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0- and 2/3-magnetization plateaus in three-leg antiferromagnetic Heisenberg spin-1/2 ladders with leg-dimerization

Rui-Xue Li [a], Shu-Ling Wang [a], Yun Ni [a], Kai-Lun Yao [a,b,*], Hua-Hua Fu [a]

[a] School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, Wuhan 430074, China
[b] International Center of Materials Physics, Chinese Academy of Sciences, Shenyang 110015, China

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ABSTRACT

Magnetic properties of three-leg antiferromagnetic Heisenberg spin-1/2 ladders with different dimerization patterns have been studied using the bond mean-field theory. Our results show that rung-columnar ladders are thermodynamically stable states for large rung-to-leg coupling ratios. Magnetization curves of leg-columnar and leg-staggered ladders always exhibit 0- and 2/3-magnetization plateaus, which do not appear in rung-columnar and rung-staggered ladders. In leg-dimerized ladders, the formation of spin dimers in the three legs results in the appearance of the 0- and 2/3-magnetization plateaus. Spin configuration in the 2/3-magnetization plateau can be understood from the mean-field bond parameters.

1. Introduction

The antiferromagnetic Heisenberg ladders have attracted a significant attention in the past decades as a relatively ideal model for revealing the transitional behavior from one-dimensional chain to two-dimensional square lattice [1–4]. Many compounds of such ladder structure have been realized experimentally, and lots of theoretical techniques have been explored to study them [3–12]. Due to the special ladder structure, spin ladders with open boundary condition (OBC) in rung direction have unusual low-energy excitations which are dependent on the number of legs. It has been observed that spin-1/2 ladders with even legs have gapped low-energy excitations while odd-leg spin ladders have gapless low-energy excitations [3,5,13–18]. Spin ladders with periodic boundary condition (PBC) in rung direction are usually called spin tubes. With theoretical analysis and numerical calculation, it is found that for the strong-rung coupling regime, odd-leg spin-1/2 tubes have gapped ground-states due to the frustration along the rung [14,19–22].

Much effort has been made to study the critical and gapped phases in the *N*-leg ladders [13,18,22]. Strong-rung three-leg spin ladders with OBC in rung direction have a magnetization plateau at one-third of the saturation magnetization (1/3-magnetization plateau). Except for the 1/3-magnetization plateau, strong-rung three-leg spin tubes can have additional plateaus at zero and two-third of the saturation magnetization (0- and 2/3-magnetization plateaus) [19–26]. Other examples include three-leg ladders with leg-columnar dimerization which have a gap in the low energy spectrum. Three-leg ladders with leg-staggered dimerization have gapped ground-state except at the quantum critical point where a quantum phase transition occurs as the rung-to-leg coupling ratio and the leg-dimerization parameter change [27–29]. However, the magnetic properties of leg-dimerized three-leg ladders have not been studied yet and very little is known about the rung-dimerized three-leg ladders, so it is necessary to consider.

Here, we concentrate on the three-leg spin ladders with leg- and rung-dimerizations, as shown in Fig. 1. The ground-states and magnetic properties of three-leg ladders with different dimerization patterns are investigated. This paper is organized as follows: In Section 2, we study the dimerized three-leg ladders in a uniform magnetic field using the bond mean-field theory (BMFT). In Section 3, the ground-state energy and magnetization are presented. Mean-field bond parameters are plotted to understand the spin configuration in the plateau states. In the end, conclusions are drawn in Section 4.

2. Model and method

The Hamiltonian of the three-leg spin ladders with dimerizations is given by

* Corresponding author at: School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, Wuhan 430074, China. Tel.: +86 27 87558523; fax: +86 27 87556264.
E-mail address: klyao@mail.hust.edu.cn (K.-L. Yao).

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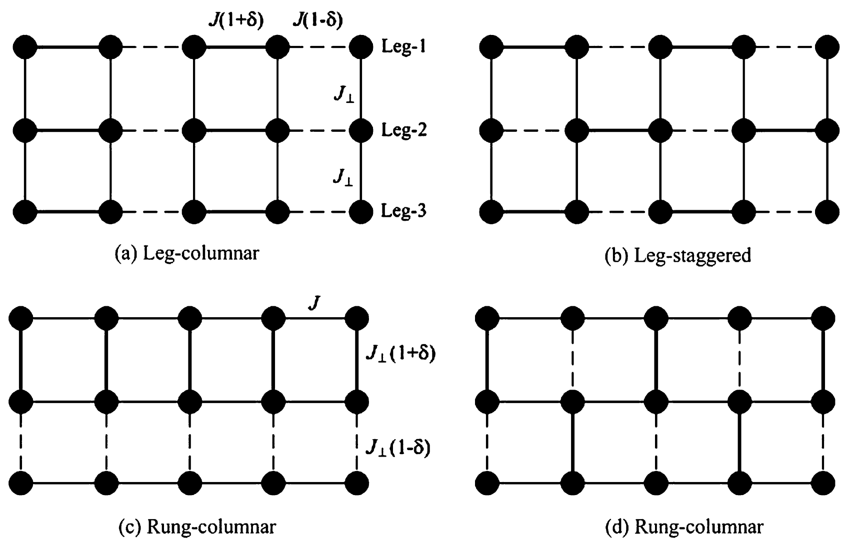

Fig. 1. Three-leg spin ladders with different dimerization patterns: (a) leg-columnar; (b) leg-staggered; (c) rung-columnar; (d) rung-staggered.

$$\begin{aligned} H_{3L} = {} & \sum_{a=1}^{3}\sum_{n=1}^{N} J_a(n) S_a(n) S_a(n+1) \\ & + \sum_{a=1}^{2}\sum_{n=1}^{N} J_{\perp a}(n) S_a(n) S_{a+1}(n) \\ & - g\mu_B B \sum_{a=1}^{3}\sum_{n=1}^{N} S_a^z(n). \end{aligned} \tag{1}$$

The dimerization patterns are defined as

$$J_a(n) = J\big[1+(-1)^{n+a}\delta\big], \quad J_{\perp a}(n) = J_\perp \quad \text{(leg-staggered)}, \tag{2}$$

$$J_a(n) = J\big[1+(-1)^{n}\delta\big], \quad J_{\perp a}(n) = J_\perp \quad \text{(leg-columnar)}, \tag{3}$$

$$J_a(n) = J, \quad J_{\perp a}(n) = J_\perp\big[1+(-1)^{a}\delta\big] \quad \text{(rung-columnar)}, \tag{4}$$

$$J_a(n) = J, \quad J_{\perp a}(n) = J_\perp\big[1+(-1)^{n+a}\delta\big] \quad \text{(rung-staggered)}, \tag{5}$$

$J>0$ and $J_\perp>0$ are the antiferromagnetic Heisenberg exchange couplings along the legs and the rungs, respectively. In the following discussions, we set $J=1.0$ as the energy unit and $\alpha = J_\perp/J$ is the rung-to-leg coupling ratio. δ is the dimerization parameter. B is the applied magnetic field, g is the Landé factor, and μ_B designates the Bohr magneton. We define $h = g\mu_B B$ for simplicity. PBC along the legs and OBC in the rung direction are adopted.

Using the two-dimensional generalized Jordan–Wigner transformation mentioned in Ref. [30], the spin operators at different sites are written as follows:

$$\begin{aligned} & S_1^-(n) = c_{n,1} e^{i\phi_{n,1}}, \quad \phi_{n,1} = \pi \sum_{d=0}^{n-1}\sum_{f=1}^{3} n_{d,f}, \\ & S_2^-(n) = c_{n,2} e^{i\phi_{n,2}}, \quad \phi_{n,2} = \phi_{n,1} + \pi n_{n,1}, \\ & S_3^-(n) = c_{n,3} e^{i\phi_{n,3}}, \quad \phi_{n,3} = \phi_{n,2} + \pi n_{n,2}, \\ & S_a^z(n) = c_{n,a}^+ c_{n,a} - \frac{1}{2} = n_{n,a} - \frac{1}{2}. \end{aligned} \tag{6}$$

The Hamiltonian (1) can be changed to

$$\begin{aligned} H_{3L} = {} & \sum_{a=1}^{3}\sum_{n=1}^{N} \frac{J_a(n)}{2}\big(c_{n,a}^+ e^{-i\phi_{n,a}} c_{n+1,a} e^{i\phi_{n+1,a}} + \text{h.c.}\big) \\ & + \sum_{a=1}^{3}\sum_{n=1}^{N} J_a(n)\left(c_{n,a}^+ c_{n,a} - \frac{1}{2}\right)\left(c_{n+1,a}^+ c_{n+1,a} - \frac{1}{2}\right) \\ & + \sum_{a=1}^{2}\sum_{n=1}^{N} \frac{J_{\perp a}}{2}\big[c_{n,a}^+ e^{-i\phi_{n,a}} c_{n,a+1} e^{i\phi_{n,a+1}} + \text{h.c.}\big] \\ & + \sum_{a=1}^{2}\sum_{n=1}^{N} J_{\perp a}\left(c_{n,a}^+ c_{n,a} - \frac{1}{2}\right)\left(c_{n,a+1}^+ c_{n,a+1} - \frac{1}{2}\right) \\ & + g\mu_B B \sum_{a=1}^{3}\sum_{n=1}^{N}\left[c_{n,a}^+ c_{n,a} - \frac{1}{2}\right]. \end{aligned} \tag{7}$$

The hopping terms of Hamiltonian (7) can be rewritten using the BMFT, which approximates the sum of the phase differences by $\pi, 0, \pi, 0$ along the legs [25,30–34]. The quartic Ising terms are decoupled using the mean-field bond parameters [27,31,33]. Take leg-columnar for example, the mean-field bond parameters are below:

$$Q_{1S} = \langle c_{2n,a} c_{2n,a}^+ \rangle, \quad a = 1,3 \quad \text{(for stronger bonds in leg-1 and leg-3)}, \tag{8}$$

$$Q_{1W} = \langle c_{2n+1,a} c_{2n+1,a}^+ \rangle, \quad a = 1,3 \quad \text{(for weaker bonds in leg-1 and leg-3)}, \tag{9}$$

$$Q_{2S} = \langle c_{2n,a} c_{2n,a}^+ \rangle, \quad a = 2 \quad \text{(for stronger bonds in leg-2)}, \tag{10}$$

$$Q_{2W} = \langle c_{2n+1,a} c_{2n+1,a}^+ \rangle, \quad a = 2 \quad \text{(for weaker bonds in leg-2)}, \tag{11}$$

$$P = \langle c_{n,a} c_{n,a+1}^+ \rangle, \quad a = 1,2 \quad \text{(for rung)}. \tag{12}$$

After the Fourier transformation and Bogoliubov transformation, the Hamiltonian (7) can be diagonalized. Then the correlation functions and magnetizations can be obtained using the self-consistent numerical calculations.

3. Results and discussions

As shown in Fig. 2, the ground-state energies of dimerized three-leg spin ladders have been compared. For a certain rung-to-leg coupling ratio α, the ground-state energies of the three-leg spin ladders with four different dimerization patterns decrease with increasing δ. For small α ($\alpha = 1.0$), the leg-dimerized spin ladders have lower ground-state energies than the rung-dimerized spin ladders, and the leg-columnar spin ladders which