Dimerization transition of three-leg Heisenberg tube

Satoshi Nishimoto
Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, D-01171 Dresden, Germany
E-mail: s.nishimoto@ifw-dresden.de

Mitsuhiro Arikawa
Institute of Physics, University of Tsukuba 1-1-1 Tennodai, Tsukuba Ibaraki 305-8571, Japan
E-mail: arikawa@sakura.cc.tsukuba.ac.jp

Abstract. We study the ground-state properties of three-leg $S = \frac{1}{2}$ Heisenberg tube with antiferromagnetic interleg couplings $J_{\perp} > 0$. The spin gap, dimerization-order parameter, and Berry phase are calculated with the density-matrix renormalization group method. We find that the system is spontaneously dimerized and all the spin excitations are gapped whether intraleg couplings $J_{\parallel}$ are antiferromagnetic or ferromagnetic. Also, the phase diagram is divided into three regimes according to topological configuration of the spin-singlet pairs: (i) Haldane-gap-like regime for $J_{\perp}/J_{\parallel} < 0$, (ii) intraleg-singlet regime $0 < J_{\perp}/J_{\parallel} \leq 5$, and (iii) intrarung-singlet regime for $J_{\perp}/J_{\parallel} \geq 5$.

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 two experimental candidates for odd-leg spin tubes. One of them is vanadium oxide $\text{Na}_2\text{V}_2\text{O}_7$ [2], which may be regarded as a nine-leg Heisenberg spin tube system. The other is three-leg compound $[(\text{CuCl}_2\text{tachH})_3\text{Cl}]\text{Cl}_2$ [3], which is composed of alternating $(\text{CuCl}_2\text{tachH})_3$ triangles along the crystallographic $c$ axis. For the former compound, the first-principle calculations [4, 5] have estimated effective exchange interactions to be antiferromagnetic for the interleg and ferromagnetic for the intraleg couplings.

Theoretically, the spin-tube systems only with antiferromagnetic exchange interactions has been extensively studied. It was suggested that all the spin excitations of three-leg Heisenberg tube are gapped due to a frustration-induced spin-Peierls (or dimerization) transition [6, 7]. Further several studies [8, 9, 10, 11, 12, 13, 14, 15, 16] have been also carried out. However, the cases including ferromagnetic exchange interactions are still open issue.
Figure 1. Berry phases on the rung bond, $\gamma_{\text{rung}}$, and leg bond, $\gamma_{\text{leg}}$. A schematic picture of the valence-bond-solid state for each phase is also shown. Two dots linked by bold line denote a spin-singlet pair.

2. Model and method
For simplicity, we consider a three-leg $S = \frac{1}{2}$ Heisenberg tube; however, it contains the essential features of low-energy physics of any odd-leg spin tube. The Hamiltonian is given by

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

where $S_{\alpha,i}$ is a spin-$\frac{1}{2}$ operator at rung $i$ and leg $\alpha (= 1, 2, 3)$. The parameter $J_\parallel$ is intraleg and $J_\perp (> 0)$ is interleg exchange interactions (see Figure 1). It is known that the system is spontaneously dimerized to avoid intrarung frustration and spin excitations are gapped for $J_\parallel > 0$. In this paper, the case of $J_\parallel < 0$ is also considered. We take $|J_\parallel| = 1$ as the unit of energy hereafter.

The density-matrix renormalization group (DMRG) technique [17] is applied to study the ground-state properties of (1). We investigate tubes with several kinds of length up to $L = 312$, i.e., $L \times 3$ ladder, under the open boundary conditions (OBC) in the leg direction. The density-matrix eigenstates up to $m = 2400$ are kept in the renormalization procedure and all quantities are extrapolated to the limit $m \to \infty$. In this way, the discarded weight is less than $1 \times 10^{-7}$, while the maximum error in the ground-state energy is less than $10^{-7} - 10^{-6}$.

3. Physical quantities
In order to explore the presence or absence of the dimerization transition for $J_\parallel < 0$, we calculate the spin gap and dimerization-order parameter. Furthermore, we investigate the quantized Berry phase for determining topological configuration of spin-singlet pairs in the spin-gapped ground state.

3.1. Spin gap
The spin gap $\Delta$ is evaluated by an energy difference between singlet ground state and first triplet excited state,

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

where $E(L, S_z)$ is the ground-state energy of a system of length $L$ with the $z$-component of total spin $S_z$. We note that the system length must be taken as $L = 2l$, with $l(> 1)$ being an integer to maintain total spin of the ground state as $S = 0$.

3.2. Dimerization-order parameter
The dimerization order is characterized by long-range alternation of nearest-neighbor spin-spin correlations, $S(i) = - \langle S_{\alpha,i} \cdot S_{\alpha,i+1} \rangle$, where $\langle \cdots \rangle$ denotes the ground-state expectation value.
We plot the results of \( \Delta = 0 \) insets are extended figures for (a) \(-2 \leq J_\perp/J_\parallel \leq 1 \) and (b) \(-2 \leq J_\perp/J_\parallel \leq 0.5 \).

Since the translational symmetry is broken under the OBC, the dimerized state is directly observable due to the Friedel oscillation. In general, the amplitude of Friedel oscillation at the center of system decays as a function of system size. If the amplitude persists for arbitrarily large system size, there exists a long-range order. Thus, we define the dimerization-order parameter as

\[
D = \lim_{L \to \infty} |S(L/2) - S(L/2 + 1)|. \tag{3}
\]

Nonzero value of \( D \) indicates the dimerization (or spin-Peierls) order in our model (1).

3.3. Berry phase
The Berry phase is defined by

\[
\gamma = -i \int_0^{2\pi} A(\phi) d\phi, \tag{4}
\]

where \( A(\phi) \) is the Abelian Berry connection, \( A(\phi) = \langle \psi_\phi | \partial_\phi \psi_\phi \rangle \) with the ground state \( |\psi_\phi \rangle \) [18]. The Berry phase is quantized as 0 or \( \pi \) (mod \( 2\pi \)) if the system has spin gap during the adiabatic continuation and time reversal symmetry ; and “undefined” if a gapless excitation exists. We introduce a local perturbation by a local twist of the nearest-neighbor connection, \( \vec{S}_{\alpha,i} \cdot \vec{S}_{\alpha',j} \to \frac{1}{2} (e^{-i\phi} S_{\alpha,i} S_{\alpha',j} + e^{i\phi} S_{\alpha,i} S_{\alpha',j}^* ) + S_{\alpha,i}^z S_{\alpha',j}^z \). In this paper, we pick up a dimerized pair of triangles, including six spins, and evaluate the Berry phase of the leg bond \( (\gamma_{\text{leg}}) \) for \( \alpha = \alpha', j = i + 1 \) and of the rung bond \( (\gamma_{\text{rung}}) \) for \( \alpha \neq \alpha', j = i \).

4. Results
4.1. Spin gap
In Figure 2 (a), the results of \( \Delta \) as a function of \( J_\perp/J_\parallel \) are shown. We see that the spin gap opens except at \( J_\parallel = 0 \). For both \( J_\parallel > 0 \) and \( J_\parallel < 0 \), roughly speaking, \( \Delta \) starts to increase proportionally to \( J_\perp \) and shift into almost constant for larger \( J_\perp \). It means that the lowest singlet-triplet excitation is approximately scaled by \( J_\perp \) in the small (large) \( J_\parallel \) regime, though the mechanism of gap opening is invariant for the entire \( J_\parallel \) regime. In fact, the spin gap in \( J_\perp/J_\parallel < 0 \) is about a factor of 6 smaller than that in \( J_\perp/J_\parallel > 0 \). Consequently, we obtain \( \Delta = 0.0437 \) in the limit of \( J_\perp/J_\parallel = -\infty \); \( \Delta = 0.254 \) in the limit of \( J_\perp/J_\parallel = \infty \).

4.2. Dimer-order parameter
We plot the results of \( D \) as a function of \( J_\perp/J_\parallel \) in Figure 2 (b). As expected, the \( J_\perp \)-dependence of \( D \) looks similar to that of \( \Delta \) but except when \( |J_\perp/J_\parallel| \) is small. It is because that the binding energy of spin-singlet pairs is scaled with the dimerization strength. Let us now see the small \( |J_\perp/J_\parallel| \) regime. The behaviors of \( D \) are quite different between \( J_\perp/J_\parallel > 0 \) and \( J_\perp/J_\parallel < 0 \): in
the former case, $D$ is discontinuously enhanced when $J_\perp$ is switched on, then goes through a minimum around $J_\perp = 0.1$, and increases almost linearly from $J_\perp \approx 0.2$ to 5; in the latter case, $D$ increases gradually with increasing $J_\perp$ like $D \sim \exp[-O(1/J_\perp)]$. In the limit of $J_\perp \rightarrow \infty (-\infty)$, $D$ is saturated to $D \sim 0.0673 (0.0183)$.

4.3. Berry phase

Figure 1 shows the Berry phase on the rung and leg bonds of couple of two triangles. We find that there are three kinds of phases dependently on $J_\perp/J_\parallel$. For antiferromagnetic $J_\parallel$, the spin excitations are always gapped and there exists a reconstruction of the valence bonds at $J_\perp/J_\parallel \approx 5$. This is consistent with a crossover between the constant $\Delta$ region and the proportional $\Delta$ region around $J_\perp/J_\parallel \approx 5$. For ferromagnetic $J_\parallel$, the valence bond are detected on the rung bond and the gapless excitation ($S = 1$) is involved in the leg bond; however, the spin excitations are gapped in bulk limit as shown above. If the coupled triangles are connected along the leg direction, the Haldane state could be realized as seen in the $S = 1$ Heisenberg model.

5. Summary

Using the DMRG method, we study the ground-state properties of three-leg Heisenberg tube with antiferromagnetic interleg exchange interactions. We confirm that all the spin excitations are gapped for both antiferromagnetic and ferromagnetic intraleg exchange interactions. Also, we find that there exist three phases according to topological configuration of the spin-singlet pairs: (i) Haldane-gap-like regime for $J_\parallel < 0$, (ii) intraleg singlet regime $0 < J_\parallel \leq 5$, and (iii) interleg singlet regime for $J_\parallel \geq 5$.

Acknowledgments

The work was supported in part by Grants-in-Aid for Scientific Research, Grant No.20654034 from JSPS and No.220029004 (Physics of New Quantum Phases in Super-clean Materials) and No.20046002 (Novel States of Matter Induced by Frustration) on Priority Areas from MEXT (Japan).

References

[1] Dagotto E and Rice T M 1996 Science 271 618; Dagotto E 1999 Repts. Prog. Phys. 62 1525.
[2] Millet P, Henry J Y, Mila F, and Galy J 1999 J. Solid State Chem. 147 676.
[3] Seeber G, Kogerler P, Kariuki B M, and Cronin L 2004 Chem. Commun. (Cambridge) 2004 1580.
[4] Mazurenko V V, Mila F, and Anisimov V I 2006 Phys. Rev. B 73 014418.
[5] Zaharko O, Gavilano J L, Strassle Th, Miclea C F, Mota A C, Filinchuk Y, Chernyshov D, Deen P P, Rahaman B, Saha-Dasgupta T, Valenti R, Matsushita Y, Donni A, and Kitazawa H 2008 Phys. Rev. B 78 214426.
[6] Schulz H J 1996 Correlated Fermions and Transport in Mesoscopic Systems, edited by T. Martin, G. Montambaux and T. Trân Thanh Vân (Editions Frontiers, Gif-sur-Yvette, France) 1996 p. 81.
[7] Kawano K and Takahashi M 1997 J. Phys. Soc. Jpn. 66 4001.
[8] Sakai T, Matsumoto M, Okumichi K, Okamoto K, and Sato M 2005 Physica E 29 633; Sakai T, Sato M, Okumichi K, Otsuka Y, Okamoto K, Ito C 2008 Phys. Rev. B 78 184415.
[9] Cabra D C, Honecker A, and Pujol P 1997 Phys. Rev. Lett. 79 5126.
[10] Cabra D C, Honecker A, and Pujol P 1998 Phys. Rev. B 58 6241.
[11] Citro R, Oregina E, Andrei N, Ito C, and Qin S J. Phys.:Condens. Matter 12, 3041 (2000).
[12] Sato M and Sakai T 2007 Phys. Rev. B 75 014411; Sato M 2007 Phys. Rev. B 75 174407.
[13] Lüscher A, Noack R M, Misguich G, Kotov V N, and Mila F 2004 Phys. Rev. B 70, 060405(R).
[14] Okumishi K, Yoshikawa S, Sakai T, Miyashita S 2005 Prog. Theor. Phys. Suppl. 159 297.
[15] Fouet J B, Läuchli A, Pilgram S, Noack R M, and Mila F 2006 Phys. Rev. B 73 014409.
[16] Nishimoto S and Arikawa M 2008 Phys. Rev. B 78 054421.
[17] White S R 1992 Phys. Rev. Lett. 69 2863; 1993 Phys. Rev. B 48 10345.
[18] Hatsugai Y 2006 J. Phys. Soc. Jpn. 75 123601.