Divergence of the entanglement range in low-dimensional quantum systems

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We study the pairwise entanglement close to separable ground states of a class of one-dimensional quantum spin models. At $T=0$ we find that such ground states separate regions, in the space of the Hamiltonian parameters, which are characterized by qualitatively different types of entanglement, namely parallel and antiparallel entanglement; we further demonstrate that the range of the concurrence diverges while approaching separable ground states, therefore evidencing that such states, with uncorrelated fluctuations, are reached by a long range reshuffling of the entanglement. We generalize our results to the analysis of quantum phase transitions occurring in bosonic and fermionic systems. Finally, the effects of finite temperature are considered: At $T>0$ we evidence the existence of a region where no pairwise entanglement survives, so that entanglement, if present, is genuinely multipartite.

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I. INTRODUCTION

Quantum fluctuations may disorder the ground state of a system, especially at low dimensions. A paradigmatic example in this sense are quantum phase transitions [1], where different phases can be achieved at $T=0$ by adjusting a control parameter of the system. Paradoxically enough, quantum effects can provide also classical-like ground states (CGS). In fact, for certain values of the control parameter, quantum fluctuations may become completely uncorrelated; thereby the ground state of the system gets factorized and identical to the lowest-energy state of the classical counterpart of the original quantum system. This phenomenon was evidenced by Kurmann *et al.* [2] in the early eighties, for $S=1/2$ Heisenberg antiferromagnetic chains in an external magnetic field h.

The study of entanglement in quantum many-body systems has been providing a new angle in statistical mechanics [3–7], particularly at low temperature where cooperative phenomena are dominated by quantum mechanics. Thanks to a proper analysis of certain entanglement estimators, the result by Kurmann *et al.* was recently retrieved [8] and generalized to two-dimensional spin systems [9]; moreover, numerical evidence arose for it to hold in spin chains with long-ranged interaction [10].

Special interest has been devoted to bipartite entanglement of formation in connection with quantum criticality: In fact, though quantum critical points are rather marked by the enhancement of multipartite entanglement [8,9,11], the variation of the pairwise entanglement at criticality captures the nonanalyticity of the ground state of the system [12]. On the other hand, the naive guess that the range of pairwise entanglement should diverge at a quantum phase transition, in analogy with the divergence of the correlation length of the two-point correlators, has never been evidenced [3,4].

In this paper we show that, in the space of the Hamiltonian parameters, the special points where CGS occur (hereafter called *separable* points) mark a separation between regions characterized by different types of entanglement, (called antiparallel and parallel entanglement in Ref. [13]), which correspond to qualitatively different spin configurations. The transition from one region to the other is found to be characterized by the divergence of the range of pairwise entanglement in the immediate neighborhoods of the CGS [see Eqs. (12) and (13) below].

Spin-off in systems of strongly interacting bosons in a lattice are also found: We evidence that the superfluid-insulator quantum phase transition at commensurate filling fractions is in fact a transition between a phase (superfluid) where solely particle-hole entanglement is present and a phase (insulator) with no pairwise entanglement at all: the particle-hole entanglement is easily seen to correspond to antiparallel entanglement and the range of the concurrence is found to diverge while approaching the transition [see the paragraph below Eq. (13)].

Finally, we study how robust CGS are with respect to temperature: We evidence the emergence of a region in the h-T plane, fanning out from separable points (see Fig. 3) where pairwise entanglement vanishes. In such a region, if entanglement is present in the system, it necessarily is of multipartite type. Our study also sheds light on the result by Kurmann *et al.* (see the concluding paragraph).

II. MODELS

We focus our attention on the class of one-dimensional (1D) spin models described by the Hamiltonian

$$\mathcal{H}(j_x,j_y,j_z) = J\sum_i (j_x S_i^x S_{i+1}^x + j_y S_i^y S_{i+1}^y + j_z S_i^z S_{i+1}^z - h S_i^z), \qquad (1)$$

where i runs over the sites of the chain, S_i^α $(\alpha=x,y,z)$ are quantum angular momentum operators corresponding to $S=1/2$, j_α are the anisotropy parameters $(|j_\alpha|\leq 1)$, $h\equiv g\mu_{\rm B}H/J$ is the reduced magnetic field, and J is the exchange integral, assumed positive and hereafter set to unity.

In Ref. [2] it was demonstrated that CGS are obtained for $h=h_f\equiv\sqrt{(j_x+j_z)(j_y+j_z)}$; although the model (1) cannot be solved exactly for generic j_α, the above result is rigorous. In order to analyze quantum correlations, which are crucial for understanding the behavior of the system at and near a separable point, we restrict the parameters in the Hamiltonian (1) so as to rely on exact results: We therefore consider the solvable cases $\mathcal{H}(1+\gamma,1-\gamma,0)\doteq\mathcal{H}_{XY}$ with $0\leqslant\gamma\leqslant 1$, and $\mathcal{H}(1,1,j_z)\doteq\mathcal{H}_{XXZ}$ corresponding to the *XY* and *XXZ* models in a transverse field, respectively.

The quantitative analysis of the pairwise entanglement between two spins sitting on sites l and m of the chain is addressed via the concurrence C_r with $r\equiv|l-m|$ (translational invariance is assumed) [14]. In terms of correlation functions $g_r^{\alpha\alpha}=\langle S_l^\alpha S_{l+r}^\alpha\rangle$ and magnetization $M_z=\langle S^z\rangle$, the concurrence reads [15]

$$C_r=2\max\{0,C_r',C_r''\}, \tag{2}$$

$$C_r'=|g_r^{xx}+g_r^{yy}|-\sqrt{\left(\frac{1}{4}+g_r^{zz}\right)^2-M_z^2}, \tag{3}$$

$$C_r''=|g_r^{xx}-g_r^{yy}|+g_r^{zz}-\frac{1}{4}, \tag{4}$$

where C_r' and C_r'' measure the pairwise entanglement related with the occurrence of antiparallel and parallel Bell states, respectively, as discussed in Ref. [13] both for pure and mixed states. We will also consider the one-tangle [15,16]

$$\tau_1=1-4\sum_\alpha M_\alpha^2, \tag{5}$$

the two-tangle

$$\tau_2=2\sum_r C_r^2, \tag{6}$$

and the ratio τ_2/τ_1 which estimates the fraction of the total entanglement stored in pairwise correlations [8]. Although $g_r^{\alpha\alpha}$ and M_z do not show any anomaly at a separable point, they unveil it when combined in C_r, which is found to drop to zero in a nonanalytic way at this point. Such circumstances come together with the vanishing of τ_1, and with a highly nontrivial behavior of the ratio τ_2/τ_1 [8].

III. RESULTS

A. Zero temperature

Let us first consider the completely integrable [17,18] *XY* model in a transverse field. Besides the quantum critical point $h=h_c=1$, its $T=0$ phase diagram [19] is characterized by the circle $h^2+\gamma^2=1$ (hereafter called the *separable circle*) where CGS occur in the form

$$|GS^{XY}\rangle=\prod_i|\phi_i^{XY}\rangle,$$

$$|\phi_i^{XY}\rangle\equiv(-1)^i\cos\left(\frac{\theta_\gamma}{2}\right)|\downarrow_i\rangle+\sin\left(\frac{\theta_\gamma}{2}\right)|\uparrow_i\rangle,$$

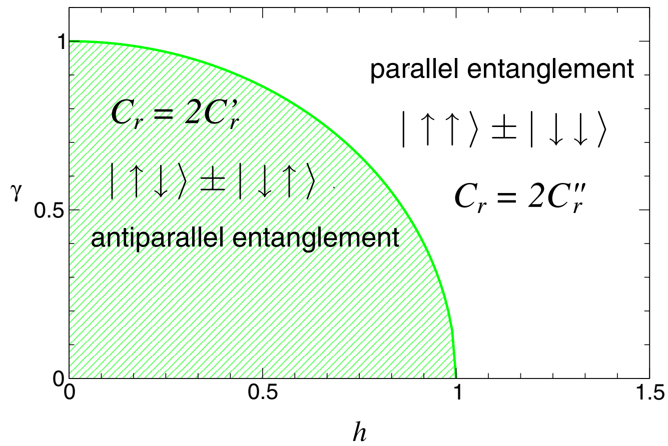

FIG. 1. (Color online) Entanglement phase diagram in the h-γ plane. Points on the circle correspond to models whose ground state is separable.

$$\cos(\theta_\gamma)=\sqrt{\frac{1-\gamma}{1+\gamma}},$$

where $|\phi_i^{XY}\rangle$ is the state of the spin sitting on the ith site.

Since the early papers on the model it is known that the functional form of M_z and $g_r^{\alpha\alpha}$ depends substantially on whether the parameters of the system fix a point sitting inside, outside, or on the circle itself [19]; however, it had never been noticed that the simplicity of the exact solution at $h_f^{XY}=\sqrt{1-\gamma^2}$ is ultimately due to the factorization of the ground state. In fact, this is clearly evidenced by the concurrence, whose expression on the separable circle reads

$$C_r=2C_r'=2C_r''=\frac{\gamma}{1+\gamma}+2M_z^2-\frac{1}{2}\quad\forall\, r, \tag{7}$$

and hence, being $M_z=\frac{1}{2}\sqrt{(1-\gamma)/(1+\gamma)}$,

$$C_r=C_r'=C_r'=0,\quad\forall\, r. \tag{8}$$

Moreover, it is $C_r'\geqslant 0$ (and $C_r''\leqslant 0$) inside the circle, and $C_r'\leqslant 0$ (and $C_r''\geqslant 0$) outside the circle, no matter the sign of the exchange interaction and the value of r. According to the analysis presented in Ref. [13] this means that inside (outside) the circle pairwise entanglement exclusively originates from the occurrence of antiparallel (parallel) Bell states.

We remark that whether the system has parallel or antiparallel pairwise entanglement at $T=0$ uniquely depends on the Hamiltonian parameters γ and h: As a consequence, we can draw an "entanglement phase diagram" in the h-γ plane, where different phases are characterized by the presence of parallel or antiparallel entanglement. The separable circle $h^2+\gamma^2=1$ marks a boundary in such diagram (see Fig. 1) suggesting that the occurrence of a CGS is a necessary step for switching from parallel to antiparallel entanglement. We notice that the same scenario emerges from the numerical analysis of more complicated models, both in one [8] and two dimensions [9].

As the transition from parallel to antiparallel entanglement involves the whole system, we study how the pairwise entanglement propagates along the chain in the vicinity

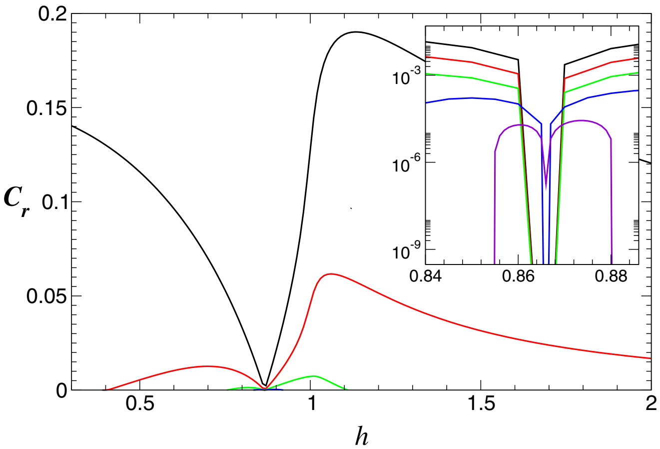

FIG. 2. (Color online) Concurrence for the XY model at $T=0$: curves are C_r vs h for $r=1,2,3,4,5$ (top to bottom), and $\gamma=0.5$. The inset is a zoom near the factorizing field, in logarithmic scale.

of a separable point: for doing that, we introduce the range R of the $T=0$ pairwise entanglement, which is defined as the maximum distance between two spins such that the concurrence is nonvanishing:

$$C_r > 0 \quad \text{for } r \leqslant R \quad \text{and} \quad C_r = 0 \quad \text{for} \quad r > R. \tag{9}$$

We underline that the exact vanishing of C_r for $r>R$ and $h \neq h_{\mathrm{f}}$ follows from the definition of the concurrence Eq. (2), in the sense that C_r vanishes whenever C'_r and C''_r are both negative. On the other hand, at the factorizing field, $C_r=C'_r=C''_r=0$ for all values of r due to the fact that the correlation functions do not depend upon r on the separable circle. In Fig. 2 we show the exact results for C_r with r ranging from 1 to 5. Results for larger r are also available and show the same qualitative behavior: C_r fans out from the separable point with nonzero derivative, reaches a maximum, and then vanishes, both for $h>h_f$ and $h<h_f$, though not symmetrically with respect to h_f.

The observed behavior suggests the divergence of R for $h \to h_{\mathrm{f}}$: by expanding the exact expressions of the correlation functions up the first order in (h-h_{f}) we find [20]

$$C_r = \frac{\Gamma^{2r-1}}{2\gamma}|h\text{-}h_{\mathrm{f}}| + O((h\text{-}h_{\mathrm{f}})^2), \tag{10}$$

where $\Gamma \equiv \sqrt{(1-\gamma)/(1+\gamma)}$. Equation (10) confirms that all C_r get progressively positive for h approaching the factorizing field, as clearly seen in Fig. 2: This means that the range of the concurrence R diverges at h_{f}.

In order to analyze how R diverges with the field, we push forward the expansion in (h-h_{f}), meanwhile considering the large-R expressions for the correlation functions, given in Refs. [19,21]. The result for $h>h_{\mathrm{f}}$ reads

$$C''_r = \frac{\Gamma^{2r-1}}{4\gamma}(h\text{-}h_{\mathrm{f}}) - [A^2 + B(r)](h\text{-}h_{\mathrm{f}})^2 + O((h\text{-}h_{\mathrm{f}})^3) \tag{11}$$

where $A^2 \equiv \Gamma^2(3+\gamma)/(32\gamma^3)$ and $B(r)$ is a coefficient which vanishes for $r\to\infty$. The range of the concurrence is implicitly obtained from Eq. (11) by requiring $C''_R=0$. In fact, for sufficiently large r, it is $[A^2+B(r)]^{-1} \simeq A^{-2}[1-B(r)/A^2]$, and hence, by substituting into Eq. (11), C''_r is found to vanish both for $h=h_{\mathrm{f}}$ and h-$h_{\mathrm{f}}=\Gamma^{2r-1}/(4\gamma A^2)$, leading to the logarithmic divergence

$$R^{XY} \propto \left(\ln \frac{1-\gamma}{1+\gamma}\right)^{-1} \ln |h\text{-}h_{\mathrm{f}}|^{-1}, \tag{12}$$

where we have introduced the symbol R^{XY} to make clear that the functional form of the divergence is in general model dependent.

For $h<h_{\mathrm{f}}$ the expression for C'_r is different from Eq. (11), and to this difference we ascribe the asymmetric behavior of C_r with respect to the separable point observed in Fig. 2; however, for $h\to h_{\mathrm{f}}^-$ the above result is still valid, though just for the (thermal) ground state with unbroken symmetry [4,22]. It is to be noticed that, in the thermodynamic limit (here considered) and while approaching the CGS, the fact that the concurrences C_r become progressively positive for larger and larger r goes together with their getting vanishingly small: this is due both to the monogamy of the entanglement [23,24] and to the proximity of the separable point itself.

The divergence of R implies, as a consequence of the monogamy of the entanglement, that the role of pairwise entanglement is enhanced while approaching the separable point; in fact, the ratio τ_2/τ_1 is found to have a cusp minimum at the critical point and to increase while moving towards the CGS, in full analogy with the result of Refs. [8,9]. In the particular case of the Ising model (i.e., $\gamma=1$), we find that for $h\to h_{\mathrm{f}}=0$ the ratio τ_2/τ_1 goes to unity at the separable point. For $\gamma\neq 1$ and $h_{\mathrm{f}}<h<h_c$ our data show that τ_2/τ_1 monotonically increases for $h\to h_{\mathrm{f}}^+$ and that the value $(\tau_2/\tau_1)|_{h_{\mathrm{f}}^+}$ increases with γ.

We remark that the divergence of R^{XY} while approaching the separable circle cannot be recognized as a critical effect, since the ground state is nonsingular at h_{f} and the long-ranged pairwise entanglement does not survive either inside or outside the separable circle.

A complementary view on the physics of CGS is obtained by the analysis of $\mathcal{H}_{XXZ}$, that can be done resorting to Bethe ansatz results [25]. In this case h_{f} coincides with the saturation field $h_{\mathrm{s}}=(1+j_z)$, and $|GS^{XXZ}\rangle=\Pi_i|\uparrow_i\rangle$. Also, and distinctively from the XY case, the factorized state extends over a finite portion of the h-j_z phase diagram of the model. In fact, h_{s} separates a gapless *quasiordered* phase (with power law decay of the in-plane correlation functions) from the gapped, fully polarized phase (with $\langle S_z\rangle=1/2$). Due to the in-plane symmetry of the model (implying $g_r^{xx}=g_r^{yy}$) C''_r is always negative and therefore pairwise entanglement, if present, is of the antiparallel type. Combining the exact results of Refs. [26,27], we find that R diverges approaching the band transition as follows:

$$R^{XXZ} \propto (h_{\mathrm{s}} - h)^{-\theta/4}, \tag{13}$$

where

$$\theta = 2 + \frac{4\sqrt{h_s - h}}{\pi \tan\left(\frac{\pi\eta}{2}\right)\tan(\pi\eta)}, \quad \text{and } \eta = \frac{1}{\pi}\arccos(-j_z). \tag{14}$$

The divergence of R in the isotropic case ($j_z=1$), specifically determined in Ref. [13], results from Eq. (13) with $\theta=2$. We underline that saturation is not related to a spontaneous symmetry breaking, and the divergence of R while approaching h_s does not mark a critical phenomenon.

Let us now consider strongly interacting hard-core bosons/spinless fermions in 1D: We shall find that the occurrence of CGS plays a fundamental role for such systems.

Hard-core bosons with repulsive Coulomb interaction are described by the quantum lattice gas [28], whose dynamics is described by $\mathcal{H}_{XXZ}$ phrasing the spins in terms of hard-core bosonic operators: $a=S^-$, $a^\dagger=S^+$, $a^\dagger a=S^z+1/2$. The relevant energies $t\to j_x$ (here $j_x=j_y=1$), $U\to j_z$, and $\mu\to h+j_z$ are the hopping amplitude, the Coulomb interaction, and the chemical potential, respectively. By this mapping, the superfluid and insulating behaviors of the quantum lattice gas at commensurate filling are related to the quasiordered (partially filled band) and fully polarized (filled band) phase of the XXZ spin model, respectively; therefore, the *band transition* observed at $\mu=t+2U$, corresponds to saturation occurring at $h_s=(1+j_z)$.

Based on the above analysis, we state that the insulator-superfluid band transition is characterized by the divergence of the range of the concurrence. Remarkably, the antiparallel character of the pairwise entanglement present in the XXZ model reflects the fact that close to the superfluid-insulator transition exclusively particle-hole entanglement plays a role. Arguments along the same line can be applied to spinless fermion models obtained via a Jordan-Wigner transformation of $\mathcal{H}_{XXZ}$ [29]: The band-transition there observed is from an insulating regime to a gapless phase equivalent to a Luttinger liquid.

B. Finite temperature

We now switch on a finite temperature in the system. We consider questions like: What is the effect fanning out from CGS on the thermal (mixed) states of the system? Particularly: How meaningful is the characterization of the system in terms of parallel or antiparallel pairwise entanglement for mixed states? To answer these questions we consider the XY model where both parallel and antiparallel entanglement are present at $T=0$. The analysis of τ_2 evidences that in the h-T plane exists a region, fanning out from the CGS, where pairwise entanglement vanishes (white region in Fig. 3) and the entanglement, if present, is shared between three or more parties. This means that a CGS may evolve into a quantum mixed state with genuinely multipartite entanglement *by increasing temperature*. In order to determine whether this happens or not, we need to know if entanglement is present in the system: the one-tangle, which accomplishes this task at $T=0$, is not a proper estimator for the entanglement content of the system at finite temperature; therefore, we have to refer to some entanglement witness. Following the results by Tóth [30], entanglement is present if

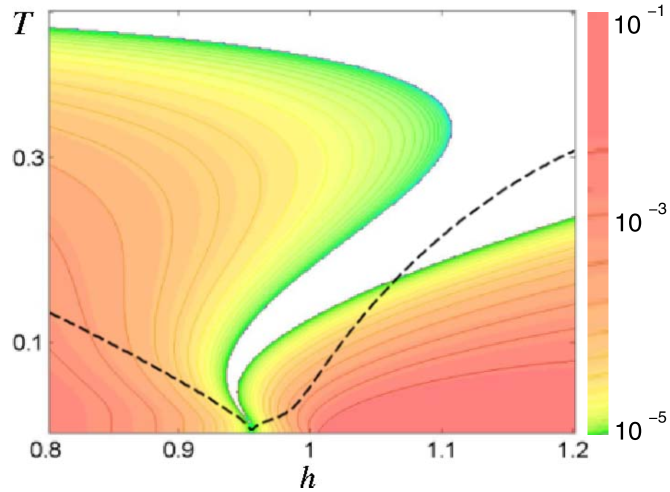

FIG. 3. (Color online) Contour plot of τ_2 in the h-T plane, for $\gamma=0.3$ (i.e., $h_f=0.9539\cdots$). The white area indicates where $\tau_2=0$. Condition (15) is fullfilled below the dashed line, which is defined by $\langle\mathcal{H}\rangle=E_{\text{sep}}$.

$$\langle\mathcal{H}\rangle - E_{\text{sep}} < 0, \tag{15}$$

where E_{sep} is the ground state energy of the corresponding classical model. The region below the dashed line in Fig. 3 is where condition 15 is fulfilled, i.e., where entanglement of whatever type is present in the system. We further observe that, in contrast to the analysis of the ground state, at finite temperature we cannot characterize the two separate phases of parallel and antiparallel entanglement. In fact, the two types of entanglement (though well defined also for mixed states) can swap by varying T and/or r (see Fig. 4). The exchange between parallel and antiparallel entanglement occurs in a nontrivial way, that ultimately produces the temperature "reentrance" of τ_2 seen in Fig. 3. We also find a regime where C_r can be a nonmonotonic function of r, so that, for instance, one spin is not entangled with its nearest neighbor while being entangled with its next-nearest

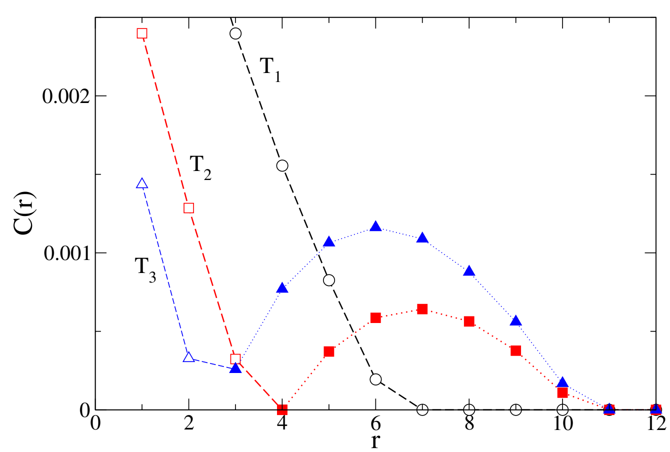

FIG. 4. (Color online) C_r versus r for $\gamma=0.01$ and $h=1.1$. Circles, squares, and triangles correspond to three different temperatures: $T_1=4\ 10^{-3}$, $T_2=4.7\ 10^{-3}$, and $T_3=5\ 10^{-3}$, respectively. Full symbols mean $C_r=C_r'$ and empty symbols mean $C_r=C_r''$.

neighbor. Such situations occur in the vicinity of the region where C_r vanishes, as seen in Fig. 4 and it is due to the nonmonotonic behavior [19] of the correlation functions.

IV. CONCLUSIONS AND PERSPECTIVES

Summarizing, we have studied the occurrence of CGS in relation with pairwise entanglement, in a class of $S=1/2$ spin chains. Our results show that at $T=0$ the space of the Hamiltonian parameters is divided into regions where either exclusively parallel or exclusively antiparallel pairwise entanglement is present, no matter the distance between the considered spins: Therefore, an entanglement phase diagram can be unambiguously drawn. Transition lines in such a diagram corresponds to separable ground states, and are further characterized by the fact that the range of the concurrence diverges while moving toward them. Due to the monogamy of the entanglement, such divergence goes together with the asymptotic vanishing of the value of the concurrence itself.

We further provide (to our knowledge for the first time) an explanation of the phenomenon described by Kurmann *et al.* [2]: the factorization of the ground state is a necessary step for antiparallel entanglement to be fully replaced by parallel entanglement. We observe that in the global reshuffling of the ground state which leads to a CGS, and involves all the spins of the chain, a long range entanglement appears as a crucial ingredient. Moreover, our results for the entanglement ratio τ_2/τ_1 confirm that multipartite entanglement dominates at a genuine quantum critical point, while pairwise entanglement is essential for understanding the mechanism leading to CGS in quantum systems.

Our analysis is of relevance also for bosonic systems undergoing a superfluid-insulator transition. It is intriguing to conjecture that the divergence of the range of C_r at a CGS goes beyond model dependency. In fact, Anfossi *et al.* [11] have observed a similar divergence of the range of C_r also in the bond-charge extended Hubbard model at certain transition lines.

For finite temperature the entanglement in the system cannot be characterized by the single parameter h and a much more complicated scenario emerges: In particular we find that, by increasing T, the factorized (pure) ground state evolves into a thermal (mixed) state with null pairwise entanglement: This opens the possibility for the existence of an experimentally accessible finite-temperature region where entanglement, if present, is genuinely multipartite.

Finally, we notice that the possibility of controlling via a proper tuning of the external magnetic field whether two spins are entangled or not, and whether they share parallel or antiparallel entanglement, might be of interest both from the experimental point of view and for applicative purposes.

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