Divergence of the entanglement range in low dimensional quantum systems

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(Dated: September 9, 2018)

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 correlation 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.

PACS numbers: 03.67.Mn, 75.10.Jm, 73.43.Nq, 05.30.-d

I. INTRODUCTION

Quantum fluctuations may disorder the ground state of a system, especially at low dimensions. Paradigmatic example in this sense are quantum phase transitions \(T=0\), 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. 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 \(\mathbf{1,2,3,4,5,8},\) 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 \(\mathbf{8}\) and generalized to two-dimensional spin systems \(\mathbf{9};\) moreover, numerical evidences arose for it to hold in spin chains with long-ranged interaction \(\mathbf{10};\).

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 \(\mathbf{8,9,11};\) the variation of the pairwise entanglement at criticality captures the non analyticity of the ground state of the system \(\mathbf{12};\) 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 \(\mathbf{3,4};\).

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. \(\mathbf{12}\), 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. \(\mathbf{12}\) and \(\mathbf{13}\) below).

Spin-off in systems of strongly interacting bosons are also found: We evidence that the superfluid-insulator quantum phase transition at commensurate filling 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. \(\mathbf{13}\)).

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. \(\mathbf{9}\) where pairwise entanglement vanishes. In such region, if entanglement is present in the system, it necessarily is of multipartite type. Our study does also shed light on the result by Kurmann et al. (see the concluding paragraph).
II. MODELS

We focus our attention on the class of one-dimensional spin models described by the Hamiltonian
\[ H(j_x, j_y, j_z) = J \sum (j_x S_i^x S_{i+1}^x + j_y S_i^y S_{i+1}^y + j_z S_i^z S_{i+1}^z - h S_i^z), \] (1)
where \( i \) runs over the sites of the chain, \( S_i^a (a = x, y, z) \) are quantum angular momentum operators corresponding to \( S = 1/2 \), \( j_a \) are the anisotropy parameters (\( |j_a| \leq 1 \)), \( h \equiv \mu_B H/J \) 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 \( h = h_f \equiv \sqrt{(j_x + j_z)/(j_x + j_y)} \); although the model cannot be solved exactly for generic \( j_a \), 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 \( H(1 + \gamma, 1 - \gamma, 0) \equiv H_{XY} \) with \( 0 \leq \gamma \leq 1 \), and \( H(1, 1, j_z) \equiv H_{XXZ} \) 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 \( r = |l - m| \) (translational invariance is assumed) \( \text{(1)} \). In terms of correlation functions \( g_{r}^{\alpha \alpha} \equiv \langle S_i^{\alpha} S_{i+r}^{\alpha} \rangle \) and magnetization \( M_z = \langle S_i^z \rangle \), the concurrence reads \( \text{(1)} \):
\[ C_r = 2 \max[0, C'_r, C''_r], \] (2)
\[ C'_r = |g_{r}^{xx} + g_{r}^{yy} - \sqrt{\frac{1}{4} + g_{r}^{zz}}|^2 - M_z^2, \] (3)
\[ C''_r = |g_{r}^{xx} - g_{r}^{yy}| + g_{r}^{zz} - \frac{1}{4}, \] (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 \( \text{[14]} \) and the two-tangle \( \text{[15]} \)
\[ \tau_1 = 1 - 4 \sum_{\alpha} M_z^2, \] (5)
\[ \tau_2 = 2 \sum_{r} C_r^2, \] (6)
and the ratio \( \tau_2/\tau_1 \) which estimates the fraction of the total entanglement stored in pairwise correlations \( \text{[8]} \). 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 non-analytic way at this point. Such circumstance comes together with the vanishing of \( \tau_1 \), and with a highly non-trivial behavior of the ratio \( \tau_2/\tau_1 \) \( \text{[8]} \).

III. RESULTS

A. Zero Temperature

Let us first consider the completely integrable \( \text{[17] [18]} \) \( XY \) model in a transverse field. Besides the quantum critical point \( h = h_c = 1 \), its \( T = 0 \) phase diagram \( \text{[19]} \) is characterized by the circle \( h^2 + \gamma^2 = 1 \) (hereafter called the separable circle) where CGS occur in the form
\[ |GS_{XY}^r > = \prod_i | \phi_i^{XY} > , \]
\[ |\phi_i^{XY} > \equiv (-1)^i \cos(\theta_i/2)| \downarrow_i > + \sin(\theta_i/2)| \uparrow_i > , \]
\[ \cos(\theta_i) = \sqrt{1 - \gamma^2}, \]
where \( |\phi_i^{XY} > \) is the state of the spin sitting on the \( i \)-th 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 \( \text{[19]} \); however, it had never been noticed that the simplicity of the exact solution at \( h_{XY} = \sqrt{1 - \gamma^2} \) 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
\[ C_r = 2C'_r = 2C''_r = \frac{\gamma}{1 + \gamma} + 2M_z^2 - \frac{1}{2}, \quad \forall r, \] (7)
and hence, being \( M_z = \frac{1}{2}\sqrt{(1 - \gamma)/(1 + \gamma)} \),
\[ C_r = C'_r = C''_r = 0, \quad \forall r. \] (8)

Moreover, it is \( C'_r \geq 0 \) (and \( C''_r \leq 0 \)) inside the circle, and \( C'_r \leq 0 \) (and \( C''_r \geq 0 \)) outside the circle, no matter the sign of the exchange interaction and the value of \( r \). According to the analysis presented in Ref.18 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 \( \gamma \) and \( h \); As a consequence, we can draw an “entanglement phase diagram” in the \( h - \gamma \) 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 \( \text{[8]} \) and two dimensions \( \text{[8]} \).

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 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 non vanishing:

\[
C_r > 0 \quad \text{for} \quad r \leq R \quad \text{and} \quad C_r = 0 \quad \text{for} \quad r > R .
\]

We underline that the exact vanishing of \( C_r \) for \( r > R \) and \( h \neq h_t \) 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 behaviour: \( C_r \) fans out from the separable point with non-zero 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 behaviour suggests the divergence of \( R \) for \( h \to h_t \): by expanding the expressions of the correlation functions up the first order in \( (h - h_t) \) we find

\[
C_r = \frac{\Gamma^{2r-1}}{2\gamma}|h - h_t| + \mathcal{O}((h - h_t)^2),
\]

where

\[
\Gamma = \sqrt{(1 - \gamma) / (1 + \gamma)}.
\]

Eq. (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 \( h_t \).

In order to analyze how \( R \) diverges with the field, we push forward the expansion in \( (h - h_t) \), meanwhile considering the large-\( R \) expressions for the correlation functions, given in Refs. [15] and [24]. The result for \( h > h_t \) reads

\[
C''_r = \frac{\Gamma^{2r-1}}{4\gamma}(h - h_t) - [A^2 + B(r)](h - h_t)^2 + \mathcal{O}((h - h_t)^3)
\]

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 \((A^2 + B(r))^{-1} \approx \Gamma^{-2}(1 - B(r)/A^2)\), and hence, by substituting into Eq. (11), \( C''_r \) is found to vanish both for \( h = h_t \) and \( h - h_t = \Gamma^{2r-1}/(4\gamma A^2) \), leading to the logarithmic divergence

\[
R_{XY} ^{\gamma} \propto \left( \ln \frac{1 - \gamma}{1 + \gamma} \right)^{-1} \ln |h - h_t|^{-1},
\]

where we have introduced the symbol \( R_{XY} ^{\gamma} \) to make clear that the functional form of the divergence is in general model-dependent.

For \( h < h_t \) the expression for \( C'_r \) is different from Eq. (11), and to this difference we ascribe the asymmetric behaviour of \( C_r \) with respect to the separable point observed in Fig. 2: however, for \( h \to h^- \) 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 \( C_r \) becomes 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 \( \tau_2/\tau_1 \) is found to have a cusp minimum at the critical point and to increase with respect of CGS, in full analogy with the result of Refs. 8 and 9. In the particular case of the Ising model (i.e. \( \gamma = 1 \)), we find that for \( h \to h_t = 0 \) the ratio \( \tau_2/\tau_1 \) goes to unity at the separable point. For \( \gamma \neq 1 \) and \( h_t < h < h_c \), our data show that \( \tau_2/\tau_1 \) monotonically increases for \( h \to h_t^+ \) and that the value \((\tau_2/\tau_1)|_{h_t^+} \) increases with \( \gamma \).
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 non-singular at \(h_f\) and the long-ranged pairwise entanglement does not survive neither inside nor outside the separable circle.

A complementary view on the physics of CGS is obtained by the analysis of \(H_{XXZ}\), that can be done resorting to Bethe ansatz results. In this case \(h_f\) coincides with the saturation field \(h_s = (1 + j_z)\), and \(|\text{GS}^{XXZ}\rangle = \prod_i |\uparrow_i\rangle\). 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 quasi-ordered 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 \(g_x = g_y\)) \(C'\) is always negative and therefore pairwise entanglement, if present, is of antiparallel type. Combining the exact results of Refs.\(^{26,27}\) we find that \(R\) diverges approaching the band transition as

\[
R^{XXZ} \propto (h_s - h)^{-\theta/4},
\]

where

\[
\theta = 2 + \frac{4\sqrt{h_s - h}}{\pi \tan(\frac{\pi}{2}) \tan(\pi \eta)}, \text{ and } \eta = \frac{1}{\pi} \arccos(-j_z).
\]

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 occurence 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 \(H_{XXZ}\) 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 \(t \rightarrow j_z\) (here \(j_z = j_{xy} = 1\)), \(U \rightarrow j_z\), and \(\mu = h + j_z\) 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 quasi-ordered (partially filled band) and fully-polarized (filled band) phase of the XXZ spin model, respectively; therefore, the band transition observed at \(\mu = t + 4U\), 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 fermions models obtained via Jordan-Wigner transformation of \(H_{XXZ}\). 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 \(\tau_2\) evidences that in the \(h - T\) plane it 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

\[
\langle \mathcal{H} \rangle - E_{\text{sep}} < 0,
\]

where \(E_{\text{sep}}\) 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
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Distance between the considered spins: Therefore, an entanglement is present, no matter the regions where either exclusively parallel or exclusively antiparallel pairwise entanglement is present, no matter the space of the Hamiltonian parameters is divided into regions where either exclusively parallel or exclusively antiparallel pairwise entanglement is present, no matter the space of the Hamiltonian parameters is divided into regions where either exclusively parallel or exclusively antiparallel pairwise entanglement is present, no matter the space of the Hamiltonian parameters is divided into regions where either exclusively parallel or exclusively antiparallel pairwise entanglement is present, no matter the space of the Hamiltonian parameters is divided into regions where either exclusively parallel or exclusively antiparallel pairwise entanglement is present, no matter the space of the Hamiltonian parameters is divided into regions where either exclusively parallel or exclusively 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Transition lines in such diagram corresponds to separable ground states, and are further characterized by the fact that the range of the concurrence diverges while moving towards 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.\cite{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 $\tau_2/\tau_1$ 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.\cite{14} 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.

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 diagram corresponds to separable ground states, and are further characterized by the fact that the range of the concurrence diverges while moving towards them. Due to the monogamy of the entanglement, such divergence goes together with the asymptotic vanishing of the value of the concurrence itself.

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V. ACKNOWLEDGEMENTS

P.V. wishes to thank S. Bose and D. Burgarth for valuable discussions. Comments by T. Roscilde are gratefully acknowledged. This work sets in the framework of the PRIN2005029421 project.

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