Global entanglement in XXZ chains

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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 non-zero global negativities are shown to depend on the asymmetry \( \Delta \) 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 \( \Delta = 1 \), 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 \( \Delta \).

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I. INTRODUCTION

Quantum entanglement is a fundamental trait of quantum mechanics, representing the non-local correlations with no classical analogue that can be exhibited by composite quantum systems. Interest on entanglement has provided a new perspective for the analysis of correlations and transitions in many-body quantum systems [6–10]. In systems at finite temperature, 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 \( \rho \) 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., \( \rho = \sum_{a} q_{a} \rho_{a}^{A} \otimes \rho_{a}^{B} \), with \( q_{a} > 0 \), \( \sum_{a} q_{a} = 1 \) and \( \rho_{a}^{A} \), \( \rho_{a}^{B} \) density matrices for each component. Otherwise, \( \rho \) 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 an 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 \( \{ m \} \) 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 \( \rho \) 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 closed as desired to \( I/d \) for sufficiently high \( T \). In particular, no bipartite entanglement can arise if \( \text{Tr} (\rho - I/d)^{2} \leq [d(d-1)]^{-1} \) [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 an 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, 20, 32, 33], revealing rich phenomena. In small XXZ chains [29, 31] it has been shown that there is no pairwise entanglement for \( T \geq 0 \) 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 \( \Delta \) if \( n \) is odd (vanishing \( \Delta \) 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 \( n \geq 4 \) and \( T > 0 \), implying a thermal reentry. Moreover, limit temperatures for non-zero global negativities do not saturate for \( \Delta \to -\infty \) in odd systems, but diverge in both the ferro- and antiferromagnetic cases, even for \( n = 3 \). These temperatures are
independent of the magnetic field but dependent on $\Delta$ and the bipartition, displaying crossings as $\Delta$ 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 an $XXZ$ Hamiltonian for $n$ qubits or spins of the form

$$H = b S_z - \sum_{i<j} [v^{ij}_z (s^i_z s^j_z + s^i_y s^j_y) + v^{ij}_y s^i_z s^j_z],$$

(1)

where $s_i$ denotes the spin operator at site $i$, $S_z = \sum_i s^i_z$ is the total spin $z$-component, $b$ accounts for the Zeeman coupling to a uniform magnetic field and $s^i_z s^j_z + s^i_y s^j_y = (s^i_1 s^j_1 + s^i_2 s^j_2)/2$ is the hopping or entangling term. Our attention will be centered on a cyclic chain with nearest neighbor coupling ($v^{ij}_d = v_0 \delta_{i,j+1}$ for $\alpha = z, z$, with $n + 1 \equiv 1$), although some results for the fully connected case ($v^{ij}_d = v_0 \forall i < j$) 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 ($s^i_y \rightarrow (-1)^i s^i_y$). 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

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

(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

$$N_p[\rho] = \frac{1}{2} \mathrm{Tr}(|\rho^p| - 1),$$

(3)

where $p \equiv \{m\} - \{n-m\}$ denotes the bipartition and $\rho^p$ the ensuing partial transpose of $\rho$ [23]. Eq. (13) is just the absolute value of the sum of the negative eigenvalues of $\rho^p$ (as $\mathrm{Tr}\rho^p = 1$), so that according to the PPT criterion [23, 24], $N_p[\rho] > 0$ indicates entanglement between the $m$ selected qubits and the rest. Eq. (13) satisfies as well properties of an entanglement measure [20], being a convex function of $\rho$ 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 GHZ states [23]). For pure states $\rho = |\Psi\rangle\langle\Psi|$ it can be shown, by means of the Schmidt decomposition

$$\mathbb{E} |\Psi\rangle = \sum_\alpha \sqrt{\lambda_\alpha} |\alpha_m\rangle |\alpha_{n-m}\rangle,$$

that

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

(4)

where $\lambda_\alpha^p$ 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 $\rho^2 = \rho$). Eq. (14) differs from the entanglement of formation [18] $E[\rho] \propto -\sum_\alpha \lambda_\alpha^p \log_2 \lambda_\alpha^p$, but is as well a measure of the disorder of the reduced system (see Appendix), satisfying $N_p[\rho] \geq N_p[\rho']$ if $\lambda^p < \lambda'^p$, where $\prec$ denotes “majorized by” (or “more mixed than”) [5]: $\sum_{\alpha=1}^k \lambda_\alpha^p \leq \sum_{\alpha=1}^k \lambda'^p_\alpha$ for $k = 1, \ldots, d_m$, where $\lambda_\alpha^p$, $\lambda'^p_\alpha$ are sorted in decreasing order and $d_m = 2^m$ is the subsystem dimension ($m \leq n/2$). 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 non-pure 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 3-qubit chain $abc$ there is single distinct global negativity $N_{a-bc} = N_{a-c} = N_{c-ba}$, whereas for $n = 4$ qubits $abcd$, there are three distinct negativities $N_{a-bcd}$, $N_{a-cbd}$ and $N_{a-c-bd}$, which measure respectively the entanglement between: one qubit and the rest, adjacent pairs, non-adjacent 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 monotonic (even entanglement vanishing plus reentry may occur for $T < T_p$ [24-26]). A remarkable feature of these global limit temperatures is that for Hamiltonians of the form (11), 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] $\sum_{\{k\} - \{m-k\}} |\rho_{(m)}| \leq N_{(k)-\{m-1-k\}}[\rho_{(m+1)}]$, as tracing out one qubit is a LOCC operation. The associated limit temperatures will then satisfy $T_{(k)-\{m-k\}} \leq T_{\{k\}-\{m+1-k\}}$, being thus higher for global bipartitions. In particular, the negativity of one qubit with the rest ($N_{a-\cdot}$) is an upper bound to all pairwise negativities $N_{a-b}$, $N_{a-c}$, etc., so that $T_{a-\cdot}$ 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 $N_{a-b}[\rho_{ab}]$ ≤ $N_{a-b}[\rho_{ab}]$, while for four qubit chain there is one distinct three-qubit density $\rho_{abc} = \mathrm{Tr}_d \rho$, with two different negativities $N_{a-bc}[\rho_{abc}]$, $N_{a-cb}[\rho_{abc}]$, satisfying $N_{a-bc} \leq (N_{a-bcd}, N_{a-cbd})$, $N_{a-cb} \leq (N_{a-bcd}, N_{a-c-bd})$. There are
also two different pair densities $\rho_{ab} = Tr_{ad}\rho$, $\rho_{ac} = Tr_{bd}\rho$, whose negativities $N_{a-b}$, $N_{a-c}$, measure the entanglement of contiguous and non-contiguous qubits and satisfy $N_{a-b} \leq (N_{a-bc}, N_{b-ac})$, $N_{a-c} \leq N_{a-bc}$. 

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 $v \equiv v_z$. At $T = 0$ and fixed $b \neq 0$, the ground state of the Hamiltonian will experience a series of $[n/2]$ transitions $|M| \rightarrow |M| + 1$ as $\Delta$ increases, starting from $|M| = 0$ ($1/2$) for $n$ even (odd) and large negative $\Delta$, 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 $|\Psi_0\rangle = |\downarrow \cdots \downarrow\rangle$ 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 ($|\Psi_1\rangle \propto \sum_{i=1}^{n} s_i^a |\Psi_0\rangle$ for $b > 0$), is $E_1 = E_0 + |b| + v_z - v$, so that the transition occurs at

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

Eq. (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 non-zero global negativities are independent of the field $b$, so will be the concomitant borders $\Delta_c^s(T)$. 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 $\Delta \geq 1$ if $n \geq 4$.

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 $v_{12}^2$ in (11)). $H$ can be rewritten in these cases in terms of the total spin components $S_n = \sum_{i=1}^{n} s_i^a$ as

$$H = b S_z - \frac{1}{2} [v (S_z^2 + S_x^2) + v_z S_x^2] + E_0, \quad (6)$$

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

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

where $S = 0, 1$, for $n = 2$, and $S = 1/2$ (two-fold degenerate), $3/2$, for $n = 3$, with $|M| \leq S$. In the fully connected case Eqs. (6)-(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 $|SM\rangle = |\uparrow\uparrow\rangle$) or maximally entangled (the Bell states $|SM\rangle = |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle \propto |\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle$), 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 $ho = \sum_{S,M} p_M^S |SM\rangle \langle SM|$ is entangled whenever

$$|p_0 - p_0^0| > 2 \sqrt{p_1^1 p_1^1}, \quad (8)$$

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

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

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 $\Delta$ (see Fig. 1), that vanishes for $\Delta \rightarrow 1$ and diverges for $\Delta \rightarrow -\infty (\Delta \leq 1 - 2t \ln(2t) \forall \Delta > 0)$.

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 $\Delta < \Delta_c(b)$ ($|SM\rangle = |\uparrow\uparrow\rangle \propto |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\down\rangle$) for $b > 0$, with global negativity $N_{a-bc} = \sqrt{2}/3 \approx 0.47$ and pair negativity $N_{a-b} = (1 - \sqrt{3})/6 \approx 0.21$, becoming the aligned state $|\uparrow\down\rangle$ for $\Delta > \Delta_c(b)$. Let us add that if $b = 0$, the states $\{|\uparrow\down\rangle, \down\rangle\rangle$ become degenerate but their mixture $\frac{1}{2} \sum_{S=1/2}^{3} |S\rangle^3 M^3 (\rangle \langle M)$ (the $\rho(T)$ for $\Delta < \Delta_c(b)$) remains entangled, with lower values $N_{a-bc} = (3\sqrt{3}/1)\approx 0.24, N_{a-b} = 1/6$.

On the other hand, for any 3-qubit mixed state $\rho = \sum_{S,M} p_M^S |SM\rangle \langle SM|$, where $p_M^S$ denotes the projector onto the subspace with total spin $S$ and component $M$, the global negativity $N_{a-bc}$ will be non-zero if and only if (see Appendix)

$$|p_{v/2}^{3/2} - p_{v/2}^{1/2}| > \sqrt{3p_{v/2}^{3/2} p_{v/2}^{1/2}}, \quad (10)$$

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

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

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

The behavior of the pairwise limit temperature $T_{a-b}$ for $n = 3$ is however quite different $\frac{2b}{3}$. The reduced two-qubit density $\rho_{a-b}$ is entangled in a smaller region which depends on the field $b$ and is determined by the equation (see Appendix)

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

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

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

so that global bipartite entanglement starts for $\Delta < 1/2$ ($\Delta < 1/2 - t \ln(3/2)$ for $t \ll 1$), although for $t \gg 1$ Eq. (13) and (11) are almost coincident, implying that $T_{a-bc}$ is almost the same for $v = 0$ for large negative $\Delta$ (Fig. 1). This is not the case for $T_{a-b}$, which for $v < 0$ is determined by Eq. (12) with $\gamma = 2 + \alpha$, 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 $\Delta < \Delta_{\gamma}(b) = 1/2 - |v/b|$, being then two-fold degenerate for $b \neq 0$, and to an aligned state ($|M| = 3/2$) if $\Delta > \Delta_{\gamma}(b)$. For $\Delta < \Delta_{\gamma}(b)$ and $b \neq 0$, the mixture $\rho = t^2P_{1/2, \pm 1/2}$ (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, $\rho = (1/2)(P_{1/2, 1/2} + P_{1/2, -1/2})$, 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.

**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 $\Delta < \Delta_{\gamma}(b)$ [Eq. (15)], with the transitions $|M| \to |M| + 1$ occurring at $\Delta = (1 - 2b - b^2)/(1 + b)$, $b = |b/v|$ (0 to 1), and $\Delta = \Delta_{\gamma}(b)$ (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 $N_{a-b} = 0$ (entanglement between contiguous pairs) and $N_{a-bc}$ (entanglement of one qubit with the rest) become again non-zero for $\Delta > 1$, indicating the reentry of the corresponding entanglement.

![FIG. 1: (Color online). Limit temperatures $T_{a-bc}$ for global bipartite entanglement for $n = 3$ qubits as a function of the asymmetry $\Delta = v/|v|$, 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 $b$).](image1)

![FIG. 2: (Color online). Top: Limit temperatures for global ($T_{a-bcd}$, $T_{ab-cd}$, $T_{a-bcd}$), pairwise ($T_{a-b}$, $T_{a-c}$) and three-qubit ($T_{a-bc}$, $T_{b-a}$) entropies for $n = 4$ qubits in a nearest neighbor cyclic chain, as a function of the asymmetry $\Delta$. There is global entanglement also for $\Delta > 1$. Results for reduced systems correspond to zero field. Center: The behavior of the global negativity $N_{a-bcd}$ as a function of temperature and $\Delta$ (with different scales for $\Delta < 1$ and $\Delta > 1$) for $b = 0$. Bottom: Negativities of the state (14) as a function of $\Delta$. For $b = 0$, they represent the ground state negativities for $\Delta < 1$.](image2)
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, \(N_{ac-bd} = 1/2\) (the reduced one-qubit density \(\rho_a\) 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 \(\Delta\). 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 \((\propto |\downarrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle + \ldots \) 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 \(\rho_{abc}\) and \(T_{a-b}, T_{a-c}\) for the reduced pair densities \(\rho_{ab}\) and \(\rho_{ac}\). 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 \(T_{a-b}\) (adjacent qubits) increases as \(\Delta\) decreases, diverging for \(\Delta \to -\infty\) (in contrast with the behavior for \(n = 3\)), \(T_{a-c}\) (non-adjacent 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 \([\text{14}]\) leads to \(N_{a-b} = \alpha(2\beta - \alpha)\) for \(\Delta < 7/2\) (and 0 for \(\Delta > 7/2\)), and \(N_{ac-b} = 2\alpha^2 - \beta^2\) for \(\Delta > 0\) (and 0 for \(\Delta < 0\)), with \(N_{a-b} > N_{ac-b}\) for \(\Delta < 1\). The ordering of negativities is of course in agreement with the discussion of sec. II.

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 non-contiguous \(2 - 3\) partition, \(N_{ac-bde}\), with \(T_{ac-bde}\) lying close to \(T_{ab-cde}\) (contiguous \(2-3\) partition) for \(\Delta \geq 1/2\); b) The negativity of one-qubit with the rest, \(N_{a-bcde}\), remains non-zero \(\forall \Delta\) if \(T > 0\), including the isotropic case \(\Delta = 1\), providing the highest limit temperature for 0.85 \(\leq \Delta \leq 1.35\); 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 non-zero). Besides, for \(\Delta \to -\infty\) the limit temperature for adjacent pairwise entanglement \(T_{a-b}\) approaches a finite limit \([\text{29}]\), 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 \(|M| \to |M| + 1\) are located at \(\Delta = (1 - b - b^2)/(1 + b)\) \((1/2 \to 3/2)\) and \(\Delta = (b)\) \((3/2 \to 5/2)\), collapsing into a single \(\frac{1}{2} \to \frac{3}{2}\) 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 non-zero for all \(\Delta\), 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 non-contiguous pairwise entanglement if \(v < 0\) \([\text{29}]\) \((T_{a-c} = 0)\), since the ground state is four-fold 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 \(\Delta = -(b-1/2)(4b+3+\sqrt{7})/4b+1+\sqrt{5}\) and \(\Delta = \Delta_- (b) = \frac{1}{2}(1 + \sqrt{5}) - b\), with both collapsing at \(\Delta_- (0) \approx 0.81\) for \(b = 0\). Again, for \(\Delta > \Delta_- (0)\) there is no two- 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 \(ab\ldots gh\), consisting of \(N_{a-}\) (one qubit with the rest), and those between different pairs and the rest \((N_{ab-}, N_{ac-}, N_{ad-}, N_{ac-})\), three qubits and the rest \((N_{abc-}, N_{abd-}, N_{abc-}, N_{ac-}, N_{ac-})\) and four qubits and the rest \((N_{abcd-}, N_{abc-}, N_{abc-}, N_{abcd-}, N_{abde-}, N_{abf-}, N_{abf-}, N_{abf-}, N_{abf-})\). All these temperatures remain non-zero \(\forall \Delta\), including the region \(\Delta \geq 1\) 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 non-contiguous \(4-4\) partition \((T_{acceg-})\) for \(\Delta \lesssim 0.5\), but changes to that between non-contiguous pairs of adjacent qubits \((T_{abf-})\) for \(\Delta \gtrsim 0.5\) (in this region \(T_{acceg-}\) 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

![FIG. 3: (Color online). The set of limit temperatures for global negativities, \(T_{a-bcd}, T_{b-cde}, T_{ac-bde}\) for \(n = 5\) qubits in the cyclic chain as a function of \(\Delta\) 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 \((T_{a-c})\) negativity for \(b = 0\) are also depicted. \(T_{a-c}\) vanishes for \(v < 0\) and \(b = 0\).](image-url)
well below the bundle of global limit temperatures, while those of non-adjacent pairs are small and non-zero just in a small interval between $\Delta = 0$ and $\Delta = 1$, where the ground state negativity is non-zero. 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.

Finally, Fig. 4 compares results for the entanglement between one qubit with the rest for different $n$, assuming $v > 0$. As previously stated, $N_{a-\cdots}$ and hence $T_{a-\cdots}$ are upper bounds to all pairwise negativities and limit temperatures. It is first seen in the upper panel that the global limit temperatures $T_{a-\cdots}$ 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 $N_{a-\cdots}$ [Eq. (4)], it can be much larger than 1 for non-pure states).

The corresponding global negativities $N_{a-\cdots}$ 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 $n$, $N_{a-\cdots}$ starts at its maximum value 1/2 at $T = 0$, since the reduced one-qubit density $\rho_a$ 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 $b \neq 0$, $N_{a-\cdots}$ would start at $\approx 0.47$ 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.

FIG. 4: (Color online). The limit temperatures of all seventeen 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 non-adjacent pairwise entanglement for $b = 0$ are also depicted.

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 $n \geq 4$ (and $\Delta \geq 1$ if $n \geq 5$), 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 $\Delta$ increases from negative to large positive values. Many of our results rapidly saturate as $n$ increases (Fig. 4), 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 multi-spin parties may be more resistant to the effects of thermal randomness.

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Appendix

Negativity of pure states. Eq. (4) can be rewritten as

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

where

\[ S_f(\rho_{\{m\}}) = \text{Tr}\{f(\rho_{\{m\}})\}, \quad f[\rho] = \sqrt{\rho - \rho^*}, \]

is a simple non-additive entropy of \(\rho_{\{m\}}\), since the function \(f\) is concave in \([0,1]\) and satisfies \(f(0) = f(1) = 0\). As a consequence, \(S_f(\rho_{\{m\}}) \geq 0\), being maximum for \(\rho_{\{m\}} = I/d_m\) and zero when \(\rho_{\{m\}}\) is pure, and satisfies \(S_f(\rho_{\{m\}}) \geq S_f(\rho'_{\{m\}})\) if \(\rho_{\{m\}} \leq \rho'_{\{m\}}\), where the last condition means that the eigenvalues of \(\rho_{\{m\}}\) are majorized by those of \(\rho'_{\{m\}}\). 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.

Independence of global limit temperatures from the uniform magnetic field \(b\). Let us consider a Hamiltonian

\[ H = bs_2 + V, \]

where \(V\) is independent of \(b\) and satisfies \([V, s_2] = 0\). For an arbitrary bipartition \(p = \{m\} - \{n - m\}\) of an \(n\)-qubit system and a standard basis of states \([M_{\{m\}}, M - M_{\{m\}}]\), where \(M\) is the eigenvalue of the total spin component \(s_2\) and \(M_{\{m\}}\) that for the first subsystem (remaining labels omitted), the partial transpose of the exponential \(D(b) = \exp[-H/T] = \exp[-bs_2/T]\exp[-V/T]\) in the previous basis satisfies \(25\):

\[ D^{Tr}(b) = \exp[-bs_2/2T]D^{Tr}(0)\exp[-bs_2/2T], \]

where \(D^{Tr}(0)\) 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 \(D^{Tr}(b)\) will not, since exp\([-bs_2/2T]\) is real and positive, being the same as those for \(D^{Tr}(0)\). Global limit temperatures will then be independent of \(b\). This applies in particular to any XXZ type Hamiltonian.

Negativity of mixtures of two- and three-qubit states with good angular momentum. The negativity \(N_{a-b}\) of any two qubit mixed state of the form

\[ \rho = \sum_{S=0,1} \sum_{M=-S}^S p_{S_M}^a |SM\rangle\langle SM|, \]

where \(|SM\rangle\rangle\) denotes the states with good total spin \(S\) and component \(M\), can be shown to be \(36\):

\[ N_{a-b} = \frac{1}{2} \text{Max}\left[\sqrt{(p_1^a-p_0^a)^2 + (p_1^1-p_0^1)^2} - p_1^a - p_1^1, 0\right] \]

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

For \(n = 3\) qubits, a set of 8 orthonormal states with good total spin \(S\) and spin component \(M\), is given by

\[ |ads\rangle = (|\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\rangle)/\sqrt{2}, \quad |\uparrow\uparrow\downarrow\rangle = (|\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\downarrow\rangle)/\sqrt{2}, \quad |\uparrow\downarrow\downarrow\rangle = (|\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\rangle)/\sqrt{2}, \]

and the corresponding partners for \(M \to -M\). For a three-qubit density of the form

\[ \rho = \sum_{S=1/2,3/2} \sum_{M=-S} p_M^S \rho_M^S, \]

where \(\rho_M^S\) 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 \(\rho\) yields the following expression for the global negativity

\[ N_{a-b} = N_{ab-c} = N_{ca-b}. \]

The condition \(N_{a-b} > 0\) leads then to Eq. (10). The ensuing reduced two qubit density \(\rho_{a-b} = \text{Tr}_c \rho\) (identical to \(\rho_{a-c}, \rho_{b-c}\)) has again the form \(15\), with

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

The condition \(8\) for pairwise entanglement leads then to

\[ |\sum_{\nu=\pm 1/2} p_{\nu/2}^3 - p_{-\nu/2}^1| > \prod_{\nu=\pm 1} \sqrt{3p_{\nu/2}^3 + p_{\nu/2}^3 + 2p_{\nu/2}^1}. \]

In the thermal case for the Hamiltonian \(11\), Eq. (19) leads to Eq. (12).
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