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Entanglement and quantum phase transition in a mixed-spin Heisenberg chain with single-ion anisotropy

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ABSTRACT

We study the ground-state and thermal entanglement in the mixed-spin $(S, s) = (1, 1/2)$ Heisenberg chain with single-ion anisotropy D using exact diagonalization of small clusters. In this system, a quantum phase transition is revealed to occur at the value $D = 0$, which is the bifurcation point for the global ground state; that is, when the single-ion anisotropy energy is positive, the ground state is unique, whereas when it is negative, the ground state becomes doubly degenerate and the system has the ferrimagnetic long-range order. Using the negativity as a measure of entanglement, we find that a pronounced dip in this quantity, taking place just at the bifurcation point, serves to signal the quantum phase transition. Moreover, we show that the single-ion anisotropy helps to improve the characteristic temperatures above which the quantum behavior disappears.

1. Introduction

In recent years, many efforts have been made to comprehend the relation between entanglement and quantum phase transitions [1–4]. An obvious advantage in determining quantum critical points using measures of entanglement is that we do not require *a priori* knowledge of the order parameter and the symmetries of the system. Most of the systems which have been studied previously are Heisenberg spin-1/2 systems, as there exists a good measure of entanglement for a two-spin system: the concurrence [5], which is applicable to an arbitrary state of two qubits. On the other hand, entanglement in mixed-spin or higher-spin systems has not been well studied, due to the lack of good operational measures of entanglement. There have been several initial studies along this direction [6–8]; however, these works are restricted to the case of only two-particle systems. For the case of general bipartite systems, a non-entangled state has necessarily a positive partial transpose according to the Peres–Horodecki criterion [9,10]. Fortunately, due to the SU(2) symmetry of the Heisenberg Hamiltonian, it can be shown [6] that a positive partial transpose is also sufficient for a separate state in the case of spin mixtures of the type $(S, 1/2)$. This allows us to investigate entanglement features in this kind of mixed-spin system, such as the well-known family of bimetallic chains [11,12] of general formula $ACu(pbaOH)(H_2O)_3nH_2O$ with A = Ni, Co, Fe, Mn, in which the largest spin varies from $S = 1$ to $5/2$.

There are very few papers on the study of entanglement in quantum mixed-spin chain models. Li et al. [13] have considered a polymerized antiferromagnetic mixed-spin chain in which the ground-state entanglement transition found is closely related to the valence-bond solid phase transition. Sun et al. have studied the entanglement properties and their relation to quantum phase transitions in the isotropic [14] and the XXZ anisotropic [15,16] $(1, 1/2)$ spin chain, respectively. Thermal entanglement has also been studied in more general spin mixtures such as the $(S, 1/2)$ and the $(S, 1)$ systems [17–19] ; here, the main interest is focused on the characteristic temperature for an entangled thermal state. The effects of external magnetic fields on the entanglement properties have also received attention recently [20–22], since they play an important role in improving the characteristic temperature and enlarging the region of entanglement in the system.

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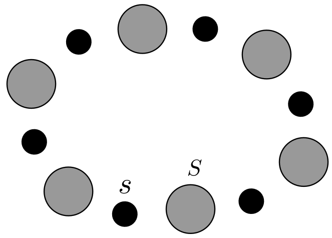

Fig. 1. Schematic representation of an alternating mixed-spin (S, s) chain arranged on a ring.

To the best of our knowledge, entanglement and its relation with quantum phase transitions have never been investigated in mixed-spin chains with single-ion anisotropy. This anisotropy (also known as magnetocrystalline or crystal-field anisotropy) is very realistic from an experimental point of view, and it can be increased locally by adding non-magnetic defects in the system [23]. As an example of this anisotropy in mixed-spin chain compounds, the chain $NiCu(pba)(D_2O)_3 2D_2O$, which has the spin mixture $(1, 1/2)$, would possibly have single-ion anisotropy on the Ni $(S = 1)$ ion [24].

Motivated by the above facts, in this paper we investigate the mixed-spin $(S, s) = (1, 1/2)$ Heisenberg system with single-ion anisotropy D. We chose this particular spin mixture just for computational convenience, but we have shown, using the interacting spin-wave theory together with density matrix renormalization group calculations, that the ground-state properties for general S and s are qualitatively similar [25], so our main results here are expected not to depend on the specific spin mixture. Having said this, the Hamiltonian of our system can be written as

$$\mathcal{H} = J\sum_{j=1}^{N}[\boldsymbol{S}_j \cdot \boldsymbol{s}_j + \boldsymbol{s}_j \cdot \boldsymbol{S}_{j+1} + D(S_j^z)^2], \tag{1}$$

where $\boldsymbol{S}_j$ and $\boldsymbol{s}_j$ are spin operators at the unit cell denoted by j, and we adopt periodic boundary conditions in a system with N unit cells, as sketched in Fig. 1. In what follows, the strength of the exchange interaction J is set to unity. An important result regarding this model (in any dimension) has been obtained recently by Tian and Lin [26]. They rigorously proved that, for an arbitrary bipartite lattice and spin mixture (S, s) with $S > s$, the global ground state is nondegenerate and has the total spin-z component $\mathcal{S}_z = 0$ when $D > 0$. On the other hand, when $D < 0$, the ground state becomes doubly degenerate with $\mathcal{S}_z = \pm N(S-s)$, and each state is antiferromagnetically ordered. When $D = 0$, the model reduces to the isotropic Heisenberg model, whose properties have been thoroughly studied. In particular, the Lieb–Mattis theorem [27] states that the system has total spin $\mathcal{S} = N(S - s)$, and therefore its ground state is highly degenerate. So the value $D = 0$ is a critical (bifurcation) point indicating the reconstruction of the energy spectrum of the system, and we expect that the entanglement, which is closely related to the structure of the ground state, will present a special behavior at the critical point. The aim of this paper is to investigate this characteristic behavior, which serves to indicate the quantum phase transition without reference to any specific order parameter. Moreover, we go beyond the ground state to study the effects of finite temperatures on the entanglement properties of the system. We do this by using the exact diagonalization of the Hamiltonian in Eq. (1) for small clusters.

2. Negativity as a measure of entanglement

In the previous section, we commented that the Peres–Horodecki criterion is very useful in determining whether a state is entangled in high-dimensional bipartite systems. The quantitative version of the Peres–Horodecki criterion was developed by Vidal and Werner [28], who presented a measure of entanglement, called the negativity, that can be computed effectively for any mixed state ρ of an arbitrary bipartite $(\mathcal{A} \otimes \mathcal{B})$ system and does not increase under local manipulations of the system. It essentially measures the degree to which the partial transpose $\rho^{T_\mathcal{A}}$ fails to be positive definite, by summing over its negative eigenvalues μ_i:

$$\mathcal{N}(\rho) = \left|\sum_i \mu_i\right| = \frac{\|\rho^{T_\mathcal{A}}\|_1 - 1}{2}. \tag{2}$$

In the second equality, the trace norm of $\rho^{T_\mathcal{A}}$ is equal to the sum of the absolute values of the eigenvalues of $\rho^{T_\mathcal{A}}$. With this definition, if $\mathcal{N} > 0$, the system is in an entangled state. The negativity has been used to quantify the entanglement in a chain of harmonic oscillators [29,30], in distant regions of XY spin chains at criticality [31], in free one-dimensional Klein–Gordon fields [32], in the spin-chain Kondo model [33], amongst others.

Another quantity which is useful in the investigation of the structure of the ground state is the purity,

$$\mathcal{P}(\rho) = \mathrm{Tr}(\rho^2). \tag{3}$$

This is used to measure the degree of mixedness of a state described by the density operator ρ. For a pure state, we have $\mathcal{P} = 1$, whereas for a maximally mixed state, it reaches a minimum. The relation between entanglement and mixedness has attracted much attention in the last decade [34–38]. In fact, for a composite system in an *global pure state*, the purity is