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Ground-state properties of the one-dimensional antiferromagnetic chain with frustrated side spins

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ABSTRACT

The properties of the one-dimensional antiferromagnetic chain with frustrated side spins are studied by means of the spin wave theory, the exact diagonalization method and the density matrix renormalization group method. The results show that the Lieb–Mattis type ferrimagnetic state is always the ground state when $\alpha < \alpha_{c_1}$. The system undergoes a first-order phase transition accompanied by a spontaneous symmetry breaking and its acoustic excitation spectrum softens completely near $k = 0$ at the critical point α_{c_1}. In the intermediate parameter region $\alpha_{c_1} < \alpha < \alpha_{c_2}$, the ground state is a nonmagnetic state called dimer-tetramer state with a small spin gap. A gapped-gapless Berezinskii-Kosterlitz-Thouless phase transition occurs at another critical point α_{c_2} beyond which the nonmagnetic dimer–monomer state becomes the ground state. The value of the critical point α_{c_2} can be precisely determined not only by the level-spectroscopy method, but also the method based on comparing the magnitude of the two types of correlation functions and the method of a scaling analysis of the gap.

1. Introduction

The study of low-dimensional quantum spin chains with frustration has attracted continuous attraction since Anderson pointed out that there is a close connection between spin liquids and high-Tc superconductivity of strongly correlated systems [1–14]. The classical magnetic order of these quantum spin chains does not usually exist in the quantum case due to the interplay of quantum effects and frustration. One typical example is the one-dimensional spin-1/2 $J_1 - J_2$ chain. Despite its simple structure, the model can be used to describe the properties of the compound $CuGeO_3$ [15]. The classical phase diagram of that model is composed of the Neel phase and the spiral phase. Those two phases are separated by a second-order phase transition at the critical point $\alpha_c = J_2/J_1 = 0.25$ at which the system evolves from the Neel state to the spiral state. However, the two classical phases vanish in the quantum phase diagram of the model [1,2]. As is well known, the ground state (GS) of the model is the disordered gapless spin fluid state in the absence of frustration [1]. Although the model cannot been exactly solved in the presence of the frustration J_2, the past research discloses that the spin fluid phase can extend to a critical point $\alpha_c \approx 0.2411$ beyond which the system is in the famous gapped dimerized state with a valence-bond-crystal order [1,2,16]. The above quantum phase transition is of the Berezinskii-Kosterlitz-Thouless (BKT) type [17]. This type of phase transition was first discovered in the two-dimensional XY model [18,19]. And then people found that the BKT transition also exists in many other spin systems, such as the $S = 1$ XXZ Chains with uniaxial single-ion-type anisotropy and the $S = 1/2$ two-leg XXZ spin ladder system [20,21]. It is very difficult to determine the BKT transition point using traditional method because this type of transition occurs with essential singularity. However, K. Okamoto and K. Nomura succeeded in proposing the level spectroscopy method based on the conformal field theory to solve this difficulty [1].

As the classical magnetic order state is rigorously ruled out in the quantum phase diagram due to quantum fluctuation, a question arises as how to recover the magnetic ordered state of the one-dimensional spin chain. To solve this problem, the impurity spin (called side spin) was added beside the same sublattice of the one-dimensional spin chain as is displayed in Fig. 1(a) in the past research [22]. It is exactly proved that the GS of that model possesses the ferromagnetic long-range order [23]. If one also considers the interaction between the side spin and the next nearest neighbor spin on the chain as is shown in Fig. 1(b), the competition between the interaction between the side spin and the nearest neighbor spin on the chain and that between the side spin and the next nearest neighbor spin on the chain generates frustration. Obviously, the frustration existing in the model presented in Fig. 1 (b) is symmetric in geometry shape. In Ref. [24], we investigate the

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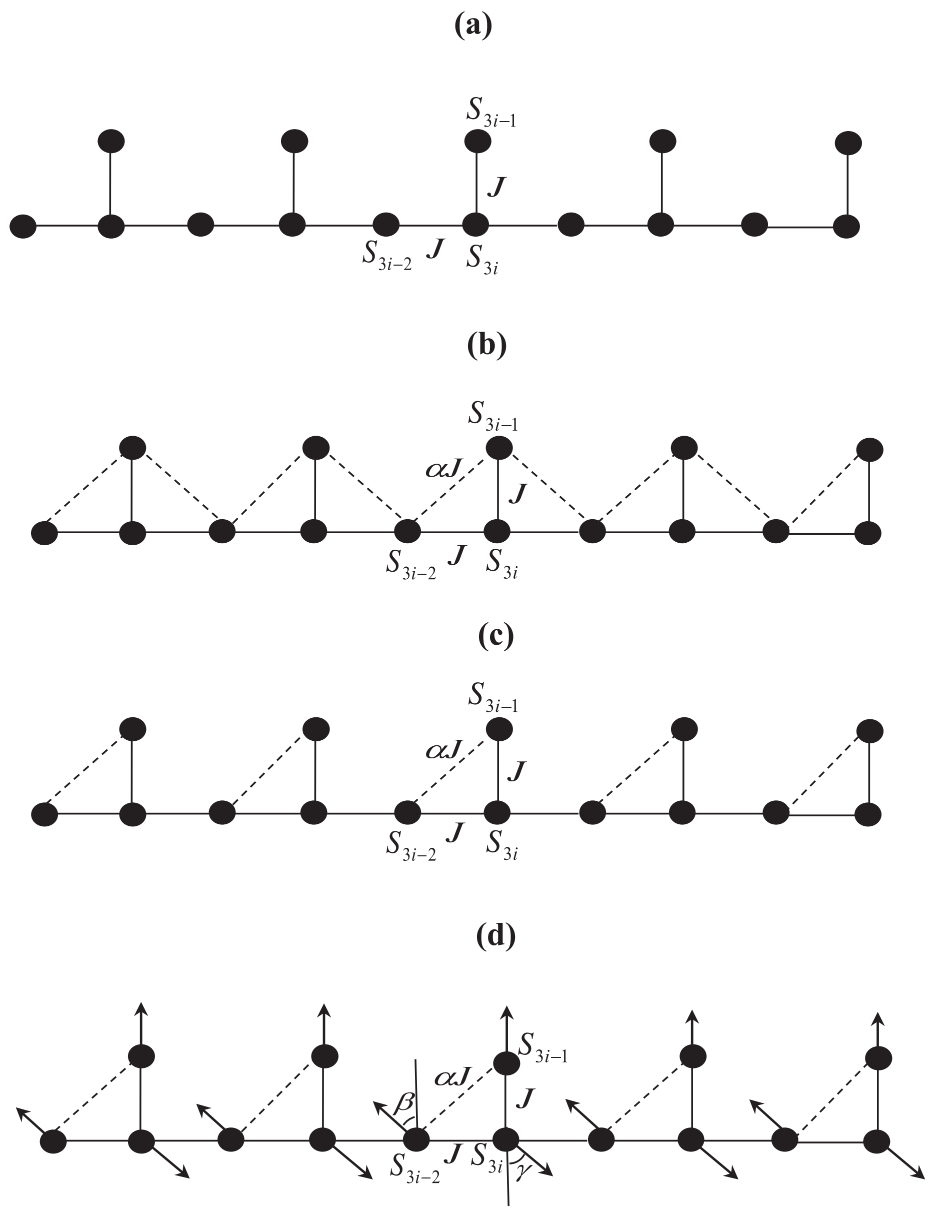

Fig. 1. The structure of the one-dimensional spin chain with side spin studied in Ref. [22] (a), Ref. [24] (b) and the present paper (c). (d) The classical canted state of the model investigated in the present paper. Spins S_{3i-2} (S_{3i}) make angles β (γ) to the z-axis (-z-axis).

properties of the one-dimensional spin chain with side spin with geometrical symmetric frustration. The results show that both the two classical phases of that model which are the ferrimagnetic phase and the canted phase survive in the quantum phase diagram, although the latter only exists in a very narrow parameter region. Besides the above two phases, the model in Fig. 1(b) also has an exotic quantum tetramer-dimer state with no classical counterpart which dominates the GS of that model in most of the parameter spaces.

In the present work, we use the analytical spin-wave theory (SWT), the numerical exact diagonalization (ED) and density matrix renormalization group (DMRG) methods to investigate the properties of the one-dimensional spin chain with side spin with geometrical asymmetric frustration as is shown in Fig. 1(c). The Hamiltonian of the model is

$$H = J\sum_{i=1}^{L}\left(\vec{S}_{3i-2}\cdot\vec{S}_{3i} + \vec{S}_{3i}\cdot\vec{S}_{3i+1} + \vec{S}_{3i-1}\cdot\vec{S}_{3i}\right) + \alpha J\sum_{i=1}^{L}\vec{S}_{3i-2}\cdot\vec{S}_{3i-1} \quad (1)$$

where $\vec{S}_{3i-2}$, $\vec{S}_{3i-1}$ and $\vec{S}_{3i}$ are spin-1/2 operators, L is the number of the unit cells, J ($J > 0$) is the coupling constant along the chain and between the side spin and the nearest neighbor spin on the chain, and αJ ($\alpha \geqslant 0$) is the coupling constant between the side spin and the next nearest neighbor spin on the chain in the same unit cell. For convenience, we set $J = 1$ in what follows. The frustration existing in the model comes from triangles, each consisting of antiferromagnetically interacting three spins. Such kind of frustration was also called geometrical frustration in the past research [25]. The spin systems with geometrical frustration, such as the two-dimensional triangular Heisenberg antiferromagnet and the antiferromagnetically coupled spin triangles chain, have been studied extensively in recent years [26–28]. We note that, in the case of $\alpha = 1$, although the GS properties of model (1) can be obtained accurately by using DMRG under open boundary condition (OBC) in a previous research [28], the spin gap of the model has not been clarified clearly. Thus, that problem needs to be further investigated.