatures in each sector are specially indicated. The limit temperatures for adjacent and nonadjacent pairwise entanglement for $b=0$ are also depicted.

$|M|\to|M|+1$ are located at $\Delta=(1-\bar{b}-\bar{b}^2)/(1+\bar{b})(\frac{1}{2}\to\frac{3}{2})$ and $\Delta_c(b)$ $(\frac{3}{2}\to\frac{5}{2})$, collapsing into a single $\frac{1}{2}\to\frac{5}{2}$ transition at $\Delta=1$ if $b=0$.

Global limit temperatures for $n=5$ and $v<0$ (lower panel) are quite close to the previous ones. The main difference is that *all* of them remain nonzero for all Δ, the most persistent negativity corresponding to N_{ac-bde} if $\Delta\lesssim 0.5$ and N_{ab-cde} if $\Delta\gtrsim 0.5$. Limit temperatures for pairwise entanglement exhibit more significant differences. For $b=0$ there is no noncontiguous pairwise entanglement if $v<0$ [29] ($T_{a-c}=0$), since the ground state is fourfold degenerate and leads to $N_{a-c}=0\ \forall\ \Delta$, while T_{a-b} is lower (saturating again for $\Delta\to-\infty$). For $v<0$, the ground state transitions $|M|\to|M|+1$ occur at $\Delta=-[(\bar{b}-1/2)(4\bar{b}+3+\sqrt{5})]/(4\bar{b}+1+\sqrt{5})$ and $\Delta=\Delta_c^-(b)=\frac{1}{4}(1+\sqrt{5})-\bar{b}$, with both collapsing at $\Delta_c^-(0)\approx 0.81$ for $b=0$. Again, for $\Delta>\Delta_c(0)$ there is no two-qubit nor three-qubit negativity, but there is four-qubit entanglement.

In order to appreciate the trend for larger n, Fig. 4 depicts the set of limit temperatures of the 17 distinct global negativities existing for $n=8$ qubits $ab\cdots gh$, consisting of N_{a-*} (one qubit with the rest), and those between different pairs and the rest (N_{ab-*}, N_{ac-*}, N_{ad-*}, N_{ae-*}), three qubits and the rest (N_{abc-*}, N_{abd-*}, N_{abe-*}, N_{ace-*}, N_{acf-*}), and four qubits and the rest (N_{abcd-*}, N_{abce-*}, $N_{abcf-*}=N_{abde-*}$, N_{abef-*}, N_{abdf-*}, N_{abdg-*}, N_{aceg-*}). *All* these temperatures remain nonzero $\forall\ \Delta$, including the region $\Delta\geqslant 1$ where the ground state is aligned for any b, confirming the tendency observed for $n=4$ and 5. The highest limit temperature corresponds to the full noncontiguous 4-4 partition (T_{aceg-*}) for $\Delta\lesssim 0.5$, but changes to that between noncontiguous pairs of adjacent qubits (T_{abef-*}) for $\Delta\gtrsim 0.5$ (in this region T_{aceg-*} becomes the lowest global limit temperature). Again, the "depth" of the entanglement for $\Delta>1$ is up to four-qubit subsystems, being zero all pairwise and three-qubit negativities. The limit temperature for adjacent pairwise entanglement for $b=0$ lies well below the bundle of global limit temperatures, while those of nonadjacent pairs are small and nonzero just in a small interval between $\Delta=0$ and $\Delta=1$, where the ground state negativity is nonzero. Let us also remark that the revival for $\Delta>1$ is sensitive to the interaction range. For instance, there is no entanglement revival in the analogous fully connected case.

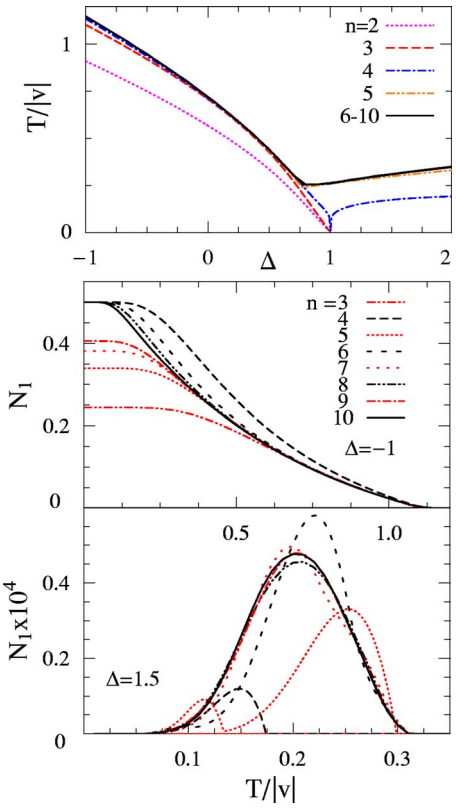

FIG. 5. (Color online) Top: Limit temperatures for nonzero negativity between one qubit and the remaining $n-1$ qubits, for $v>0$ and $n=2-10$. Center and bottom: The thermal behavior of these negativities for $\Delta=-1$ and 1.5, for $b=0$.

Finally, Fig. 5 compares results for the entanglement between one qubit with the rest for different n, assuming $v>0$. As previously stated, N_{a-*} and, hence, T_{a-*} are upper bounds to all pairwise negativities and limit temperatures. It is first seen in the upper panel that the global limit temperatures T_{a-*} for different n rapidly converge to a common value, results for $n=6-10$ being undistinguishable in the scale and range of the figure. This temperature exhibits a slope discontinuity around $\Delta\approx 0.8$, where the number k of negative eigenvalues of the partial transpose exhibits a minimum (while in the case of pure states $k=1$ for N_{a-*} [Eq. (4)], it can be much larger than 1 for nonpure states).

The corresponding global negativities $N_1 \equiv N_{a-*}$ also approach a limit curve for $\Delta<1$, as seen in the central panel for $b=0$ and $\Delta=-1$. Note that for *all* even n, N_{a-*} starts at its maximum value 1/2 at $T=0$, since the reduced one-qubit density ρ_a for the $M=0$ ground state is *maximally mixed*, and Eq. (4) reaches then its maximum value. At fixed $T>0$, they tend initially to decrease for increasing n, rapidly approaching the limit curve. On the other hand, for n odd and $b=0$, the ground state for $\Delta=-1$ has $M=\pm 1/2$ and is degenerate, so that the initial value is lower than in the even case (see the comment for $n=3$), although it increases as n increases and approaches the limit curve (for $b\neq 0$, N_{a-*} would start at ≈ 0.47 for $n=3$, increasing then with n). The lower panel depicts the reentry of the negativity for $T>0$ at $\Delta=1.5$ for increasing n. The behavior is less monotonous than in the previous case, although the difference between results for neighboring odd-even values of n tend to decrease as n increases.

IV. CONCLUSIONS

The present results demonstrate that limit temperatures for global bipartite entanglement in *XXZ* chains may differ considerably from those limiting pairwise entanglement between two qubits in the same chain. In contrast with the latter, global limit temperatures are independent of the field b and do not saturate for $\Delta\to-\infty$ in odd chains. Moreover, global thermal entanglement in nearest neighbor cyclic chains may naturally arise at low levels even for $\Delta>1$ if $n\geqslant 4$ (and $\Delta\geqslant 1$ if $n\geqslant 5$), i.e., in anisotropic and isotropic chains with fully separable ground states, generating entangled bipartitions of the whole system as well as of subsystems with no less than four qubits. The ordering of global limit temperatures also changes as Δ increases from negative to large positive values. Many of our results rapidly saturate as n increases (Fig. 5), indicating that they may remain stable for chains with a larger number of qubits. The present study provides thus a more comprehensive understanding of the borders of thermal entanglement in *XXZ* spin chains, suggesting that quantum schemes based on entanglement between multispin parties may be more resistant to the effects of thermal randomness.

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APPENDIX

1. Negativity of pure states

Equation (4) can be rewritten as

$$N_p[\rho]=\tfrac{1}{2}\{[S_f(\rho_{\{m\}})+1]^2-1\},$$

where

$$S_f(\rho_{\{m\}})=\mathrm{Tr}\, f(\rho_{\{m\}}),\quad f(\rho)\equiv\sqrt{\rho}-\rho,$$

is a simple nonadditive entropy of $\rho_{\{m\}}$ [15], since the function f is concave in [0, 1] and satisfies $f(0)=f(1)=0$. As a consequence, $S_f(\rho_{\{m\}})\geqslant 0$, being maximum for $\rho_{\{m\}}=I/d_m$ and zero when $\rho_{\{m\}}$ is pure, and satisfies $S_f(\rho_{\{m\}})\geqslant S_f(\rho'_{\{m\}})$ if $\rho_{\{m\}}\prec\rho'_{\{m\}}$, where the last condition means that the eigenvalues of $\rho_{\{m\}}$ are majorized by those of $\rho'_{\{m\}}$ [15]. These properties are then also satisfied by the pure state negativity N_p since it is an increasing function of S_f that vanishes for $S_f=0$ and ensure that it cannot increase under LOCC.

2. Independence of global limit temperatures from the uniform magnetic field *b*

Let us consider a Hamiltonian

$$H = bS_z + V,$$

where V is independent of b and satisfies $[V,S_z]=0$. For an arbitrary bipartition $p=\{m\}-\{n-m\}$ of a n-qubit system and a standard basis of states $|M_{\{m\}},M-M_{\{m\}}\rangle$, where M is the eigenvalue of the total spin component S_z and $M_{\{m\}}$ that for the first subsystem (remaining labels omitted), the partial transpose of the exponential $D(b)=\exp[-H/T]=\exp[-bS_z/T]\exp[-V/T]$ in the previous basis satisfies [25]

$$D^{t_p}(b) = \exp[-bS_z/2T]D^{t_p}(0)\exp[-bS_z/2T],$$

where $D^{t_p}(0)$ has matrix elements between states with total spin component M and $M\pm 2k$, with k integer. While the negativity will depend on b, the limits for the positivity of $D^{t_p}(b)$ will not, since $\exp[-bS_z/2T]$ is real and positive, being the same as those for $D^{t_p}(0)$. Global limit temperatures will then be independent of b. This applies in particular to any *XXZ*-type Hamiltonian.

3. Negativity of mixtures of two-qubit and three-qubit states with good angular momentum

The negativity N_{a-b} of any two qubit mixed state of the form

$$\rho = \sum_{S=0,1} \sum_{M=-S}^{S} p_M^S |SM\rangle\langle SM|, \tag{A1}$$

where $|SM\rangle$ denotes the states with good total spin S and component M, can be shown to be [36]

$$N_{a-b} = \tfrac{1}{2}\max[\sqrt{(p_0^1-p_0^0)^2+(p_1^1-p_{-1}^1)^2}-p_1^1-p_{-1}^1,0]. \tag{A2}$$

The condition $N_{a-b}>0$ leads then to Eq. (8). Note also that the single-qubit density is $\rho_a=\mathrm{Tr}_b\,\rho=\sum_{\nu=\pm 1/2} q_\nu|\nu\rangle\langle\nu|$, with $q_\nu=p_\nu^1+\frac{1}{2}(p_0^0+p_0^1)$.

For $n=3$ qubits, a set of eight orthonormal states with good total spin S and spin component M is given by $|\tfrac{3}{2}\tfrac{3}{2}\rangle=|\uparrow\uparrow\uparrow\rangle$, $|\tfrac{3}{2}\tfrac{1}{2}\rangle=(|\downarrow\uparrow\uparrow\rangle+|\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\rangle)/\sqrt{3}$, $|\tfrac{1}{2}\tfrac{1}{2}a\rangle=(|\downarrow\uparrow\uparrow\rangle-|\uparrow\downarrow\uparrow\rangle)/\sqrt{2}$, $|\tfrac{1}{2}\tfrac{1}{2}b\rangle=(|\downarrow\uparrow\uparrow\rangle+|\uparrow\downarrow\uparrow\rangle-2|\uparrow\uparrow\downarrow\rangle)/\sqrt{6}$, and the corresponding partners for $M\to -M$. For a three-qubit density of the form

$$\rho = \sum_{S=1/2,3/2} \sum_{M=-S}^{S} p_M^S P_M^S, \tag{A3}$$

where P_M^S denotes the projector onto the subspace with total spin S and spin component M, an analytic evaluation of the eigenvalues of the partial transpose of ρ yields the following expression for the global negativity $N_{a-bc}=N_{ab-c}=N_{ca-b}$,

$$N_{a-bc} = \frac{1}{6}\sum_{\nu=\pm 1} \max [\sqrt{(3p_{-3\nu/2}^{3/2}-2p_{\nu/2}^{3/2}-p_{\nu/2}^{1/2})^2+8(p_{-\nu/2}^{3/2}-p_{-\nu/2}^{1/2})^2} - 3p_{-3\nu/2}^{3/2}-2p_{\nu/2}^{3/2}-p_{\nu/2}^{1/2},0]. \tag{A4}$$

The condition $N_{a-bc}>0$ leads then to Eq. (10). The ensuing reduced two-qubit density $\rho_{a-b}=\mathrm{Tr}_c\,\rho$ (identical to ρ_{a-c}, ρ_{b-c}) has again the form (A1), with

$$p_{\pm 1}^1 = (3p_{\pm 3/2}^{3/2}+p_{\pm 1/2}^{3/2}+2p_{\pm 1/2}^{1/2})/3,$$

$$p_0^1 = [2(p_{1/2}^{3/2}+p_{-1/2}^{3/2})+p_0^0]/3, \quad p_0^0 = p_{1/2}^{1/2}+p_{-1/2}^{1/2}.$$

The condition (8) for pairwise entanglement leads then to

$$\left|\sum_{\nu=\pm 1} p_{\nu/2}^{3/2}-p_{\nu/2}^{1/2}\right| > \prod_{\nu=\pm 1}\sqrt{3p_{3\nu/2}^{3/2}+p_{\nu/2}^{3/2}+2p_{\nu/2}^{1/2}}. \tag{A5}$$

In the thermal case for the Hamiltonian (1), Eq. (A5) leads to Eq. (12).

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