Entanglement in a second-order quantum phase transition

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We consider a system of mutually interacting spins 1/2 embedded in a transverse magnetic field which undergoes a second-order quantum phase transition. We analyze the entanglement properties and the spin squeezing of the ground state and show that, contrarily to the one-dimensional case, a cusplike singularity appears at the critical point λ_c in the thermodynamical limit. We also show that there exists a value $\lambda_0 \geqslant \lambda_c$ above which the ground state is not spin squeezed despite a nonvanishing concurrence.

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Entanglement is a truly specific property of the quantum world and one of its deepest signatures, as it was already recognized in the early days of quantum mechanics. It is at the heart of the celebrated Einstein-Podolsky-Rosen (EPR) paradox [1,2] and plays a key role in the measurement problem as well as in the quantum to classical transition [3]. Entanglement is also central in quantum computation [4,5] where the most interesting operations cannot be completely fulfilled through the manipulation of separable states.

Recently, entanglement properties of systems undergoing quantum phase transitions [6] have attracted much attention [7–11]. Interestingly, the concurrence of the ground state, which is related to the entanglement of formation [12], has been shown to be strongly affected at the critical point [7,8]. More precisely, in the one-dimensional (1D) Ising model in a transverse field, Osterloh *et al.* have shown that the derivative of the concurrence with respect to the coupling constant diverges at the transition point [8] although the concurrence itself is not maximum. These pioneering results raise the question of the universality of these behaviors. Apart from 1D quantum spin models, there has been, up to now, no other analysis of the ground-state entanglement in systems displaying quantum phase transitions except in the Kagomé lattice [9]. Actually, the lack of exact solutions especially in higher dimensions implies a numerical treatment which often restricts the study to a small number of degrees of freedom. Such approaches do not allow, in general, an accurate description of the thermodynamical properties.

In this paper, we study the entanglement properties of a quantum system made up of N spins 1/2 on a simplex (each spin interacts with all others) embedded in a magnetic field. The permutation symmetry of this system allows us to restrict the ground-state determination to an N-dimensional subspace and, consequently, to deal with a large number of spins (about 1000). We analyze the concurrence and the spin squeezing of the ground state which are, in this case, closely related [13]. Contrarily to what happens in the 1D Ising model, the concurrence of the ground state is maximum and displays a cusplike singularity at the critical point. Moreover, at the transition point, the ground state is maximally spin squeezed and its squeezing parameter [14] vanishes in the thermodynamical limit. Finally, we show that there exists a special line in the parameter space where the concurrence vanishes and above which the ground state is not spin squeezed although the concurrence is nonzero.

Let us consider the following Hamiltonian first introduced by Lipkin *et al.* [15]:

$$H = -\frac{\lambda}{N}\sum_{i<j}\left(\sigma_x^i\sigma_x^j + \gamma\sigma_y^i\sigma_y^j\right) - \sum_i \sigma_z^i \tag{1}$$

$$= -\frac{2\lambda}{N}\left(S_x^2 + \gamma S_y^2\right) - 2S_z + \frac{\lambda}{2}(1+\gamma), \tag{2}$$

where the σ_α's are the Pauli matrices and $S_\alpha = \Sigma_i \sigma_\alpha^i/2$. We focus here on the ferromagnetic case ($\lambda > 0$) and we mainly consider the case $0 \leqslant \gamma \leqslant 1$. The prefactor $1/N$ is necessary to get a finite free energy per spin in the thermodynamical limit.

The Hamiltonian H preserves the total spin and does not couple states having a different parity of the number of spin pointing in the magnetic field direction, namely:

$$[H, \mathbf{S}^2] = 0, \tag{3}$$

$$\left[H, \prod_i \sigma_z^i\right] = 0, \tag{4}$$

for all γ. In the isotropic case $\gamma = 1$, one further has $[H, S_z] = 0$ so that H is diagonal in the standard eigenbasis $\{|S,M\rangle\}$ of $\mathbf{S}^2$ and S_z.

For any γ, this system displays a second-order quantum phase transition at $\lambda_c = 1$ which is characterized by the mean-field exponents [16,17]. Nevertheless, a mean-field approach cannot provide nontrivial entanglement properties since it essentially turns the Hamiltonian into a sum of single-body Hamiltonians. It is thus necessary to use numerical diagonalizations of H for finite N. The dimension of the Hilbert space is 2^N but the study of the ground state reduces to a problem linear with N since it lies in the fully symmetric representation corresponding to the maximum total spin $S = N/2$. In this subspace spanned by the Dicke states [18] $|M\rangle = |N/2, M\rangle$ with $M = -N/2, \ldots, +N/2$, one has

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$$H|M\rangle=\left[-\frac{\lambda}{N}(1+\gamma)(N^2/4-M^2)-2M\right]|M\rangle - (a^-_{M-1}a^-_M|M-2\rangle+a^+_{M+1}a^+_M|M+2\rangle) \times\frac{\lambda(1-\gamma)}{2N}, \quad (5)$$

where $a^{\pm}_M=\sqrt{(N/2)(N/2+1)-M(M\pm1)}$. In the following, we will denote by $\mathcal{E}_{\pm}$ the orthogonal subspaces spanned by the Dicke states $|M\rangle$, such that $\Pi_i\sigma^i_z|M\rangle=\pm|M\rangle$ which corresponds to even or odd values of $(N/2-M)$.

When $\lambda<\lambda_c$ and for any γ, the ground state is nondegenerate. By contrast, for $\lambda>\lambda_c$, the ground state is doubly degenerate in the thermodynamical limit for any $\gamma\neq1$ but remains unique in the isotropic case ($\gamma=1$). In this limit, the magnetization (per spin) in the z direction of the ground state is simply given by [16,17]

$$\frac{1}{N}\langle S_z\rangle=\frac{1}{2} \quad \text{for } \lambda\leqslant\lambda_c, \quad (6)$$

$$\frac{1}{N}\langle S_z\rangle=\frac{1}{2\lambda} \quad \text{for } \lambda>\lambda_c, \quad (7)$$

for all γ.

To analyze the entanglement properties of the ground state $|\psi\rangle$, we have computed for several values of γ the concurrence introduced by Wootters [12], which is defined as follows. Let us denote by ρ the reduced density matrix obtained from $|\psi\rangle$ by tracing out over $(N-2)$ spins. Of course, in our system, the choice of the two spins kept is irrelevant contrarily to the 1D Ising model [7,8]. Next, we introduce the spin-flipped matrix $\tilde{\rho}=\sigma_y\otimes\sigma_y\rho^*\sigma_y\otimes\sigma_y$ where ρ^* is the complex conjugate of ρ. The concurrence C is then defined by

$$C=\max\{0,\mu_1-\mu_2-\mu_3-\mu_4\}, \quad (8)$$

where the μ_j are the square roots of the four real eigenvalues, classified in decreasing order, of the non-Hermitian product matrix $\rho\tilde{\rho}$. This concurrence vanishes for an unentangled two-body state whereas $C=1$ for a maximally entangled one. Finally, since H couples every spin with each other, the two-body entanglement is somewhat ''diluted'' between all spins and eventually goes to zero in the thermodynamical limit. To get nontrivial information about the entanglement, it is thus crucial to consider the rescaled concurrence $C_R=(N-1)C$ where the prefactor is simply the coordination number of each spin. In symmetric multiqubit systems, this rescaled concurrence has recently been related to the spin squeezing parameter [13]

$$\xi^2=\frac{4(\Delta S_{\vec{n}_\perp})^2}{N}, \quad (9)$$

which measures the spin fluctuations in a correlated quantum state [14]. The subscript $\vec{n}_\perp$ refers to an axis perpendicular to the mean spin $\langle\vec{S}\rangle$ where the minimal value of the variance is obtained. More precisely, for any state belonging to $\mathcal{E}_+$ or $\mathcal{E}_-$, one has

$$\xi^2=1-C_R \quad (10)$$

if the matrix elements of the reduced density matrix ρ written in the standard basis $\{|\uparrow\uparrow\rangle,|\uparrow\downarrow\rangle,|\downarrow\uparrow\rangle,|\downarrow\downarrow\rangle\}$ satisfy $|\rho_{14}|\geqslant\rho_{22}$ [13,19]. In the opposite case, the states are not spin squeezed ($\xi^2=1$).

Let us first recall the results in the isotropic case $\gamma=1$ which is exactly solvable. As it can be straightforwardly obtained from Eq. (5), the (nondegenerate) ground state is the Dicke state $|N/2\rangle$ for $\lambda<\lambda_c$ and switches from one state $|M\rangle$ to a state $|M'<M\rangle$ as λ increases [17]. The concurrence of a Dicke state $|M\rangle$ can be determined analytically [20,21]:

$$C_R=\frac{1}{2N}\{N^2-4M^2-\sqrt{(N^2-4M^2)[(N-2)^2-4M^2]}\}. \quad (11)$$

In the thermodynamical limit, this rescaled concurrence vanishes for $\lambda<\lambda_c$, jumps to 2 at the critical point λ_c, and decreases, by discrete steps, to 1 at large λ. This singular behavior at the transition point is similar to the one obtained in the 1D Ising model [7,8,10,11], except that in this latter case, the nearest-neighbor concurrence $C(1)$ is not maximum at the critical point. Concerning the spin squeezing, its behavior is trivial since all Dicke states are not spin squeezed [20], and no singularity can thus be observed on this quantity at the transition.

For $\gamma\neq1$, the situation is more complex. Indeed, as mentioned above, the ground state is doubly degenerate for $\lambda>\lambda_c$ in the thermodynamical limit so that, in this region, we should, in principle, study the entanglement obtained from the thermal density matrix (at zero temperature)

$$\rho_{\text{th}}=\frac{1}{2}(|+\rangle\langle+|+|-\rangle\langle-|), \quad (12)$$

where $|+\rangle$ and $|-\rangle$ are *any* two orthogonal ground states. Of course, for finite N, the ground state is nondegenerate and lies, depending on λ, either in $\mathcal{E}_+$ or in $\mathcal{E}_-$. In the thermodynamical limit, the reduced density matrices $\rho\pm$ built from the corresponding ground state $|\psi_\pm\rangle$ by tracing out over $(N-2)$ spins become identical. Therefore, we have analyzed the entanglement of the true finite N ground state ($|\psi_+\rangle$ or $|\psi_-\rangle$).

We have displayed in Fig. 1 the rescaled concurrence of the ground state as a function of λ for various anisotropy parameters $0\leqslant\gamma\leqslant1$. For all γ, the rescaled concurrence C_R develops a singularity at the critical point λ_c as already pointed out for $\gamma=1$. However, as can be seen in Fig. 2, the rescaled concurrence goes to 1 in the thermodynamical limit contrarily to the isotropic case where it jumps to 2. More precisely, for all $\gamma\neq1$, one has

$$1-C_R(\lambda_M)\sim N^{-0.33\pm0.01}, \quad (13)$$

$$\lambda_M-\lambda_c\sim N^{-0.66\pm0.01}, \quad (14)$$

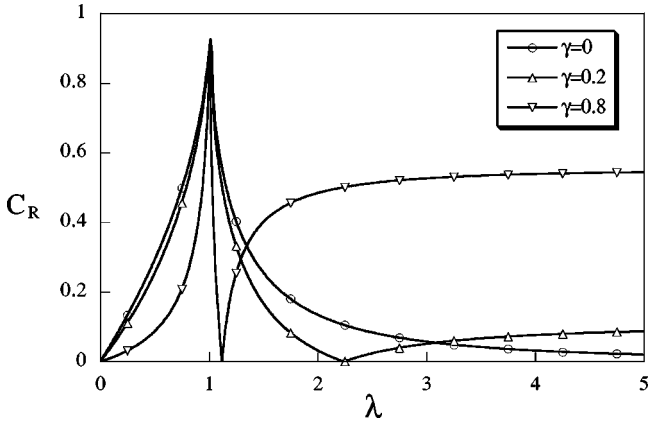

FIG. 1. Rescaled concurrence of the ground state as a function of λ for different values of γ and for $N=1000$.

where λ_M is the value of λ for which C_R is maximum. In the thermodynamical limit, $C_R(\lambda_M)$ goes to 1 while λ_M goes to λ_c so that the ground state is maximally spin squeezed at the critical point ($\xi^2=0$).

To analyze the formation of the singularity at $\lambda=\lambda_c$, we have focused on the case $\gamma=0$ and plotted in Fig. 3 the behavior of $\partial_\lambda C_R$ near the critical point for different values of N.

Denoting by λ'_M (respectively, λ'_m) the value of λ for which $\partial_\lambda C_R$ is maximum (respectively, minimum), one has

$$\partial_\lambda C_R(\lambda'_M)\sim N^{0.33\pm 0.01}, \tag{15}$$

$$\partial_\lambda C_R(\lambda'_m)\sim -N^{0.33\pm 0.03}, \tag{16}$$

$$\lambda_c-\lambda'_M\sim N^{-1\pm 0.01}, \tag{17}$$

$$\lambda'_m-\lambda_c\sim N^{-0.66\pm 0.01}, \tag{18}$$

for all $\gamma\neq 1$ and at large N. In the thermodynamical limit, a real cusplike singularity is thus observed at the quantum critical point. We underline that although we are not able to exactly compute the exponent giving the large-N behaviors of C_R, $\partial_\lambda C_R(\lambda'_M)$, and $\partial_\lambda C_R(\lambda'_m)$, we conjecture that it

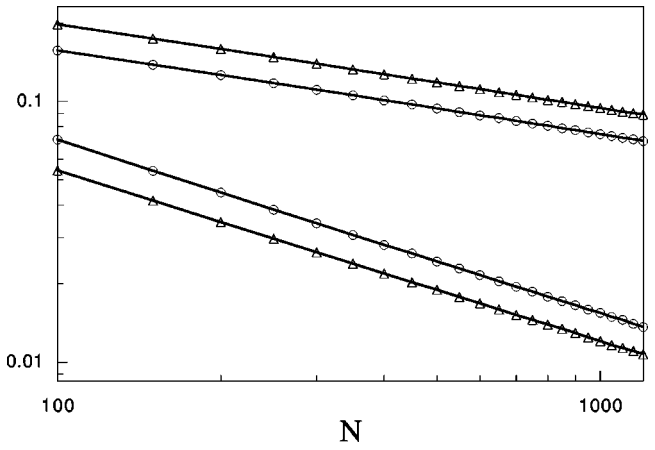

FIG. 2. Behaviors of $1-C_R(\lambda_M)$ (upper curves) and λ_M-1 (lower curves) as a function of N for $\gamma=0$ ($\bigcirc$) and $\gamma=1/2$ ($\triangle$).

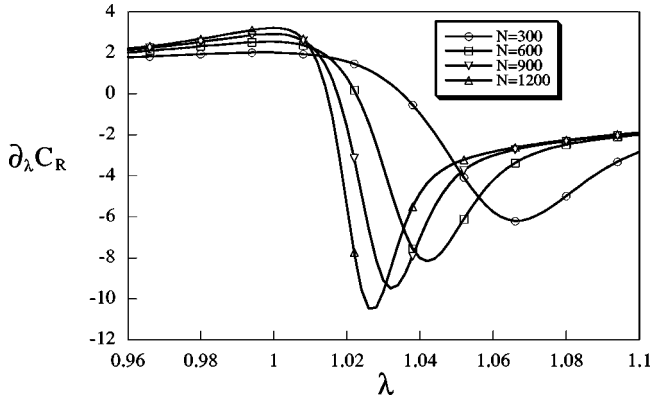

FIG. 3. Finite-N behavior of $\partial_\lambda C_R$ for $\gamma=0$ near the critical point $\lambda_c=1$.

equals 1/3. Note that it is also the one guessed in Refs. [16,17] for the scaling of the magnetization at the critical point.

The behaviors of C_R and $\partial_\lambda C_R$ are notably different from those observed in the 1D case [8]. Indeed, in the fully connected system considered here, C_R and $\partial_\lambda C_R$ are extrema at λ_c whereas in the 1D Ising model, $\partial_\lambda C(1)$ is the only quantity affected by the transition [$C(1)$ is surprisingly maximum below the critical point]. In addition, the scaling behavior of the concurrence and of its derivative are different in both models. This simply reflects the fact that they do not belong to the same universality class as was already known from the calculations of critical exponents.

In the zero-coupling limit ($\lambda=0$), the rescaled concurrence obviously vanishes since the ground state is in this case the fully polarized Dicke state $|N/2\rangle$ and, accordingly, $\xi^2=1$. More interestingly, for $\gamma\neq 0$, there exists another special value $\lambda_0(\gamma)$ for which C_R vanishes. For $\lambda\geqslant\lambda_0(\gamma)$, the rescaled concurrence is nonzero but the ground state is not spin squeezed ($\xi^2=1$), whereas for $\lambda<\lambda_0(\gamma)$, the spin squeezing is given by Eq. (10). This behavior of ξ^2 is due to a change in the sign of $|\rho_{14}|-\rho_{22}$ which is always negative above $\lambda_0(\gamma)$. For $\gamma=0$, such a situation never occurs and the ground state is always spin squeezed. This is a surprising result since it singularizes the case $\gamma=0$, which, from the phase transition viewpoint, belongs to the same universality class as the case $\gamma\neq 0$ [16,17].

We have displayed in Fig. 4 the "critical line" $\lambda_0(\gamma)$. Apart from the very specific case $\gamma=1$ for which the ground state is never spin squeezed, this line is given, in the thermodynamical limit, by $\lambda_0=1/\sqrt{\gamma}$. We emphasize that this formula is also valid for $\gamma>1$ though, in this region, the critical point is readily obtained by a rescaling of the coupling constant and is given by $\lambda_c=1/\gamma$.

At this stage, we do not completely understand why the entanglement properties are so strongly affected by the quantum critical point. In particular, the extremization of the (rescaled) concurrence does not seem to be a generic characteristic since this phenomenon is not observed in the 1D Ising model in a transverse magnetic field [7,8], at least for $C(1)$ [22]. Note, however, that in both models the variation of the concurrence is extremal at λ_c. Although in the present case

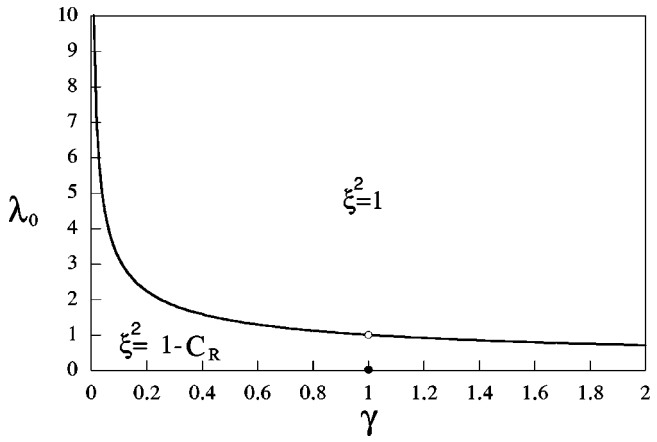

FIG. 4. Phase diagram for the ground-state spin squeezing in the plane (γ,λ_0). Note that for the isotropic case $\gamma=1$, the ground state which is a Dicke state is never spin squeezed ($\xi^2=1$ for any λ).

we have not exactly related the scaling exponent of the entanglement to the critical exponents, there may certainly exist some deep relations between them which deserve further investigations. It would also be interesting to analyze the scaling of the Von Neumann entropy which has been, very recently, related to the central charge of the conformal theory associated with 1D quantum spin models [10,11].

Several important issues remain open. In other systems displaying a quantum phase transition, the behavior of the spin squeezing has never been investigated so far. It would be worth determining whether it is always minimum at the critical point or not. Indeed, if the concurrence is not always maximum at the transition, nothing prevents the spin squeezing from being minimum as is the case in the present study. Another challenging question concerns the quantum dynamics. For nonstationary states, one may wonder how the proximity of a quantum critical point influences the time evolution of the entanglement. For a simple initial state fully polarized along the field direction, we have already some indications that in the fully connected system analyzed here, the rescaled concurrence vanishes, at large times, for $\lambda \geqslant \lambda_c$. Though we cannot assert that it is a generic situation, it is likely that the entanglement of all eigenstates is modified at the critical point and, consequently, the one of any quantum states built from them. Such a study would be of primary interest in exactly solvable models.

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