Entanglement and Factorized Ground States in Two-Dimensional Quantum Antiferromagnets

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Making use of exact results and quantum Monte Carlo data for the entanglement of formation, we show that the ground state of anisotropic two-dimensional $S = 1/2$ antiferromagnets in a uniform field takes the classical-like form of a product state for a particular value and orientation of the field, at which the purely quantum correlations due to entanglement disappear. Analytical expressions for the energy and the form of such states are given, and a novel type of exactly solvable two-dimensional quantum models is therefore singled out. Moreover, we show that the field-induced quantum phase transition present in the models is unambiguously characterized by a *cusp minimum* in the pairwise-to-global entanglement ratio R, marking the quantum-critical enhancement of *multipartite* entanglement.

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The study of entanglement in quantum many-body systems is an emerging field of research which promises to shed new light on our understanding of complex quantum models. Entanglement represents indeed a unique form of correlation that quantum states do not share with their classical counterparts, and it thus accounts for the purely quantum aspects of the many-body behavior. Given that collective phenomena show up in a dramatic fashion at phase transitions, the study of entanglement in quantum-critical systems represents an intriguing subject [1,2]. The main focus has been so far the study of spin-1/2 chains, mainly because they provide paradigmatic examples of exactly solvable quantum systems showing a quantum phase transition [3]. Only few studies [4] have explored models in two dimensions and higher, and it is therefore hard to tell to which extent the behavior of entanglement observed at one-dimensional (1D) transitions reflects universal critical features [5].

A similarly intriguing question in this framework is: can we learn anything from entanglement that we did not know already from conventional equilibrium observables? In general, entanglement at $T = 0$ gives a unique insight on the global properties of the ground-state wave function, measuring in a sense how far the quantum ground state sits from any possible classical counterpart. Therefore, entanglement is a powerful tool to detect the occurrence, concrete albeit surprising, of classical-like states in strongly interacting quantum systems.

The aim of this Letter is to show that a proper analysis of entanglement estimators, applied to interacting quantum spin systems in arbitrary dimensions, not only exhibits universal features at continuous quantum phase transitions, but also unveils the occurrence of unexpected ground-state features.

We consider the two-dimensional (2D) antiferromagnetic spin-1/2 XYZ model in a uniform magnetic field:

$$\hat{\mathcal{H}}/J = \sum_{\langle ij \rangle} [\hat{S}_i^x \hat{S}_j^x + \Delta_y \hat{S}_i^y \hat{S}_j^y + \Delta_z \hat{S}_i^z \hat{S}_j^z] - \sum_i \boldsymbol{h} \cdot \hat{\boldsymbol{S}}_i, \quad (1)$$

where $J > 0$ is the exchange coupling, $\langle ij \rangle$ runs over the pairs of nearest neighbors, and $\boldsymbol{h} \equiv g\mu_B \boldsymbol{H}/J$ is the reduced magnetic field. For the sake of simplicity we will hereafter understand the canonical transformation $\hat{S}_i^{x,y} \to (-1)^I \hat{S}_i^{x,y}$ with $I = 1(2)$ for i belonging to sublattice 1(2). Equation (1) is the most general Hamiltonian for an anisotropic spin-1/2 system with exchange spin-spin interactions. However, as real compounds usually display axial symmetry, we will henceforth consider either $\Delta_y = 1$ or $\Delta_z = 1$. Moreover, we will apply the field along the z axis, i.e., $\boldsymbol{h} = (0, 0, h)$. The case $\Delta_y = 1$ corresponds to the XXZ model in a longitudinal field, where no genuine quantum phase transition occurs upon changing the applied field.

This Letter focuses on the less investigated case $\Delta_z = 1$, defining the XYX model in a field. Because of the noncommutativity of the Zeeman and the exchange term, for $\Delta_y \neq 1$ this model is expected to show a field-induced quantum phase transition on any D-dimensional bipartite lattice, with the universality class of the D-dimensional Ising model in a transverse field [6]. The two cases $\Delta_y < 1$ and $\Delta_y > 1$ correspond to an easy-plane (EP) and easy-axis (EA) behavior, respectively. The ordered phase in the EP (EA) case arises by spontaneous symmetry breaking along the x (y) direction, which corresponds to a finite value of the order parameter M^x (M^y) below the critical field h_c. At the transition, long-range correlations are destroyed, and the system is left in a partially polarized state with field-induced magnetization reaching saturation only as $h \to \infty$.

This picture has been verified so far in $D = 1$ only, both analytically [7] and numerically [8,9].

We investigate the ground-state properties of the *XYX* model on a $L \times L$ square lattice making use of stochastic series expansion quantum Monte Carlo (QMC) simulations using a modified version of the directed-loop algorithm [9,10] to account for the low symmetry (Z_2 only) of the Hamiltonian. With this numerical approach we can reach sizes as big as $L = 28$ at very low temperatures ($T/J = 1/2L$), such that the $T = 0$ limit of the model, and, in particular, its quantum-critical behavior, is captured.

The main focus of our simulations is on entanglement properties, analyzed through *one-tangle* and *concurrence*. The one-tangle quantifies the entanglement between a spin and the remainder of the system. It is defined as $\tau_1 = 4\det\rho^{(1)}$, where $\rho^{(1)}$ is the one-site reduced density matrix [11,12]. In terms of the magnetic observables, τ_1 takes the simple form $\tau_1 = 1 - 4\sum_\alpha (M^\alpha)^2$, where $\alpha = x, y, z$, and $M^\alpha \equiv \langle \hat{S}^\alpha \rangle$. The one-tangle represents a *global* estimate of the entanglement in a translationally invariant system, since the vanishing of τ_1 is a necessary and sufficient condition for the ground state to be factorized. The concurrence [13] quantifies the pairwise entanglement between two spins at sites i and j. For the model of interest, in absence of spontaneous symmetry breaking (SSB), the concurrence takes the form [12] $C_{ij} = 2\max\{0, C_{ij}^{(1)}, C_{ij}^{(2)}\}$, where

$$C_{ij}^{(1)} = g_{ij}^{zz} - \frac{1}{4} + |g_{ij}^{xx} - g_{ij}^{yy}|, \quad (2)$$

$$C_{ij}^{(2)} = |g_{ij}^{xx} + g_{ij}^{yy}| - \left[\left(\frac{1}{4} + g_{ij}^{zz}\right)^2 - (M^z)^2\right]^{1/2}, \quad (3)$$

with $g_{ij}^{\alpha\alpha} \equiv \langle \hat{S}_i^\alpha \hat{S}_j^\alpha \rangle$. When SSB occurs, Syljuåsen [14] has shown that Eqs. (2) and (3) remain unchanged if the condition $C_{ij}^{(2)} < C_{ij}^{(1)}$ is satisfied; otherwise Eq. (3) provides an upper bound for the actual concurrence.

One-tangle and concurrence are related by the Coffman-Kundu-Wootters (CKW) conjecture [11] $\tau_1 \geq \tau_2 \equiv \sum_{j\neq i} C_{ij}^2$, which expresses the crucial fact that pairwise entanglement does not exhaust the global entanglement of the system, as entanglement can also be stored in 3-spin correlations, 4-spin correlations, and so on. The fact that n-spin entanglement and m-spin entanglement with $m \neq n$ are mutually exclusive is a unique feature of entanglement as a form of correlation, which puts it at odds with classical correlations. In this respect, if the CKW conjecture is verified, the *entanglement ratio* [9] $R \equiv \tau_2/\tau_1 < 1$ quantifies the relative weight of pairwise entanglement, and its deviation from unity reveals in turn the relevance of n-spin entanglement with $n > 2$. Although indirect, the entanglement ratio is the only accessible estimate of multispin entanglement that we can systematically implement at the moment.

In Fig. 1 we plot τ_1 and τ_2 for the 2D *XYX* model for two values of Δ_y in the EP and the EA case. The most striking feature is the nonmonotonic behavior of both quantities as a function of the field. Although the field is expected to suppress quantum fluctuations and entanglement only in the extreme $h \to \infty$ limit, we observe that there exists an intermediate nontrivial value h_f at which entanglement disappears completely, since τ_1 is vanishing. This signals an *exactly factorized ground state* in the 2D model, completely unknown before. Above the factorizing field h_f both τ_1 and τ_2 have a steep recovery that will later be associated with the occurrence of the quantum phase transition. Finally, we observe that the CKW conjecture is verified for any field value within error bars.

The behavior of the concurrence is found to be qualitatively the same as that observed [9] in $D = 1$ and we do not report it here; however, we underline that also in $D = 2$ its range stays extremely short and that, for all values of Δ_y studied, $C_{ij}^{(1)}$ and $C_{ij}^{(2)}$ cross each other (and vanish simultaneously) at the factorizing field. In particular, for $h > h_f$, $C_{ij}^{(1)} > C_{ij}^{(2)}$, so that Eqs. (2) and (3) are accurate above the factorizing field and all the way to the critical point.

The existence of a factorized ground state in the 1D *XYX* model has been exactly proven in Ref. [15], and its entanglement signature has been studied in Ref. [9]. The evidence for a factorized ground state in $D = 2$, coming from our QMC simulations, leads us to the 2D generalization of the exact proof of factorization: we were indeed able to demonstrate that a factorized ground state exists for the most general Hamiltonian Eq. (1) on any 2D bipartite lattice. The proof will be soon reported elsewhere [16], but we here outline the essential findings.

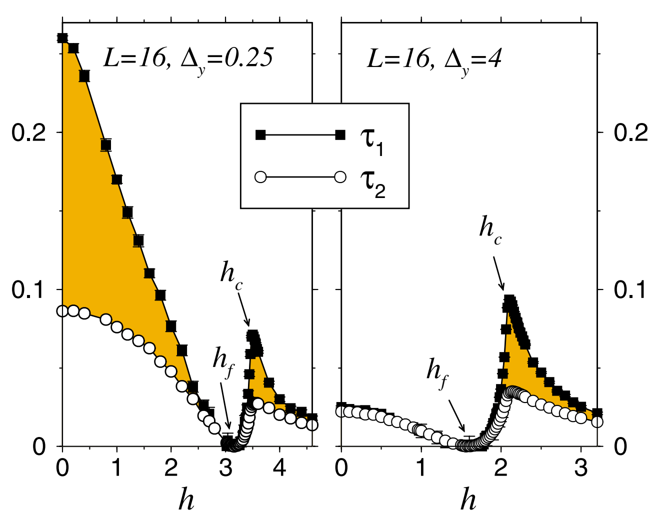

FIG. 1 (color online). One-tangle τ_1 and sum of squared concurrences τ_2 as a function of the applied field for the 2D $S = 1/2$ *XYX* model with $\Delta_y = 0.25$ and $\Delta_y = 4$. The vanishing of τ_1 signals the occurrence of an exactly factorized state, while its spike signals the quantum-critical point.

For any value of the anisotropies Δ_y and Δ_z, there exists an ellipsoid in field space

$$\frac{h_x^2}{(1+\Delta_y)(1+\Delta_z)} + \frac{h_y^2}{(1+\Delta_y)(\Delta_y+\Delta_z)} + \frac{h_z^2}{(1+\Delta_z)(\Delta_y+\Delta_z)} = 4 \qquad (4)$$

such that, when $\boldsymbol{h}$ lies on its surface, the ground state of the corresponding model is factorized, $|\Psi\rangle = \bigotimes_{i=1}^N |\psi_i\rangle$. The single-spin states $|\psi_i\rangle$ are eigenstates of $(\boldsymbol{n}_I \cdot \hat{\boldsymbol{S}})$, $\boldsymbol{n}_I = (\cos\phi_I \sin\theta_I, \sin\phi_I \sin\theta_I, \cos\theta_I)$ being the local spin orientation on sublattice I. We will hereafter indicate with $\boldsymbol{h}_\mathrm{f}$ (*factorizing* field) the field satisfying Eq. (4); at $\boldsymbol{h} = \boldsymbol{h}_\mathrm{f}$, the reduced energy per site is found to be $\epsilon = -(1+\Delta_y+\Delta_z)/2$. In the particular case of $\Delta_z = 1$ and $\boldsymbol{h} = (0, 0, h)$, the factorizing field takes the simple expression $h_\mathrm{f} = 2\sqrt{2(1+\Delta_y)}$. As for the structure of the ground state, the analytical expressions for ϕ_I and θ_I are available via the solution of a system of linear equations. The local spin orientation turns out to be different in the EP and EA cases, being $\phi_1 = 0$, $\phi_2 = \pi$, $\theta_1 = \theta_2 = \cos^{-1}\sqrt{(1+\Delta_y)/2}$ for $\Delta_y < 1$, and $\phi_1 = \pi/2$, $\phi_2 = -\pi/2$, $\theta_1 = \theta_2 = \cos^{-1}\sqrt{2/(1+\Delta_y)}$ for $\Delta_y > 1$.

The numerical and analytical findings for the location of the factorizing field in the 2D *XYX* model as a function of the anisotropy Δ_y are summarized in Fig. 2. In the same figure, we also report the line of quantum-critical fields h_c, extracted through the linear scaling of the spin-spin correlation length, $\xi^{xx}(h = h_\mathrm{c}) \sim L$. The critical scaling of the structure factor $S_{xx}(q = 0) \sim L^{\gamma/\nu - z}$ at the critical field is fully consistent with the best estimates for the critical exponents of the 2D Ising model in a transverse field, $z = 1$, $\gamma = 1.237$, and $\nu = 0.630$ [6,17]. We observe that at the Heisenberg point $\Delta_y = 1$ the critical field and the factorizing field converge to the (noncritical) saturation field $h = 4$.

It is not clear yet, not even in the 1D case, if the occurrence of a factorized ground state is related with that of the quantum phase transition in these models. In this respect we notice that the change in the analytical expression of the concurrence from $C_{ij}^{(2)}$ to $C_{ij}^{(1)}$ at $h = h_\mathrm{f}$ can be related to a qualitative change in the wave function [16] at the level of the phase coherence between any two spins. The factorized ground state could hence represent a crucial step towards a global rearrangement of the ground state, *in view* of the quantum phase transition.

Let us now move to the analysis of the critical behavior of entanglement from the point of view of the entanglement ratio R which, under the validity of the CKW conjecture, provides a new insight in the relative weights of multipartite *versus* bipartite entanglement. Figure 3 shows R as a function of the field for both the EP ($\Delta_y = 0.25$) and the EA ($\Delta = 4$) case. We observe that a pronounced dip, in the form of a cusp, is exhibited at the critical point, signaling a quantum-critical enhancement of multispin entanglement involving n spins with $n > 2$ at the expenses of pairwise entanglement.

The critical features of R in $D = 2$ are surprisingly analogous to those exhibited in the 1D case by the same class of models [9]. Such observation indicates a universal scenario for entanglement at a quantum phase transition. We specialize here to the case of *second-order* quantum phase transitions, assuming that the correct estimator of concurrence is provided by Eqs. (2) and (3), which implies

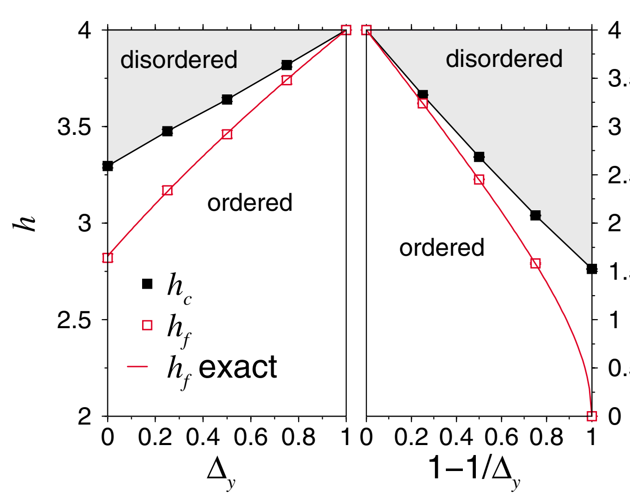

FIG. 2 (color online). Phase diagram of the 2D *XYX* model in a field in the easy-plane case ($\Delta_y < 1$, left panel) and in the easy-axis case ($\Delta_y > 1$, right panel). The squares are the QMC estimates for h_f and h_c.

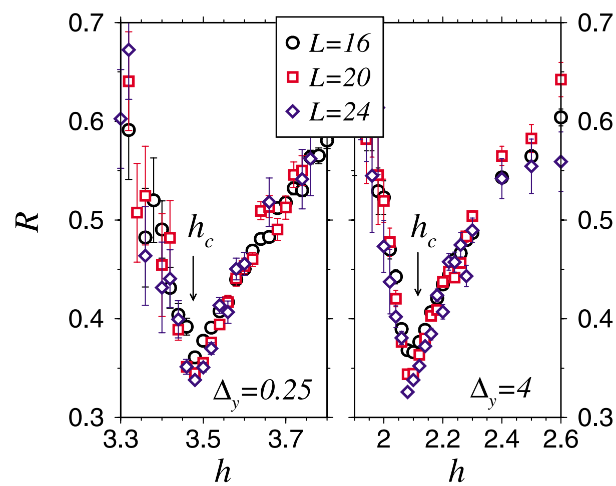

FIG. 3 (color online). Entanglement ratio $R = \tau_2/\tau_1$ around the quantum-critical point of the 2D *XYX* model ($\Delta_y = 0.25$ and $\Delta_y = 4$).

that, if not vanishing, $C_{ij} = g_{ij}^{zz} - \frac{1}{4} + |g_{ij}^{xx} - g_{ij}^{yy}|$. As τ_1 and τ_2 are continuous (and nonvanishing) functions around a quantum phase transition, R is continuous as well, and its critical behavior is best predicted from its derivative with respect to the dimensionless control parameter, hereafter indicated as λ ($\lambda = h$ in the transition under investigation).

At the quantum phase transition, one of the magnetizations, e.g., M^x, will vanish, $M^x \sim (\lambda_c - \lambda)^\beta$ for $\lambda \to \lambda_c^-$. Therefore, the λ derivative of τ_1 for $\lambda < \lambda_c$ contains the term $-\partial_\lambda (M^x)^2 \sim (\lambda_c - \lambda)^{2\beta - 1}$, which diverges to $+\infty$ if $\beta < 1/2$ (i.e., away from the mean-field limit). In presence of an applied magnetic field along, e.g., the z axis, the derivative $-\partial_\lambda (M^z)^2$ can also be divergent, this time to $-\infty$. This is indeed the case for the 1D transverse Ising model [18] where $-\partial_\lambda (M^z)^2 \sim -\ln(\lambda - \lambda_c)$. On the other hand, in the mean-field ($D = \infty$) limit no divergence of the derivative is present, but only a discontinuity jump [19]. Therefore, we expect the singularity in the derivative to become weaker when the dimensionality is increased, as our 2D results suggest when compared with the 1D results of Ref. [9]. This means that, within the Ising universality class and below the upper critical dimension, $\partial_\lambda \tau_1$ is dominated by the power-law divergence to $+\infty$ of $-\partial_\lambda (M^x)^2$. This is *a fortiori* true in the case of phase transitions with $\beta < 1/2$ in which the only "singular" magnetization is the order parameter. For $\lambda \to \lambda_c^+$, instead, $\partial_\lambda \tau_1$ is either finite or, again in presence of a field along the z axis, it might be dominated by the divergence to $-\infty$ of $-\partial_\lambda (M^z)^2$. Therefore τ_1 has a discontinuous derivative at λ_c, and, being a continuous function, it shows a *cusp maximum* at the critical point. This feature witnesses the quantum-critical enhancement of global entanglement, as estimated through τ_1.

On the other hand, τ_2 is essentially a sum of spin-spin correlators $g_{ij}^{\alpha\alpha}$ with $|i - j|$ limited by the very short range of the concurrence [1,9]. It is fair to assume that τ_2 is dominated by the nearest-neighbor (nn) concurrence, which contains the most relevant features for this analysis. In particular, the nearest-neighbor correlators building up the nn concurrence are also the fundamental ingredients of the energy, along with the magnetization M^z in presence of a field. At a $T = 0$ continuous transition the first derivative of the energy w.r.t. λ is continuous, so that either the derivative of the correlators is not singular, or, if a singularity shows up in $\partial_\lambda M^z$, it has to be compensated by an equal and opposite singularity in one of the nn correlators. This suggests that $\partial_\lambda \tau_2$ is at most as singular as $\partial_\lambda M^z$, with the same sign of the possible singularity [1,2].

Finally, we consider $\partial_\lambda R = (\partial_\lambda \tau_2)/\tau_1 - \tau_2(\partial_\lambda \tau_1)/(\tau_1)^2$. For $\lambda \to \lambda_c^-$, if $\beta < 1/2$ and under the condition of $\partial_\lambda M^z$ having a weaker singularity than $\partial_\lambda (M^x)^2$, $\partial_\lambda R$ is dominated by $-\partial_\lambda \tau_1$ with a power-law divergence to $-\infty$. On the other hand, for $\lambda \to \lambda_c^+$, $\partial_\lambda R$ might be nonsingular or, at most, as singular as $\partial_\lambda M^z$, with a divergence to $+\infty$. We therefore obtain that R has derivatives of opposite sign when approaching the critical point from left and right, and, R being a continuous function, $\lambda = \lambda_c$ can only be a *cusp minimum*.

In conclusion, through a systematic study of the entanglement of formation, we have shown that anisotropic $S = 1/2$ quantum Heisenberg antiferromagnets on the square lattice in an arbitrarily oriented uniform magnetic field display an exactly factorized state for a given field $\boldsymbol{h}_f$ [Eq. (4)]. The existence of many real compounds whose magnetic behavior is described by the Hamiltonian Eq. (1) suggests the possibility of an experimental analysis of our findings. Indeed, the existence of a classical-like ground state with flat correlators and absence of quantum fluctuations should lead to striking signatures both in the static and dynamical observables. Finally, we have also shown that the field-induced quantum phase transition occurring in these systems is characterized by critical enhancement of *multipartite* entanglement, in the form of a cusp minimum in the pairwise-to-global entanglement ratio R. Based on general scaling arguments, we conclude that such a cusp in R is a universal entanglement signature of quantum-critical points for continuous quantum phase transitions below the upper critical dimension.

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[1] A. Osterloh *et al.*, Nature (London) **416**, 608 (2002).
[2] T. J. Osborne *et al.*, Phys. Rev. A **66**, 032110 (2002).
[3] E. Barouch *et al.*, Phys. Rev. A **2**, 1075 (1970); **3**, 786 (1971).
[4] O. F. Syljuåsen, Phys. Lett. A **322**, 25 (2004).
[5] L.-A. Wu *et al.*, Phys. Rev. Lett. **93**, 250404 (2004).
[6] B. K. Chakrabarti *et al.*, *Quantum Ising Phases and Transitions in Tranverse Ising Models* (Springer, New York, 1996).
[7] D. V. Dmitriev *et al.*, J. Exp. Theor. Phys. **95**, 538 (2002).
[8] J.-S. Caux *et al.*, Phys. Rev. B **68**, 134431 (2003).
[9] T. Roscilde *et al.*, Phys. Rev. Lett. **93**, 167203 (2004).
[10] O. F. Syljuåsen *et al.*, Phys. Rev. E **66**, 046701 (2002).
[11] V. Coffman *et al.*, Phys. Rev. A **61**, 052306 (2000).
[12] L. Amico *et al.*, Phys. Rev. A **69**, 022304 (2004).
[13] W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).
[14] O. F. Syljuåsen, Phys. Rev. A **68**, 060301 (2003).
[15] J. Kurmann *et al.*, Physica A (Amsterdam) **112**, 235 (1982).
[16] A. Fubini *et al.* (to be published).
[17] A. Pelissetto and E. Vicari, Phys. Rep. **368**, 549 (2002).
[18] Th. Niemeijer, Physica (Amsterdam) **36**, 377 (1967).
[19] P. Pfeuty, Ann. Phys. (N.Y.) **57**, 79 (1970).