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Quantum phase transition and magnetic plateau in three-leg antiferromagnetic Heisenberg spin ladder with unequal J_1–J_2–J_1 legs

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ABSTRACT

Magnetic properties of spin-1/2 antiferromagnetic three-leg Heisenberg ladders, where antiferromagnetic interactions in legs are J_1, J_2 and J_1 respectively and in the rungs are $J_\perp$, have been investigated by bond-mean field method. As $J_\perp$ changes, magnetization curves show different behavior. For $J_\perp$=0.5, there are cusps in magnetization curves, while for $J_\perp$=3.0, the 1/3 magnetization plateau appears, which can be explained by energy spectra. Furthermore, for $J_\perp$=3.0 the 1/3 magnetization plateaus will become wider or narrow down with J_2 changing. In addition, the mean-field bond parameters and the concurrences, which confirm the phase transitions, are also studied.

1. Introduction

Low dimensional magnetic systems have attracted much attention due to their various fascinating magnetic properties and thermodynamic behavior in the past decades [1–5]. Particularly, spin chains and spin ladders which are typical systems have been investigated theoretically and experimentally [1,2,6–16], and it has been found that the ladders with even legs have gapped low-energy excitations while odd-leg ladders are gapless [3,4,7].

Much effort has been made to study the spin-1/2 Heisenberg ladders, which have interesting phenomena related to magnetization plateau, quantum critical properties and spin excitation behavior [2,4,6–8,11,12,17–21]. Herein, one of particular interests is the magnetic field induced quantum phase transitions (QPTs). For two leg spin ladders, investigations on both strong-rung spin ladders ($(C_5H_{12}N)_2CuBr_4$ ($(Hpip)_2CuBr_4$) [17] and strong-leg spin ladders ($(C_7H_{10}N)_2CuBr_4$ (DIMPY) [12] under different magnetic field have furthered the understanding of their phase diagram. Besides, the quantum criticality in the three-leg ladders have been also studied widely, by bond-mean-field theory (BMFT), density-matrix renormalization group (DMRG) technique, and the strong-coupling series expansion [2,4,18–20,22]. In 2008, Azzouz et al. calculated the magnetic field dependence of bond parameters and magnetization in S=1/2 three-leg antiferromagnetic Heisenberg ladders, and found that the plateau at one third of the saturation magnetization appears only when the rung-to-leg coupling exceeds a threshold value [18]. Moreover, the Spin-Peierls instability in the three-leg ladder coupled to phonons has also been studied [20–22]. Numerical results showed that the leg-dimerizations antiferromagnetic three-leg spin ladders have column and staggered dimerized patterns, and the column dimerized presented lower zero temperature energies [20]. In 2014, the three-leg ladders with leg- and rung-dimerizations have also been discussed [8]. However, studies on spin ladders with unequal legs are lacked, except several investigations about the asymmetric zigzag ladders [23,24].

Here, we concentrate on the three-leg spin ladders with unequal J_1–J_2–J_1 legs, as shown in Fig. 1. Our goal is to study the magnetic process of ladders with unequal legs, and obtain the field-induced multiple-point quantum criticality. This paper is organized as follows: In Section 2, we study the three-leg ladder in a uniform magnetic field using the bond mean-field theory (BMFT). In Section 3, the field dependence of magnetization and the mean-field bond parameters for different rung interaction are investigated. To explain the distinct features of the magnetic curves, we also plot the energy spectrum. Moreover, in order to confirm the appearance of the quantum phase transition, the entanglements are presented. In Section 4, conclusions are drawn.

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2. Model and method

The Hamiltonian for the three-leg spin ladders with different couplings along the legs is

$$H=\sum_{i}^{N}\left\{J_1 S_{i,1}S_{i+1,1}+J_2 S_{i,2}S_{i+1,2}+J_1 S_{i,3}S_{i+1,3}+\sum_{j=1}^{2}J_{\perp}S_{i,j}S_{i,j+1}\right\}-g\mu_B B\sum_{i}^{N}\sum_{j}^{3}S_{i,j}^{z} \quad (1)$$

where the index $i=0, 1,\ldots, N-1$ labels the N sites on each of the legs and $j=1$, 2, and 3 labels the legs. The periodic boundary conditions are chosen along the leg direction and the open boundary conditions along the rung direction. $J_1>0$, $J_2>0$ and $J_{\perp}>0$ are the antiferromagnetic Heisenberg exchange coupling constants along the chains and the rungs, respectively. For convenience, we define the reduced magnetic field $h=g\mu_B B$.

Using the two-dimensional generalized Jordan–Wigner transformation [25], the spin operators at site of the three legs are written as follows:

$$S_{i,1}^{-}=c_{i,1}e^{i\phi_{i,1}},\quad \phi_{i,1}=\pi\sum_{d=0}^{i-1}\sum_{f=1}^{3}n_{d,f}$$
$$S_{i,2}^{-}=c_{i,2}e^{i\phi_{i,2}},\quad \phi_{i,2}=\phi_{i,1}+\pi n_{i,1}$$
$$S_{i,3}^{-}=c_{i,3}e^{i\phi_{i,3}},\quad \phi_{i,3}=\phi_{i,2}+\pi n_{i,2}$$
$$S_{i,j}^{z}=c_{i,j}^{+}c_{i,j}-\frac{1}{2} \quad (2)$$

where $n_{i,j}=c_{i,j}^{+}c_{i,j}$ is the occupation operator for the JW fermions. The hopping terms of Eq. (1) are written using the BMFT, which approximates the sum of the phase differences by π, 0,π, 0 along the legs [18,25,26]. After the JW transformation, the Hamiltonian (1) becomes

$$\begin{aligned}H=\sum_i J_1[&\tfrac{1}{2}(c_{2i,1}^{+}c_{2i+1,1}e^{i\pi}+c_{2i-1,1}^{+}c_{2i,1}+h.c.)+\\&(c_{2i,1}^{+}c_{2i,1}-\tfrac{1}{2})(c_{2i+1,1}^{+}c_{2i+1,1}-\tfrac{1}{2})\\&+(c_{2i-1,1}^{+}c_{2i-1,1}-\tfrac{1}{2})(c_{2i,1}^{+}c_{2i,1}-\tfrac{1}{2})]\\&+J_2[\tfrac{1}{2}(c_{2i-1,2}^{+}c_{2i,2}e^{i\pi}+c_{2i,2}^{+}c_{2i+1,2}+h.c.)+\\&(c_{2i,2}^{+}c_{2i,2}-\tfrac{1}{2})(c_{2i+1,2}^{+}c_{2i+1,2}-\tfrac{1}{2})\\&+(c_{2i-1,2}^{+}c_{2i-1,2}-\tfrac{1}{2})(c_{2i,2}^{+}c_{2i,2}-\tfrac{1}{2})]\\&+J_1[\tfrac{1}{2}(c_{2i,3}^{+}c_{2i+1,3}e^{i\pi}+c_{2i-1,3}^{+}c_{2i,3}+h.c.)+\\&(c_{2i,3}^{+}c_{2i,3}-\tfrac{1}{2})(c_{2i+1,3}^{+}c_{2i+1,3}-\tfrac{1}{2})\\&+(c_{2i-1,3}^{+}c_{2i-1,3}-\tfrac{1}{2})(c_{2i,3}^{+}c_{2i,3}-\tfrac{1}{2})]\\&+J_{\perp}[\tfrac{1}{2}(c_{2i,1}^{+}c_{2i,2}+c_{2i-1,1}^{+}c_{2i-1,2}+c_{2i,2}^{+}c_{2i,3}\\&+c_{2i-1,2}^{+}c_{2i-1,3}+h.c.)\\&+(c_{2i-1,1}^{+}c_{2i-1,1}-\tfrac{1}{2})(c_{2i-1,2}^{+}c_{2i-1,2}-\tfrac{1}{2})\\&+(c_{2i,1}^{+}c_{2i,1}-\tfrac{1}{2})(c_{2i,2}^{+}c_{2i,2}-\tfrac{1}{2})\\&+(c_{2i-1,2}^{+}c_{2i-1,2}-\tfrac{1}{2})(c_{2i-1,3}^{+}c_{2i-1,3}-\tfrac{1}{2})\\&+(c_{2i,2}^{+}c_{2i,2}-\tfrac{1}{2})(c_{2i,3}^{+}c_{2i,3}-\tfrac{1}{2})]\\&-g\mu_B B\sum_i\sum_{j=1}^{3}(c_{i,j}^{+}c_{i,j}-\tfrac{1}{2})\end{aligned} \quad (3)$$

We employ the equations of motion method to calculate the retarded Green's function [27,28] for JW fermions, which is described as

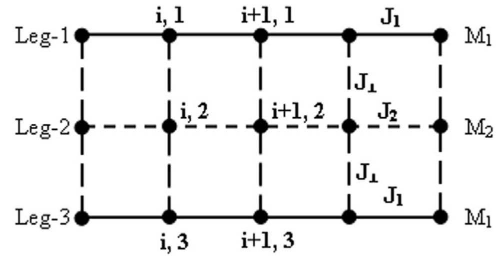

Fig. 1. The three-leg ladder with unequal J_1–J_2–J_1 legs. J_1, J_2 are the antiferromagnetic Heisenberg exchange integral along leg-1(3) and leg-2. $J_{\perp}$ is the antiferromagnetic Heisenberg exchange integral along the rung.

$$G_{ij}(t-t')=\ll a_i(t);\,b_j^{+}(t')\gg\;=-i\theta(t-t')\langle a_i b_j^{+}+b_j^{+}a_i\rangle \quad (4)$$

where the subscripts i and j label lattice sites. After the time Fourier transformation, the Green's function is put into the equation of motion,

$$\omega\ll a_i;\,b_j^{+}\gg\;=\langle[a_i;\,b_j^{+}]_{+}\rangle+\ll[a_i,H];\,b_j^{+}\gg \quad (5)$$

By using the equation of motion similar as Eq. (5) for the higher-order Green's function $\ll[a_i, H];\, b_j^{+}\gg$, it will generate the higher-order Green's function, giving rise to an infinite set of coupled equations.The quartic Ising terms are treated by Hartree–Fock approximation using the bond parameters $Q_1=\langle c_{2i,1}c_{2i+1,1}^{+}\rangle=\langle c_{2i,3}c_{2i+1,3}^{+}\rangle$ for leg-1(3) and $Q_2=\langle c_{2i,2}c_{2i+1,2}^{+}\rangle$ for leg-2, $P=\left\langle c_{i,j}c_{i,j+1}^{+}\right\rangle$ is along the rungs [18,25,26],

$$\begin{aligned}&\left(c_{i,j}^{+}c_{i,j}-\frac{1}{2}\right)\left(c_{i+1,j}^{+}c_{i+1,j}-\frac{1}{2}\right)=\\&\langle c_{i,j}c_{i+1,j}^{+}\rangle c_{i,j}^{+}c_{i+1,j}+\langle c_{i+1,j}c_{i,j}^{+}\rangle c_{i+1,j}^{+}c_{i,j}\\&+\langle c_{i,j}c_{i+1,j}^{+}\rangle\langle c_{i+1,j}c_{i,j}^{+}\rangle+\langle c_{i+1,j}^{+}c_{i+1,j}\rangle c_{i,j}^{+}c_{i,j}\\&+\langle c_{i,j}^{+}c_{i,j}\rangle c_{i+1,j}^{+}c_{i+1,j}-\langle c_{i+1,j}^{+}c_{i+1,j}\rangle\langle c_{i,j}^{+}c_{i,j}\rangle\\&-\tfrac{1}{2}c_{i+1,j}^{+}c_{i+1,j}-\tfrac{1}{2}c_{i,j}^{+}c_{i,j}+\tfrac{1}{4}\end{aligned} \quad (6)$$

For further Fourier transformation into momentum space, the Green's function can be expressed as

$$G_{ij}=\frac{1}{N}\sum_k g(k)e^{ik(i-j)} \quad (7)$$

The integral of the wave vector k is along the chain direction. So, the momentum space Green's function $g(k,\omega)$can be characterized as a function of wave vector k and the elementary excitation spectrum $\omega=\omega(k)$.

According to the standard spectral theorem, the correlation function of the fermion operators can be obtained by,

$$\langle b_j^{+}a_i\rangle=\frac{i}{2\pi N}\sum_k e^{ik(i-j)}\int\frac{d\omega}{e^{\beta\omega}+1}[g(k,\omega+io^{+})-g(k,\omega-io^{+})] \quad (8)$$

where $\beta=\frac{1}{k_B T}$, k_B and T are the Boltzman's constant and the absolute temperature, respectively.

The concurrence of the bipartite quantum state characterizing the quantum entanglement, can be calculated as

$$C=\max\{0,\ \lambda_1-\lambda_2-\lambda_3-\lambda_4\} \quad (9)$$

where λ_1, λ_2, λ_3, λ_4 are square roots of the eigenvalues of $\tilde{\rho}_{ij}\rho_{ij}$ with descending order. $\tilde{\rho}_{ij}=(\sigma_i^{y}\otimes\sigma_j^{y})\rho_{ij}^{*}(\sigma_i^{y}\otimes\sigma_j^{y})$ and σ_i^{y} is the y component of the Pauli operator. ρ_{ij}^{*} is the complex conjugation of reduced density matrix ρ_{ij} [29–31]. Herein, the reduced density matrix ρ_{ij} are the correlation functions, which can be obtained by Green's function method, and in the conventional basis $\{|\uparrow\uparrow\rangle,|\uparrow\downarrow\rangle,|\downarrow\uparrow\rangle,|\downarrow\downarrow\rangle\}$, it can take the form