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Basic properties of three-leg Heisenberg tube

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Abstract. We study three-leg antiferromagnetic Heisenberg model with the periodic boundary conditions in the rung direction. Since the rungs form regular triangles, spin frustration is induced. We use the density-matrix renormalization group method to investigate the ground-state properties. We find that the spin excitations are always gapped to remove the spin frustration as long as the rung coupling is nonzero. We also demonstrate a direct observation of spin-Peierls dimerization order in the leg direction. Both the spin gap and the dimerization order are basically enhanced as the rung coupling increases.

1. Introduction

For many years spin ladder systems have attracted much attention. The fundamental properties are well understood when the open boundary conditions are applied in the rung direction: for example, spin- $\frac{1}{2}$ ladders are gapful for an even number of legs and whereas gapless for an odd number of legs (e.g., as a review, see Ref. [1]). However, if the periodic boundary conditions are applied in the rung direction (referred as a spin tube) for odd-leg ladders, the spin states are drastically changed by associating with the occurrence of frustration. At present, there are some experimental candidates for odd-leg spin tubes [2, 3]. Theoretically, it was suggested that all the spin excitations of three-leg Heisenberg tube are gapped due to a frustration-induced spin-Peierls transition [4, 5]. Although further several theoretical studies [6, 7, 8, 9, 10, 11, 12, 13] have been carried out since then, the basic properties of odd-leg spin tube are still open.

2. Model

In general, the low-energy physics of any odd-leg spin tube may be epitomized by that of the three-leg spin tube. Therefore, we consider the three-leg antiferromagnetic Heisenberg tube, the Hamiltonian of which is given by

$$H = J \sum_{\alpha=1}^3 \sum_i \vec{S}_{\alpha,i} \cdot \vec{S}_{\alpha,i+1} + J_{\perp} \sum_{\alpha(\neq\alpha')} \sum_i \vec{S}_{\alpha,i} \cdot \vec{S}_{\alpha',i}, \quad (1)$$

where $\vec{S}_{\alpha,i}$ is a spin- $\frac{1}{2}$ operator at rung i and leg α . J (> 0) is the exchange interaction in the leg direction and J_{\perp} (> 0) is the exchange interaction between the legs (see Figure 1). We take $J = 1$ as the unit of energy hereafter.

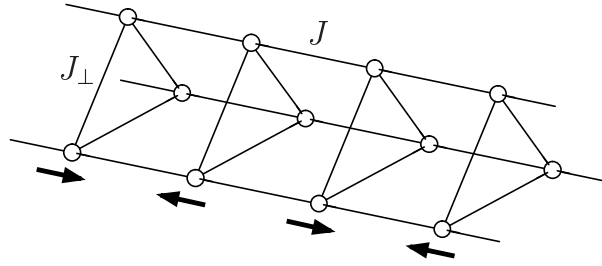


Figure 1. Lattice structure of three-leg Heisenberg tube. The arrows show an example of spin-Peierls distortion.

3. Physical quantities

In this work we employ the density-matrix renormalization group (DMRG) method which provides very accurate data for ground-state properties of one-dimensional quantum systems; for a review, see Refs. 14. We use the DMRG method to calculate the spin gap Δ_σ and the dimerization order parameter D . We study ladders with several kinds of length $L = 24$ to 312 with open-end boundary conditions in the leg direction. We keep up to $m = 2400$ density-matrix eigenstates in the renormalization procedure and extrapolate the calculated quantities to the limit $m \rightarrow \infty$. In this way, the maximum truncation error, i.e., the discarded weight, is less than 1×10^{-7} , while the maximum error in the ground-state energy is less than $10^{-7} - 10^{-6}$.

The spin gap is evaluated by an energy difference between the first triplet excited state and the singlet ground state,

$$\Delta_\sigma(L) = E(L, 1) - E(L, 0), \quad \Delta_\sigma = \lim_{L \rightarrow \infty} \Delta_\sigma(L), \quad (2)$$

where $E(L, S_z)$ is the ground-state energy of a system of length L , i.e., $L \times 3$ ladder, with z -component of the total spin S_z . Note that the number of system length must be taken as $L = 2l$, with $l (> 1)$ being an integer to maintain the total spin of the ground state as $S = 0$. All values of the spin gap shown in this paper are extrapolated to the thermodynamic limit $L \rightarrow \infty$.

Let us then define the dimerization order parameter. Since the translational symmetry is broken due to the Friedel oscillation under the application of the open-end boundary conditions, the dimerized state is directly observable. We are interested in the formation of alternating spin-singlet pairs in the leg direction, so that we calculate the nearest-neighbor spin-spin correlations,

$$S(i) = -\langle \vec{S}_{\alpha,i} \cdot \vec{S}_{\alpha,i+1} \rangle, \quad (3)$$

where $\langle \dots \rangle$ denotes the ground-state expectation value. The results for all α values are equivalent. It is generally known that the Friedel oscillations at the center of the system decay as a function of the system length. If the amplitude at the center of the system persists for arbitrarily long system length, there exists a long-ranged order. It corresponds to the spin-Peierls (dimerized) ground state in our model. We thus define the dimerization order parameter as

$$D = |S(L/2) - S(L/2 + 1)|. \quad (4)$$

It was confirmed that D is almost saturated at $L \geq 120$ in our previous paper [15], so that we here calculate for a system with fixed length $L = 120$. Nonzero value of D indicates a long-ranged spin-Peierls state with finite spin gap.

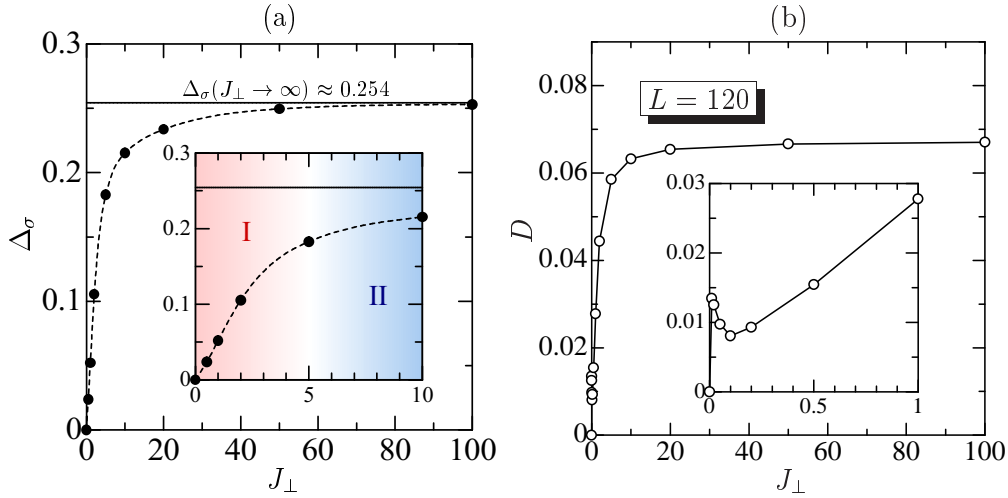


Figure 2. (a) Extrapolated values of spin gap to the thermodynamic limit $L \rightarrow \infty$ as a function of J_{\perp} . The inset shows an expanded view for $0 \leq J_{\perp} \leq 10$. Indices I and II denote on-leg and on-rung regions, respectively (see text). (b) Dimerization order parameter for $L = 120$ as a function of J_{\perp} . The inset shows an expanded view for $0 \leq J_{\perp} \leq 1$.

4. Results

4.1. Spin gap

In Figure 2 (a), we show the DMRG results of the spin gap Δ_{σ} as a function of J_{\perp} . We obtain $\Delta_{\sigma} = 0.254$ in the limit of $J_{\perp} = \infty$. It is rather smaller than a value estimated in Ref. 3 because the finite-size-scaling analysis is different. Roughly speaking, the spin gap increases proportionally to J_{\perp} in the small J_{\perp} (≤ 3) regime and keeps almost constant in the large J_{\perp} (≥ 10) regime. This behavior can be interpreted in terms of different origin of the lowest singlet-triplet excitation for each the J_{\perp} regime, although the mechanism of gap opening is invariant for the entire J_{\perp} regime. Thing is, the spin gap is approximately scaled by a binding energy of most weakly bounded spin-singlet pair in the system and it switches around $J_{\perp} \approx 5$. In fact, most weakly bounded pairs are transferred from on-leg ones in the small J_{\perp} region (on-leg region) to on-rung ones in the large J_{\perp} region (on-rung region) [in the inset of Figure 2 (a), we denote the two regions as I and II, respectively]. A more concrete description is given in the following paragraph.

For $J \ll J_{\perp}$, we can easily imagine that the on-rung spin-singlet pairs must be bounded more solidly than the on-leg ones. The spin gap is therefore scaled by the binding energy of an on-leg pair, i.e., $\Delta_{\sigma} \propto J$. Accordingly, Δ_{σ} is independent of J_{\perp} and it is consistent with the constant behavior of Δ_{σ} with J_{\perp} at $J_{\perp} \geq 10$. On the other hand, the situation is somewhat different for $J_{\perp} < \mathcal{O}(J)$: the bound state of the on-leg pairs is expected to be more solid than that of the on-rung ones. It is because that the system is strongly dimerized even with infinitesimally small J_{\perp} . The dimerization strength develops abruptly at $J_{\perp} = 0^+$ and increases rather slowly with increasing J_{\perp} (see below). Thus, the spin gap is essentially scaled by the binding energy of an on-rung pair. In addition, we may assume that the binding energy of the on-rung pair is proportional to J_{\perp} in the small J_{\perp} regime, by analogy with that of the two-leg Heisenberg system [16]. Now therefore, the spin gap is scaled by J_{\perp} , i.e., $\Delta_{\sigma} \propto J_{\perp}$, which is consistent to a linear behavior of Δ_{σ} with J_{\perp} at $J_{\perp} \leq 3$. Note that the derivative $\partial\Delta_{\sigma}/\partial J_{\perp}$ is very small (~ 0.053) due to strong spin frustration among the intra-ring spins. Consequently, a crossover between the constant Δ_{σ} region and the proportional Δ_{σ} region is seated not at $J_{\perp} \approx 1$ but

around $J_{\perp} \approx 5$. The existence of this crossover has also been confirmed by studying the J_{\perp} dependence of the dynamical spin structure factor [15].

4.2. Dimerization order parameter

We plot the DMRG results of the dimerization order parameter D as a function of J_{\perp} in Fig. 2 (b), where the system size is fixed at $L = 120$. We expect the J_{\perp} -dependence of D to be similar to that of the spin gap Δ_{σ} because the binding energy of spin-singlet pairs would be scaled with the dimerization strength. It is true that the overall behavior seems to be similar to that of the spin gap. However, surprisingly, the dimerization order parameter is discontinuously enhanced when J_{\perp} is switched on as contrasted with the linear increase of the spin gap. Then, the dimerization order parameter goes through a minimum around $J_{\perp} = 0.1$ and increases almost linearly from $J_{\perp} \approx 0.2$ to 5. In the limit of $J_{\perp} \rightarrow \infty$, the dimerization order parameter is saturated to $D \sim 0.0676$.

5. Summary

We study three-leg antiferromagnetic Heisenberg tube with the DMRG method. The spin gap and the dimerization order parameter are estimated as a function of the rung coupling. We suggest that the spin gap is scaled by the binding energy of the on-rung spin-singlet pair in the weak-coupling regime ($J_{\perp} \leq 3$); whereas, it is scaled by the binding energy of the on-leg spin-singlet pair in the strong-coupling regime ($J_{\perp} \geq 10$). Furthermore, we find that the dimerization order parameter is approximately proportional to the spin gap except when the rung coupling is very small. The dimerization strength is abruptly enhanced at $J_{\perp} = 0$.

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