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Investigation of frustrated and dimerized classical Heisenberg chains

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ABSTRACT

We have considered the 1D dimerized frustrated antiferromagnetic (ferromagnetic) Heisenberg model with arbitrary spin S. The exact classical magnetic phase diagram at zero temperature is determined using the LK cluster method. The cluster method results show that the classical ground-state phase diagram of the model is very rich, including first-order and second-order phase transitions. In the absence of dimerization, a second-order phase transition occurs between antiferromagnetic (ferromagnetic) and spiral phases at the critical frustration $\alpha_c = \pm 0.25$, a well-known result. In the vicinity of the critical points α_c, the exact classical critical exponent of the spiral order parameter is found to be $1/2$. In the case of a dimerized chain ($\delta \neq 0$), the spiral order shows stability and exists in some part of the ground-state phase diagram. We have found two first-order phase boundaries separating antiferromagnetic (uud and duu) phases from the spiral phase.

1. Introduction

In recent decades, several classical techniques such as the well-known Luttinger–Tisza method [1] and the vertex model [2] have been introduced to solve for the ground states of the classical Hamiltonian exactly. The Luttinger–Tisza method is more effective in systems with bilinear interactions and the vertex model usually applied for treating the frustrated model [3,4].

In very recent work [5], Kaplan has used a cluster method, hereafter referred to simply as the LK (following the original work of Lyons and Kaplan) method, which is based on a block of three spins, to solve the frustrated classical Heisenberg model in one dimension with added nearest-neighbor biquadratic exchange interactions. He asserted that the LK method is not limited to one dimension or to translationally invariant spin Hamiltonians [6]. This approach was expanded to determine the phase diagram of frustrated classical Heisenberg and XY models with added nearest-neighbor biquadratic exchange interactions in two dimensions [7]. In order to check the validity of Kaplan's phase diagram conjecture, we have investigated his model [5] from a quantum point of view for spin $\frac{1}{2}$ chains with an accurate algorithm (Lanczos method), and our results, which will be presented elsewhere [8], showed that the LK method, albeit a classical approach, has the capability to work for certain aspects of a quantum treatment.

Actually, these are our stimulating reasons to take a quite well-known frustrated and dimerized Heisenberg model and determine its classical ground-state phase diagram exactly with the powerful but not well-known LK method, which is able to solve problems rigorously [5]. Let us start with the definition of the dimerized and frustrated Heisenberg model as follows:

$$H = J_1 \sum_n \left[1 + (-1)^n \delta\right] \mathbf{S}_n \cdot \mathbf{S}_{n+1} + J_2 \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+2}, \tag{1}$$

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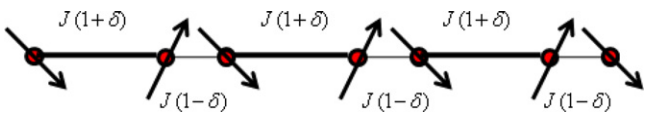

Fig. 1. (Color online) A schematic picture of a dimerized spin chain.

where $\vec{S}_n$ is the nth classical vector of length S. A spin system is frustrated when the global order because of the competition of different kinds of interaction is incompatible with the local order, so chains with both antiferromagnetic–antiferromagnetic exchanges ($J_1 > 0, J_2 > 0$) and ferromagnetic–antiferromagnetic exchanges ($J_1 < 0, J_2 > 0$), hereafter simply AF–AF and F–AF, respectively, are frustrated. We define the frustration parameter $\alpha = \frac{J_2}{J_1}$.

Studies of this model for spin-1/2 and spin-1 chains are extensive and well known [9–17]. It is found that the quantum fluctuations play a very important role at zero temperature in the ground-state phase diagram of the models. This model exhibits a dimerization transition at $\delta = \delta_c$. For $S = 1/2$, the transition point is always $\delta_c = 0$, since the Lieb–Schultz–Mattis theorem implies either gapless excitations or two-fold degeneracy of the ground states at $\delta = 0$. In fact, on the undimerized line $\delta = 0$, for the AF–AF case, there exists a critical frustration parameter $\alpha_c = 0.2411$ [18,19]. For $\alpha < \alpha_c$ the system is a gapless Tomonaga–Luttinger liquid (TLL); that is, the dimerization transition at $\delta = \delta_c = 0$ is of second order. In contrast, for $\alpha > \alpha_c$, the ground state is doubly degenerate, exhibiting a spontaneous dimerization. This implies a first-order dimerization transition at $\delta = \delta_c = 0$. For $S = 1$, on the other hand, $\delta = 0$ (for a small α) belongs to a Haldane phase and does not represent a transition line. Instead, a dimerization transition between the Haldane phase and the dimerized phase occurs [20,21] at a finite δ_c, which depends on the frustration α. Although the shape of the phase diagram is thus different, the topology of the phase diagram is rather similar to that for $S = 1/2$. In fact, also for $S = 1$, there is a critical frustration α_c; the transition is of second order, with the critical point described by a TLL, for $\alpha < \alpha_c$, and is of first order for $\alpha > \alpha_c$.

In spite of the extensive work on the phase diagram of quantum systems, there is no clear picture of different ground-state phases of this model for classical spins. On the one hand, having a classical picture helps us to know how quantum fluctuations destroy or affect different classical ordering. On the other hand, for an arbitrary large spin model, the classical and quantum pictures are the same.

In this work, we focus on 1D frustrated and dimerized systems with arbitrary spin S (see Fig. 1). To find the exact classical ground-state phase diagram of the model, the LK cluster method is used. In the absence of dimerization, by increasing the frustration, a phase transition is known to occur at $\alpha_c = +0.25\ (-0.25)$ from the antiferromagnetic (ferromagnetic) phase into the spiral magnetic phase [5]. Our results show that the dimerization parameter induces new magnetic phases including stripe-antiferromagnetic phases (or uud and duu phases [12]). The existence of these magnetic phases is independent of the length of the spins.

The outline of the paper is as follows. In the next section we will extensively explain the LK method, implementing it to our model, and in Section 3 we will summarize our results.

2. The LK cluster method

In order to implement LK method, we follow exactly the procedure in Ref. [2]. Without loss of generality, and setting periodic boundary conditions, Eq. (1) can be rewritten as

$$H_c = \sum_i h_c\left(\mathbf{S}_{i-1}, \mathbf{S}_i, \mathbf{S}_{i+1}\right), \tag{2}$$

where the "cluster energy" involve three neighboring spins is

$$h_c(\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3) = \frac{J_1}{2}\left\{(1-\delta)\,\mathbf{S}_1 \cdot \mathbf{S}_2 + (1+\delta)\,\mathbf{S}_2 \cdot \mathbf{S}_3\right\} + J_2(\mathbf{S}_1 \cdot \mathbf{S}_3). \tag{3}$$

It is clear that

$$H_c \geq \sum_j \min\ h_c(\vec{S}_{j-1},\ \vec{S}_j,\ \vec{S}_{j+1}). \tag{4}$$

To minimize h_c with respect to the spin directions, we first consider coplanar spins, and label the angles made by the end spins with the central spin θ, θ' (see Fig. 2), which in the coplanar case we set as $\phi = 0$, $\phi' = 0$. The cluster energy is given by

$$h_c(\theta, \theta') = S^2\left\{\left(\frac{1-\delta}{2}\right)\cos\theta + \left(\frac{1+\delta}{2}\right)\cos\theta' + \alpha\cos(\theta - \theta')\right\}, \tag{5}$$

where $\alpha = J_2/J_1$. Minimizing h_c with respect to θ, θ' gives the following equation:

$$\begin{aligned}
\frac{\partial h_c}{\partial \theta} &= -\frac{S^2}{2}\left[(1-\delta)\sin\theta + 2\alpha\sin(\theta - \theta')\right] = 0 \\
\frac{\partial h_c}{\partial \theta'} &= -\frac{S^2}{2}\left[(1+\delta)\sin\theta' - 2\alpha\sin(\theta - \theta')\right] = 0.
\end{aligned} \tag{6}$$