Entanglement in quantum critical spin systems

Tommaso Roscilde,1 Paola Verrucchi,2 Andrea Fubini,2,3 Stephan Haas,1 and Valerio Tognetti2,3,4

1Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484
2Istituto Nazionale per la Fisica della Materia, UdR Firenze, Via G. Sansone 1, I-50019 Sesto F.no (FI), Italy
3Dipartimento di Fisica dell’Università di Firenze, Via G. Sansone 1, I-50019 Sesto F.no (FI), Italy
4Istituto Nazionale di Fisica Nucleare, Sez. di Firenze, Via G. Sansone 1, I-50019 Sesto F.no (FI), Italy

(Dated: November 28, 2018)

I. INTRODUCTION

One of the most striking aspects of quantum coherence in a quantum many-body system is the occurrence of entanglement, namely the realization of a superposition of many-body states that cannot be factorized into a product of single-particle wave functions. An entangled state possesses correlations that cannot be accounted for by classical-like quantities; for instance an entangled state might not show any form of classical order, and nonetheless be at the same time strongly correlated. The possibility of a local description of such state is partially or completely lost, depending on the degree of entanglement contained in the state. In particular, the non-local nature of special collective quantum states is the fundamental ingredient that allows quantum communication protocols and quantum computation algorithms to outperform their classical counterparts.

The idea of entanglement as a resource naturally demands a systematic investigation of which quantum many-body systems are able to display sizable entanglement in a controllable way. An intriguing perspective is that pure-quantum correlations are strongly enhanced when a system undergoes a quantum phase transition (QPT) analogously to what classical correlations do at a thermal phase transition. Indeed quantum fluctuations show up at all length scales at a quantum critical point. In what sense quantum correlations, and thus entanglement, ‘diverge’ at a QPT has been the subject of investigation in several recent studies, although the resulting picture is still controversial. In this work we consider a quite general $S = 1/2$ quantum spin system displaying a field-induced QPT in arbitrary dimensions. In particular, we discuss how the behavior of entanglement at and around the quantum critical point shows strong features providing new insight in the drastic change of the system’s ground state under the effect of strong quantum fluctuations.

II. THE MODEL

A very general example of a quantum phase transition in spin models is offered by the the antiferromagnetic XYZ model in a field. The model Hamiltonian reads:

$$\hat{H} = J \sum_{\langle ij \rangle} \left[ \hat{S}_i^x \hat{S}_j^x + \Delta_y \hat{S}_i^y \hat{S}_j^y + \Delta_z \hat{S}_i^z \hat{S}_j^z - \frac{2h}{z} \hat{S}_i^z \right]$$

where $J > 0$ is the exchange coupling, the sum $\langle ij \rangle$ runs over the nearest neighboring sites of a bipartite lattice with coordination number $z$, and $h \equiv g \mu_B H / J$ is the reduced magnetic field. In the following we perform the canonical transformation $\hat{S}_i^y \rightarrow (-1)^i \hat{S}_i^y$ on Eq. 1, so that the relevant correlations along the $x$ and $y$ axes are ferromagnetic. The parameters $0 \leq \Delta_y, \Delta_z \leq 1$ control the anisotropy of the system. In the most general case of $\Delta_y \neq 1$ the Zeeman term in Eq. [1] does not commute with the rest of the hamiltonian. This property is at the core of the field-driven quantum phase transition occurring at a critical field $h_c(\Delta)$, which separates a Neel-ordered phase ($h < h_c$) from a partially-polarized disordered phase ($h > h_c$). When $h \leq h_c$ the field favors long-range magnetic order along the $x$-axis. This order disappears at the critical field $h_c$, where magnetic correlations along $x$ become short-ranged, while quantum fluctuations prevent the spins from being fully polarized along the field.

The case $\Delta_z = 0$ reproduces the XY model in a transverse field, which is exactly solvable in one dimension, and whose entanglement properties have been the subject of several recent investigations. When $\Delta_z \neq 0$, and/or in higher dimensions, the model is no longer exactly solvable. The one-dimensional case has been indeed investigated within approximate analytical and numerical approaches. A renewed interest in the model stems from the experimental in-field studies on the quantum spin chain compound Cs$_2$CoCl$_4$, displaying a strong planar anisotropy, $\Delta_y \approx 0.25$, $\Delta_z \approx 1$, and $J \approx 0.23$ meV.

III. LINEAR CHAIN: CRITICAL POINT AND FACTORIZED STATE

Motivated by the existing theoretical and experimental results, we first concentrate on the case of a linear chain, and on the parameter range $0 \leq \Delta_y \leq 1$, $\Delta_z = 1$, which defines the XYX model in a field. The qualitative behavior of the more general XYZ model is expected to be close to that of the XYX model in a field, since the two models share the same symmetries.
Remarkably, none of these standard magnetic observables bears signatures of the second striking feature of the model, namely the occurrence of an exactly factorized state for a field \( h = (\Delta_y) \) lower than the critical field \( h_c \). The factorizing field reads \( h = \sqrt{2(1+\Delta_y)} \) in the case of the XY model. The factorized state has the form \( |\Psi\rangle = \bigotimes_{j=1}^{L} |\psi_j\rangle \) with \( |\psi_j\rangle = \cos \theta |\uparrow\rangle + \sin \theta e^{i\phi_j} |\downarrow\rangle \) and \( \phi_j = (1+(-1)^j)\pi/2, \theta = \cos^{-1} \sqrt{(1+\Delta_y)/2} \). This corresponds to a configuration in which the spins have perfectly staggered \( x \) components but also cant out of the \( xy \) plane by an angle \( \theta \). The occurrence of such a factorized ground state is particularly surprising if one considers that we are dealing with the \( S = 1/2 \) case, characterized by the most pronounced effects of quantum fluctuations. However, in the class of models here considered, such fluctuations are fully uncorrelated at \( h = h_t \), thus leading to a classical-like ground state.

IV. ENTANGLEMENT ESTIMATORS

The study of entanglement properties in the XY model turns out to be very insightful, and it has the unique feature of unambiguously detecting both the factorized state and the quantum critical point. Our study has focussed on the entanglement of formation\(^\dagger\) which is quantified through the one-tangle and the concurrence. The one-tangle\(^\dagger\dagger\) is an estimate of the \( T = 0 \) entanglement between a single site and the remainder of the system. It is defined as \( \tau_1 = 4 \det \rho^{(1)} \), where \( \rho^{(1)} = (I + \sum_{\alpha} M^x \sigma^\alpha)/2 \) is the one-site reduced density matrix, \( M^x = \langle \hat{S}^x \rangle \), \( \sigma^\alpha \) are the Pauli matrices, and \( \alpha = x, y, z \). In terms of the spin expectation values \( M^x \), \( \tau_1 \) takes the simple form:

\[
\tau_1 = 1 - 4 \sum_{\alpha} (M^x)^2. \tag{2}
\]

The concurrence quantifies instead the pairwise entanglement between two spins at sites \( i, j \) both at zero and finite temperature. For the model of interest, in absence of spontaneous symmetry breaking \( (M^x = 0) \) the concurrence takes the form\(^\dagger\dagger\dagger\)

\[
C_{ij} = 2 \max\{0, C_{ij}^{(1)}, C_{ij}^{(2)}\}, \tag{3}
\]

where

\[
C_{ij}^{(1)} = g_{ij}^{zz} - \frac{1}{4} + |g_{ij}^{xx} - g_{ij}^{yy}|, \tag{4}
\]

\[
C_{ij}^{(2)} = |g_{ij}^{xx} + g_{ij}^{yy}| - \sqrt{\left(\frac{1}{4} + g_{ij}^{zz}\right)^2 - (M^z)^2}, \tag{5}
\]

with \( g_{ij}^{\alpha\beta} = \langle \hat{S}_i^\alpha \hat{S}_j^\beta \rangle \).

V. RESULTS

The QMC results for the model Eq. (1) with \( \Delta_y = 0.25 \) are shown in Fig. 2, where we plot \( \tau_1 \), the sum of squared
entanglement has a very steep recovery, accompanied by the quantum phase transition at $h_c > h_f$. The system realizes therefore an interesting entanglement switch effect controlled by the magnetic field.

As for the concurrence terms Eqs. (1)-(2), the factorizing field divides two field regions with different expressions for the concurrence:

$$C_{ij}^{(1)} < 0 < C_{ij}^{(2)} \quad \text{for } h < h_f,$$

$$C_{ij}^{(2)} < 0 < C_{ij}^{(1)} \quad \text{for } h > h_f,$$

whereas $C_{ij}^{(1)} = C_{ij}^{(2)} = 0$ at $h = h_t$. In presence of spontaneous symmetry breaking occurring for $h > h_c$, the expression of the concurrence is generally expected to change with respect to Eqs. (1)-(2), as extensively discussed in Ref. [3]. For the model under investigation, the expression of the concurrence stays unchanged when the condition $C_{ij}^{(2)} < C_{ij}^{(1)}$ is satisfied, i.e. for $h > h_t$. This means that our estimated concurrence is accurate even in the ordered phase above the factorizing field: in the region $0 < h < h_t$ it represents instead a lower bound to the actual $T = 0$ concurrence. Alternatively it can be regarded as the concurrence for infinitesimally small but finite temperature.

A naive analogy between classical and quantum correlations would lead to the expectation that the range of pairwise entanglement, expressed through the concurrence, is critically enhanced at a quantum phase transition, reflecting the divergence of the length scale for quantum effects. Indeed this is clearly not the case as shown in the right panel of Fig. 2 where the behavior of the spin-spin correlator $g^{xx}$ as a function of the distance is contrasted with that of the concurrence. We observe that, while the correlator becomes long-ranged below the critical field and even completely flat at the factorizing field, the concurrence remains short-ranged when passing through the transition, and it basically vanishes after four lattice spacings.
To clarify this issue, one has to consider the special nature of quantum correlations. At variance with classical correlations, entanglement has basically to satisfy a sum rule, or, as it is often phrased, is subject to a constraint of monogamy. This means that the more partners a spin is entangled with, the less entanglement will be shared with each partner. Moreover, entanglement is present not only in the form of pairwise correlations as in the case of the concurrence, but also in the form of \( n \)-spin correlations with \( n > 2 \), which, unlike classical correlations, can be completely independent of pairwise correlations. This is exemplified for instance by the maximally entangled Greenberger-Horne-Zeilinger (GHZ) state for \( n \) spins \( | \text{GHZ} \rangle = (| \uparrow \uparrow \ldots \uparrow \rangle + | \downarrow \downarrow \ldots \downarrow \rangle) / \sqrt{2} \), on which the concurrence between any two spins is vanishing. Therefore, according to monogamy, pairwise entanglement and \( n \)-wise entanglement with \( n > 2 \) are mutually exclusive, a condition which is absurd from the point of view of classical correlations.

The mathematical expression of the monogamy constraint for the entanglement is provided by the Coffman-Kundu-Wootters (CKW) conjecture, which indeed represents an approximate sum rule for entanglement correlations. Such conjecture states that \( \tau_2 \leq \tau_1 \), and, although it can be rigorously proved only in the case of three spins, it has always been verified so far in the case of an arbitrary number of spins. Indeed Fig. 2 shows that the CKW conjecture is verified also in the case of our model.

In particular, we interpret the entanglement ratio \( R = \tau_2 / \tau_1 \) as a measure of the fraction of the total entanglement stored in pairwise correlations. This ratio is plotted as a function of the field in Fig. 4. As the field increases, we observe the general trend of pairwise entanglement saturating the whole entanglement content of the system. But a striking anomaly occurs at the quantum critical field \( h_c \), where \( R \) displays a very narrow dip. According to our interpretation, this result shows that the weight of pairwise entanglement decreases dramatically at the quantum critical point in favour of multi-spin entanglement. Indeed, due to the monogamy constraint, multi-spin entanglement appears as the only possible quantum counterpart to long-range spin-spin correlations occurring at a quantum phase transition. The divergence of entanglement range has to be interpreted in the sense that, at a quantum phase transition, finite \( n \)-spin entanglement appears with \( n \rightarrow \infty \) at the expense of the pairwise one. A unique estimator for the \( n \)-spin entanglement with \( n > 2 \) has not been found yet, so that justifying the above statement on a more quantitative level is problematic. Nonetheless strong indications of the relevance of \( n \)-spin entanglement with large \( n \) at a quantum critical point are given in Ref. 8. Finally, the above results evidence the serious limitations of concurrence as a reliable estimate of entanglement at a quantum critical point. In turn, we propose the minimum of the entanglement ratio \( R \) as a novel estimator of the quantum critical point, fully based on entanglement quantifiers.

**VI. TWO-LEG LADDER**

We extend the above analysis of entanglement to the less investigated case of the XYX model on a two-leg ladder, thanks to the fact that the SSE quantum Monte Carlo approach is easily generalizable to any bipartite lattice. In this case the Hamiltonian of Eq. (1) is still expected to display a field-driven quantum phase transition, whose existence is independent of the lattice geometry and it is instead uniquely due to the non-commutativity between the exchange term and the Zeeman term. There is instead no specific reason to expect that the model still displays a perfectly factorized state for geometries other than that of the linear chain.

Fig. 4 shows the one-tangle and the sum of squared concurrences for the XYX model on the two-leg ladder with \( L = 40 \) on each leg and \( \Delta_y = 0 \). We notice that, for such a strong anisotropy, the two-leg ladder does not display a gapped Haldane phase, as shown by the finite value of the magnetization for low fields (inset of Fig. 4). Remarkably, the qualitative behavior of both \( \tau_1 \) and \( \tau_2 \) as a function of the field is the same as in the case of a single chain, and in particular the vanishing of the one-tangle signals the rigorous existence of a factorized state for a lower field than the critical one. The CKW conjecture is verified for all the field values considered, and therefore the entanglement ratio \( \tau_2 / \tau_1 \) can be still interpreted as a measure of the fraction of entanglement stored in pairwise correlations. This quantity, plotted in the inset of Fig. 4, again displays a deep minimum corresponding to the inflection point of the uniform magnetization and therefore marking the quantum critical point.
VII. CONCLUSIONS

In this paper we have shown that entanglement estimators give a precious and novel insight in the ground state properties of lattice $S = 1/2$ spin systems. In the case of anisotropic spin chains with a field-driven quantum phase transition, we have shown that the quantum critical point can be detected through a narrow dip in the pairwise-to-global entanglement ratio. Moreover, unlike the more conventional magnetic observables, entanglement estimators are able to single out the occurrence of an exactly factorized state in these systems. The use of quantum Monte Carlo techniques naturally allows to extend this analysis to different lattice geometries. In particular we have discussed here the case of a two-leg ladder, in which the calculation of entanglement estimators remarkably shows the existence of a factorized state below the quantum critical point. The entanglement ratio displays again a minimum at the critical field, confirming the generality of this feature of the entanglement behavior as a signature of a quantum phase transition. Finally, the proximity of a quantum critical point to the factorized state of the system gives rise to an interesting field-driven entanglement-switch effect. This suggests that many-body effects, driven by a macroscopic parameter as an applied field, are a powerful tool for the control of the microscopic entanglement in a multi-qubit system. The application of this kind of concepts in the design of quantum computing devices looks therefore appealing.

Acknowledgments

Fruitful discussions with L. Amico, T. Brun, P. Delsing, G. Falci, R. Fazio, A. Osterloh, and G. Vidal are gratefully acknowledged. We acknowledge support by DOE under grant DE-FG03-01ER45908 (T.R. and S.H.), by INFN, INFM, and MIUR-COFIN2002 (A.F., P.V., and V.T.).

1. M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge Univ. Press, 2000.
2. S. Sachdev, *Quantum Phase Transitions*. Cambridge University Press, Cambridge (1999).
3. T. J. Osborne and M. A. Nielsen, Phys. Rev. A 66, 032110 (2002).
4. A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) 416, 608 (2002).
5. G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).
6. F. Verstraete, M. Popp, and J. I. Cirac, Phys. Rev. Lett. 92, 027901 (2004); F. Verstraete, M. A. Martin-Delgado, and J. I. Cirac, *ibid.* 92, 087201 (2004).
7. E. Barouch, B. M. McCoy, and M. Dresden, Phys. Rev. A 2, 1075 (1970); *ibid.* 3, 786 (1971).
8. J. Kurmann, H. Thomas, and G. Mueller, Physica A, 112, 235 (1982).
9. D. V. Dmitriev, V. Ya. Krivnov, A. A. Ovchinnikov, and A. Langari, J. Exp. Th. Phys. 95, 538 (2002).
10. F. Capraro and C. Gros, Eur. Phys. J B 29, 35 (2002).
11. J.-S. Caux, F. H. L. Essler, and U. Loew, Phys. Rev. B 68, 134431 (2003).
12. M. Kenzelmann et al., Phys. Rev. B 65, 144432 (2002).
13. T. Delica and H. Leschke, Physica A 168, 736 (1990).
14. O. F. Syljuåsen and A. W. Sandvik, Phys. Rev. E 66, 046701 (2002).
15. T. Roscilde, P. Verrucchi, A. Fubini, S. Haas, and V. Tognetti, Phys. Rev. Lett. 93, 167203 (2004).
16. C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, Phys. Rev. A 54, 3824 (1996).
17. V. Coffman, J. Kundu, and W. K. Wootters, Phys. Rev. A 61, 052306 (2000).
18. L. Amico, A. Osterloh, F. Plastina, R. Fazio, and G. M. Palma, Phys. Rev. A 69, 022304 (2004).
19. W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998).
20. O. F. Syljuåsen, Phys. Rev. A 68, 060301 (2003).