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. We find that the spin excitations are always gapped to remove the spin frustration as long as the rung coupling is nonzero. We also visibly confirm 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 essentially understood when the open boundary conditions are applied in the rung direction. One of the overriding properties is that 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, it has been recognized that the spin states of odd-leg ladders are drastically changed by applying the periodic boundary conditions in the rung direction (referred as a spin tube). 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 is a still open issue.

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

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

where $\vec{S}_{\alpha,i}$ is a spin-$\frac{1}{2}$ operator at rung $i$ and leg $\alpha$. $J$ ($>0$) 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.
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 $\Delta_\sigma$ 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 $m \to \infty$. In this way, the maximum truncation error, i.e., the discarded weight, is less than $1 \times 10^{-7}$, 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,

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

(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 $L \to \infty$.

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,

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

(3)

where $\langle \cdots \rangle$ denotes the ground-state expectation value. The results for all $\alpha$ 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

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

(4)

We confirmed that $D$ is almost saturated at $L \geq 120$ in our previous paper [15], so that in this paper it is calculated for a system with length $L = 120$. Nonzero value of $D$ indicates a long-ranged spin-Peierls state with finite spin gap.
4. Results

4.1. Spin gap
In Figure 2 (a), we show the DMRG results of the spin gap $\Delta_\sigma$ 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 of the different finite-size-scaling analysis. Roughly speaking, the spin gap increases proportionally to $J_\perp$ in the small $J_\perp$ ($\leq 3$) regime and keeps almost constant in the large $J_\perp$ ($\geq 10$) 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 other words, 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, $\Delta_\sigma$ is independent of $J_\perp$ and it is consistent with the constant behavior of $\Delta_\sigma$ with $J_\perp$ at $J_\perp \geq 10$. On the other hand, the situation is somewhat different for $J_\perp \in O(J)$: 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 $\Delta_\sigma$ with $J_\perp$ at $J_\perp \leq 3$. Note that the derivative $\partial \Delta_\sigma / \partial J_\perp$ is very small ($\sim 0.053$) due to strong spin frustration among the intra-ring spins. Consequently, a crossover between the constant $\Delta_\sigma$ region and the proportional $\Delta_\sigma$ region is seated not at $J_\perp \approx 1$ but

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**Figure 2.** (a) Extrapolated values of spin gap to the thermodynamic limit $L \to \infty$ 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 $0 \leq J_\perp \leq 1$. 

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

4.2. Dimerization order parameter
We plot the DMRG results of the dimerization order parameter $D$ as a function of $J_\perp$ in Figure 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 $\Delta_\sigma$ 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 $J_\perp \to \infty$, 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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