Numerical Diagonalization Study on the S=1/2 Frustrated Three-Leg Quantum Spin Ladder Systems

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Abstract. The spin ladder systems have attracted a lot of interest in the field of low-dimensional physics. It is well known that the $S=1/2$ two-leg spin ladder has a spin gap, while the three-leg one has a gapless spin liquid ground state. Some spin liquid behaviors were observed in the recent experiments of some frustrated systems; the distorted triangular lattice and kagome lattice antiferromagnets etc.. Thus we consider the $S=1/2$ three-leg spin ladder system with the next-nearest-neighbor interaction to investigate the effect of frustration on the spin liquids. Using the exact numerical diagonalization of finite-cluster systems, we study the ground state of this system. The phase diagram with respect to some exchange interaction constants is presented. It is revealed that sufficiently large next-nearest-neighbor coupling leads to a ferrimagnetic phase, which has a frustration-induced spontaneous magnetization. In addition we find two spin liquid phases, one of which corresponds to a Néel-like spin configuration and the other a collinear spin configuration. As a result of the numerical study, we find a new phase which is different from three phases.

1. Introduction

The spin liquid has attracted a lot of interest, since the resonating valence bond was proposed as a mechanism of the high temperature superconductivity\cite{1, 2}. Recently a spin liquid-like behavior was observed in the organic triangular-lattice quantum spin system\cite{3}. In the system the spin frustration and the quantum fluctuation interplay to create the spin liquid state. The $S=1/2$ three-leg spin ladder\cite{4} is one of typical systems with the gapless spin liquid ground states. In this paper, we investigate the $S=1/2$ three-leg spin ladder model with the next-nearest-neighbor interaction, to consider a role of the frustration in the spin liquid. Using the exact numerical diagonalization, we calculate the low-lying energy levels to present the ground-state phase diagram.

2. Model

We consider the $S=1/2$ frustrated three-leg spin ladder, as shown in Fig. 1, described by the Hamiltonian,

$$H = J_l \sum_{i=1}^{3} \sum_{j=1}^{L} \vec{S}_{i,j} \vec{S}_{i,j+1} + J_r \sum_{i=1}^{2} \sum_{j=1}^{L} \vec{S}_{i,j} \vec{S}_{i+1,j} + J_d \sum_{i=1}^{2} \sum_{j=1}^{L} \vec{S}_{i+1,j} \vec{S}_{i,j+1},$$

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Figure 1. The structure of the $S = 1/2$ frustrated three-leg spin ladder. Open circles denote the locations of $S = 1/2$ spins. The AF exchange interaction constants $J_r$, $J_l$ and $J_d$ are for the neighboring spin pairs along rung, legs and diagonals viewed as the solid, broken dotted and dashed lines, respectively.

Figure 2. Schematic ground states of the $S = 1/2$ frustrated three-leg spin ladder expected for some extreme values of AF exchange interaction constants. Up arrows and down arrows are the $S_z = 1/2$ up spins and down spins in the figure. (a) $J_d \preceq J_l, J_r$. The ground-state is the Néel-like spin liquid. (b) $J_r \preceq J_l, J_d$. The ground state is the collinear spin liquid. (c) $J_l \preceq J_r, J_d$. The ground-state is the ferrimagnetic.

where $\vec{S}_{i,j}$ is the spin-$1/2$ operator and $L$ is the length of the ladder in the leg direction. The Antiferromagnetic(AF) exchange interaction constant, $J_l$, is for the neighboring spin pairs along the legs, while $J_r$ and $J_d$ are the rung and diagonal coupling constant, respectively.

3. Method
Using exact numerical diagonalization, we calculate the low-lying energy levels for finite-size systems. ($L = 4, 6, 8$.) When we calculate the energy levels for various AF-exchange parameters ($J_r, J_l, J_d$), we use the spin quantum number $S$ and wave number $k$ to identify each states. We evaluate the value of $S$ from the degree of degeneracy with respect to $S^z$. We decide a critical point of quantum phase transition by comparing some energy eigenvalues. Finally, we use all of numerical result to make a phase diagram.

4. Results
4.1. Expected phases
One can expect several different phases in the ground state for some extreme values of the coupling constants. In the limit that $J_d \preceq J_l, J_r$, the ground state is the Néel-like spin liquid as shown in Fig. 2(a). In the Néel-like spin liquid phase, the neighboring spin pairs along the legs and rungs tend to be antiparallel to each other. In the limit that $J_r \preceq J_l, J_d$, the ground state is the collinear spin liquid as shown in Fig. 2(b). In the collinear spin liquid phase, the
As a result from the numerical calculation, we make the phase diagram of \( S = 1/2 \) frustrated three-leg spin ladder with three AF-exchange interaction constants, as shown in Fig. 3. All of the phase boundaries correspond to first-order transitions, detected as level crosses in the ground state. Three phases discussed in Sec. 4.1. are shown as (I) the Néel-like spin liquid phase, (II) the collinear spin liquid phase and (III) the ferrimagnetic phase in Fig. 3. In our current study, we find the new phase shown as (IV) in Fig. 3. The size dependence of phase boundaries are so small that we can neglect them to present the phase diagram. The broken dotted line shown in Fig. 3 is the energy crossover line. On the line, a level cross between the first- and second-excited states exists.

To make sure of the validity of our numerical results, we try an analytical approach to calculate phase boundaries between ferrimagnetic phase and two spin liquid phases. We use the first-order perturbation expansion from the limit that \( J_r \cong J_l, J_d \) or \( J_d \cong J_l, J_r \). In case that \( J_r \cong J_l, J_d \), we...
diagonalize the Hamiltonian of the three-spin unit cell along the rung and take the lowest two states. We introduce a pseudospin to describe the two states as follows:

$$|⇑⟩ = \frac{1}{\sqrt{6}} (|↑↑↓⟩ - 2|↑↓↑⟩ + |↓↑↑⟩).$$

$$|⇓⟩ = -\frac{1}{\sqrt{6}} (|↓↓↑⟩ - 2|↓↑↓⟩ + |↑↓↓⟩).$$

Within the pseudospin effective theory, the nearest neighbor pairs should be $|⇑⟩\otimes |⇑⟩$ and $|⇑⟩\otimes |⇓⟩$ in the ferrimagnetic and Néel-like spin liquid phases, respectively. For each phase we calculate the expectation value of the following Hamiltonian:

$$H_{J_l;J_d} = J_l \sum_{i=1}^{3} \sum_{j=1}^{2} \vec{S}_{i,j} \cdot \vec{S}_{i,j+1} + J_d \sum_{i=1}^{2} \sum_{j=1}^{2} \vec{S}_{i+1,j} \cdot \vec{S}_{i,j+1}$$

For ferrimagnetic phase, the value $E_{\text{ferri}}$ is:

$$E_{\text{ferri}} = \langle⇑| \otimes \langle⇑| H_{J_l;J_d} |⇑⟩\otimes |⇑⟩ = \frac{1}{4} J_l - \frac{1}{9} J_d.$$ 

For Néel-like spin liquid phase, the value $E_{\text{SL}}$ is:

$$E_{\text{SL}} = \langle⇑| \otimes \langle⇓| H_{J_l;J_d} |⇑⟩\otimes |⇓⟩ = -\frac{1}{4} J_l + \frac{1}{9} J_d.$$ 

The phase boundary can be determined by $E_{\text{ferri}} = E_{\text{SL}}$. Therefore the analytical phase boundary between ferrimagnetic and Néel-like spin liquid phase is obtained as $J_d/J_l = 9/4$. In the same way, the analytical phase boundary between ferrimagnetic and collinear spin liquid phase is $J_r/J_l = 9/4$ in the case that $J_d \oplus J_l$, $J_r$. Numerical calculation results approach asymptotically to perturbation calculation results.

In the present study we found a new phase between the spin liquid and ferrimagnetic phases, as shown in Fig. 3. However, it is quite difficult to specify the spin structure of this phase with the numerical diagonalization, because many size-dependent level crosses appear. Now we can just conclude that the ground state is a singlet in this phase. Thus at the boundary of the ferrimagnetic phase the magnetization has a jump from $S = 0$ to $S = M_s/3$. In constrast, another three-leg quantum spin model which exhibits a partial ferrimagnetism was proposed[5].

5. Conclusions
We have investigated the $S = 1/2$ three-leg spin ladder model with the next-nearest-neighbor interaction, to consider a role of the frustration in the spin liquid. Using the exact numerical diagonalization, we have calculated the low-lying energy levels to present the ground-state phase diagram. We have found four ground-state phases; (I) the Néel-like spin liquid phase, (II) the collinear spin liquid phase, (III) the ferrimagnetic phase and (IV) the new phase.

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