Ground State Properties of the $S = 3/2$ Three-Leg Heisenberg Tube

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Abstract. Using the density-matrix renormalization group and exact diagonalization methods the ground-state properties of the $S = 3/2$ three-leg Heisenberg tube with leg ($J_{\parallel}$) and rung ($J_{\perp}$) exchange couplings are studied. We find that the spin-excitation gap associated with a spontaneous dimerization opens in the entire region of the coupling strength, as seen in the $S = 1/2$ three-leg tube. However, in contrast to the case of the $S = 1/2$ tube, the gap develops very slowly with increasing the rung coupling strength in the weak-coupling regime and its size remains only about 5% of the leg coupling strength even at $J_{\perp}/J_{\parallel} = 5$. We also calculate the quantized Berry phase and suggest that there exist three types of the valence-bond-solid states depending on the ratio of leg and rung coupling strengths. Moreover, an effective model is derived by the perturbative expansion to check the numerical results in the strong rung-coupling limit.

1. Introduction

The physics of spin tube has attracted much attention in recent years. So-called “spin tube” is a spin ladder with periodic boundary condition in the rung direction. It has a geometrical frustration if the number of legs is odd and the frustration poses a variety of interesting phenomena. As a simplest example the three-leg spin tube has been extensively studied for $S = 1/2$ [1, 2, 3, 4, 5] and integer-spin [6] cases. Very recently it was reported experimentally that the hexagonal compound CsCrF$_4$, which is an ideal $S = 3/2$ three-leg tube, shows a Tomonaga-Luttinger-liquid behavior at low temperature [7]. However, this observation seems to contradict our theoretical knowledge that a dimerized ground state is obtained for a half-integer spin tube. Therefore, direct investigation of the $S = 3/2$ tube is necessary.

2. Model and method

2.1. Hamiltonian

We consider the three-leg $S = 3/2$ antiferromagnetic Heisenberg tube. The Hamiltonian is given by

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

where $\vec{S}_{\alpha,i}$ is a $S = 3/2$ operator at leg $\alpha (= 1, 2, 3)$ and rung $i$. $J_{\parallel}$ and $J_{\perp}$ are the nearest-neighbor exchange couplings in the leg and rung directions, respectively.
2.2. **Strong-coupling Hamiltonian**

The ground state of a $S = 3/2$ spin triangle is four-fold degenerate with energy $-21J_\perp/4$. Since these four eigenstates are two doublets of spin-1/2 with the left and right chirality corresponding to two momenta $\pm 2\pi/3$, they can be represented by $|\uparrow R\rangle$, $|\uparrow L\rangle$, $|\downarrow R\rangle$ and $|\downarrow L\rangle$ as in the $S = 1/2$ tube [1, 2]. In the strong rung-coupling limit $J_\perp \gg J_\parallel$, we can apply the first-order degenerated perturbation theory and yield an effective Hamiltonian

$$H = \frac{J_\parallel}{3} \sum_i \tilde{S}_i \cdot \tilde{S}_{i+1} \left[ 1 + 16 \left( \tau_+^i \tau_-^{i+1} + \tau_-^i \tau_+^{i+1} \right) \right],$$

(2)

where $\tilde{S}_i$ is the effective $S = 1/2$ operator and $\tau^\pm_+$ are the chirality operators defined by $\tau_+^R = |L\rangle\langle R|$ and $\tau_-^L = |R\rangle\langle L|$. So far, it has been shown that this system is spontaneously dimerized and the spin-excitation gap opens in the ground state [2, 8, 9]. The dependence on spin magnitude appears only in the spin-chirality coupling constant and this effective model is expected to be valid for all half-integer spin cases. We take $J_\parallel = 1$ as the unit of energy from now on.

2.3. **Methods**

In order to investigate the original model (1), we employ the density-matrix renormalization group (DMRG) method [10]. The open boundary condition (OBC) or periodic boundary condition (PBC) are applied in the leg direction as needed. Using the OBC (PBC), we study the tubes with several kind of length $L = 12$ to $48$ ($L = 8$ to $24$) keeping $m = 1200$ to $2600$ ($m = 1600$ to $3200$) density-matrix eigenstates in the renormalization procedure; in this way, the typical truncation error is below $10^{-5}$ ($7 \times 10^{-5}$). All physical quantities calculated in this paper are extrapolated to the limit $m \to \infty$. The extrapolation to the thermodynamic limit $L \to \infty$ is then performed; the maximum error in the ground state energy is estimated to be less than $1 \times 10^{-3}$. Also, we use the exact diagonalization to study the effective model (2) with lengths $L = 4$ to $L = 14$ ($L = 4$ to $L = 16$) for the OBC (PBC).

3. **Results**

For a half-integer spin tube, we may expect a spontaneous dimerization in the ground state. To confirm it in the $S = 3/2$ three-leg tube (1), we calculate the spin-excitation gap and the dimerization order parameter. Furthermore, the topological structure of dimerized ground state is studied by calculating the quantized Berry phase.

3.1. **Spin-excitation gap**

The spin-excitation gap is defined by

$$\Delta = \lim_{L \to \infty} \left[ E_1(L) - E_0(L) \right],$$

(3)

where $E_0(L)$ and $E_1(L)$ are energies of the singlet ground state ($S = 0$) and the first triplet excited state ($S = 1$) for the system with length $L$, respectively. Left panel of Fig. 1 shows the values of $\Delta$ as a function of $J_\perp$. We can see that $\Delta$ is finite in the whole $J_\perp$ regime. However, $\Delta$ seems to develop very slowly for the weak-coupling $J_\perp \lesssim 5$, and increases almost linearly in the intermediate-coupling regime $5 \lesssim J_\perp \lesssim 15$ and then saturates to $\Delta = 0.6661$ in the strong-coupling limit $J_\perp \to \infty$. We also obtain $\Delta = 0.604(2)$ ($\Delta = 0.688(3)$) for the effective Hamiltonian (2) with OBC (PBC) and they are in good agreement with the DMRG result. Since $\Delta = 0.254$ in the $S = 1/2$ tube [4], the gap scales as $\Delta \propto S$ in the strong-coupling limit.
Figure 1. Spin-excitation gap (Left) and dimerization order parameter (Right) as a function of the rung coupling strength $J_{\perp}$. Both of them are extrapolated to the thermodynamic limit $L \rightarrow \infty$. The dotted lines correspond to values obtained from the effective model for strong-coupling limit (2). Insets: extended figures for small $J_{\perp}$. The error bars give differences between the second-order and cubic polynomial fittings for $\Delta(L)$.

3.2. Dimerization order parameter
The dimerization order is characterized by the long-range alternating formation of spin singlet pairs in the leg direction. We focus on the nearest-neighbor spin-spin correlations, $S(i) = -\langle \hat{S}_{\alpha,i} \cdot \hat{S}_{\alpha,i+1} \rangle$, where $\langle \cdots \rangle$ denotes an expectation value in the ground state. Since the translational symmetry is broken for the OBC, the dimerized state is directly observable due to the Friedel oscillation. If the amplitude at the center of the system persists for arbitrarily long system length, it corresponds to a long-ranged dimerization order. Thus, we define the dimerization order parameter as an extrapolated value into the thermodynamic limit,

$$D = \lim_{L \rightarrow \infty} |S(L/2) - S(L/2 + 1)|.$$ (4)

In right panel of Fig. 1, we plot the values of $D$ as a function of $J_{\perp}$. As expected from the analysis of $\Delta$, $D$ increases very slowly in the weak-coupling regime $J_{\perp} \lesssim 5$, almost linearly in the intermediate-coupling regime $5 \lesssim J_{\perp} \lesssim 15$ and saturates to $D = 0.2764$ in the strong-coupling limit. This saturation value is supported by $D = 0.271 (3)$ obtained for the effective Hamiltonian (2) with the OBC.

3.3. Quantized Berry phase
The quantized Berry phase [11] is defined by

$$\gamma = -i \int_0^{2\pi} A(\phi) d\phi,$$ (5)

where $A(\phi)$ is the Abelian Berry connection $A(\phi) = \langle \psi_\phi | \partial_\phi \psi_\phi \rangle$ with the ground state $|\psi_\phi \rangle$ depending on a parameter $\phi$. We introduce a local perturbation by a local twist of the nearest-neighbor connection, $\vec{S}_{\alpha,i} \cdot \vec{S}_{\alpha',j} \rightarrow \frac{1}{2} \left( e^{-i\phi} S^z_{\alpha,i} S^z_{\alpha',j} + e^{i\phi} S^z_{\alpha,i} S^z_{\alpha',j} \right) + S^z_{\alpha,i} S^z_{\alpha',j}$. The Berry phase is quantized as $0$ or $\pi$ (mod $2\pi$) if the system has a gap during the adiabatic continuation and time reversal symmetry. If a gapless excitation exists, the Berry phase is “undefined”. We use the small cluster with $L = 4$ for OBC and evaluate the Berry phase of the leg bond ($\gamma_{\text{leg}}$) for
Figure 2. Schematic pictures of three valence-bond-solid configurations. Each red solid circle and connection with a red line denote a spin-1/2 and a singlet pair, respectively. The large open circle represents the symmetrization of three spin-1/2’s to create a spin-3/2. Three configurations are classified by the Berry phase on the leg bond (\(\gamma_{\text{leg}}\)) and rung bond (\(\gamma_{\text{rung}}\)).

\[ \alpha = \alpha', \quad j = i + 1 \]

and of the rung bond (\(\gamma_{\text{rung}}\)) for \(\alpha \neq \alpha', \quad j = i\). The result is shown in Fig. 2. The crossover among three valence-bond-solid configurations is expected as the ratio \(J_\perp/J_\parallel\) is varied. In the strong-coupling regime, it is natural to consider that the spin excitation arises from breaking the leg bond spin-singlet because \(J_\parallel\) is much weaker than \(J_\perp\). Thus, the saturating behavior of \(\Delta\) can be explained. If we remove one spin-singlet from each rung, we recover the result of the \(S = 1/2\) tube [12] and this is consistent with having the same form of the effective Hamiltonian.

4. Summary

The ground-state properties of the \(S = 3/2\) spin tube are studied using the DMRG method. The results in the strong-coupling limit are confirmed by analysis of the effective Hamiltonian with exact diagonalization. We thus find that both the spin-excitation gap and the dimerization order parameter are finite for the whole \(J_\perp\) regime and, however, they are too small to be measured experimentally in light of typical couplings of real materials. It may give a reasonable explanation to the fact that no gap was observed for CsCrF\(_4\).

Acknowledgments

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