Melting of Ferromagnetic Order on a Trellis Ladder

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Abstract

The ground state properties of a frustrated spin-1/2 system is studied on a trellis ladder which is composed of two zigzag ladders interacting through rung interactions. The presence of rung interaction between the zigzag ladders induces a non-magnetic ground state, although, each of zigzag ladders has ferromagnetic order in weak anti-ferromagnetic leg interaction limit. The rung interaction also generates rung dimers and opens spin gap which increases rapidly with rung interaction strength. The correlation between spins decreases exponentially with the distance between them.

Keywords: Frustrated magnetic systems, Dimer phase, Density Matrix Renormalization Group Method

1. Introduction

The interaction-driven quantum phase transition in low-dimensional frustrated systems like spin chain [1, 2], ladder or any quasi-one dimensional system has been a frontier area of current research [3, 4]. Many realizations of these systems like (N₄H₂)CuCl₅ [5], LiCuSbO₄ [6], LiCuVO₄ [7], Li₂CuZrO₄ [8] are frustrated due to competing spin exchange interactions. J₁ − J₂ Heisenberg spin-1/2 model with nearest neighbor (NN) ferromagnetic (FM) J₁ and next nearest neighbor (NNN) anti-ferromagnetic (AFM) J₂ interactions is used extensively to understand the ground state magnetic properties of many of these materials [9–12]. This model can explain the gapless spin fluid, gapped dimer and incommensurate gapped spiral phases [9, 12, 13]. On the other hand, the ground state of quasi-1D ladder like structure with AFM leg and rung interactions shows the presence of gapped short-range order in the system. This kind of phase is observed in SrCu₂O₃ [14], (VO)₂P₂O₇ [15, 16], CaV₄O₉, MgV₂O₅ [17, 18] etc. The J₁ − J₂ chain can also be considered as a two-chain lattice with diagonal or zigzag like couplings. Hence it can be alternatively called as zigzag ladder. The isolated ladders like zigzag [9, 11] and normal ladder [3, 9] have been extensively studied. However, the theoretical study of the effect of inter-ladder coupling on the ladders is still an open field. One of the extended networks of the coupled ladders can form a trellis lattice like structure. The trellis lattice is composed of a number of normal ladders coupled through zigzag bonds; alternatively, it can be considered as coupled zigzag ladders through rung interactions as shown in Fig. 1. In this lattice, J₂ and J₃ are leg and rung couplings of a normal ladder, respectively and J₁ is inter-ladder coupling through zigzag bonds.

There are several theoretical studies for two coupled zigzag ladders, e.g. a two-leg honeycomb ladder is considered in Ref. [19], where both J₁ and J₂ are AFM, but J₃ can be either FM or AFM. This system shows two types of Haldane phases for the FM J₃ and, columnar dimer and rung singlet phases for the AFM J₃. Normand et al. considered the similar coupled ladders with all three AFM J₁, J₂ and J₃ interactions. They find dimerized chains for large J₂ and small J₃ limit, spiral long range order for both large J₂ and J₃ limit, Néel long range order in the small J₂ < 0.4 and for all J₃ [20]. Ronald et al. have shown the effect of inter-chain coupling on spiral ground state of J₁ − J₂ model [21]. The effect of inter-ladder coupling on spin gap and magnon dispersion has been discussed in [22] exploiting a theoretical model which has also been

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compared with the experimental data of SrCu$_2$O$_3$ and CaV$_2$O$_5$. The study of interladder coupling effect is important to explain the physical properties of some other materials like LaCuO$_{2.5}$ [23], Sr$_{14}$Cu$_{24}$O$_{41}$ [24], MgV$_2$O$_5$ [17], NaV$_2$O$_5$ [25, 26] etc. The weak interladder exchange interactions in these materials form an effective 2D trellis like structure. Recently Yamaguchi et al. showed magnetic field induced spin nematic phase in the verdazyl radical β-2,3,5-Cl$_3$V [27]. The $J_1$-$J_2$-$J_3$ spin system promises a zoo of exotic phases.

In the current paper we consider a trellis ladder which is composed of two zigzag ladders with FM $J_1$ and AFM $J_2$ and coupled by AFM $J_3$ as shown in Fig. 1. The ground state of an isolated zigzag ladder in small $J_2$ limit is FM. Our main focus of this paper is to understand the effect of rung interaction $J_3$ on the FM ground state exhibited by a single zigzag ladder in the limit of $|J_3| \ll |J_1|$, and study the transition of ground state from the FM to the singlet dimer state.

This paper is divided into four sections. In section 2, the model Hamiltonian and the numerical methods are explained. The numerical results are given in section 3. All the results are discussed and summarized in section 4.

2. Model Hamiltonian and Numerical Method

We consider four-leg ladder system where two zigzag ladders are coupled through an AFM Heisenberg interaction as shown in Fig. 1. The diagonal interactions $J_1$ in zigzag ladders are FM whereas $J_2$ bonds along the legs are AFM. Two zigzag ladders interact with each other through AFM rungs $J_3$. Thus we can write an isotropic Heisenberg spin-$1/2$ model Hamiltonian for the system as

$$H = \sum_{a=1,2} \sum_{i=1}^{N/2} J_1 \vec{S}_{a,i} \cdot \vec{S}_{a,i+1} + J_2 \vec{S}_{a,i} \cdot \vec{S}_{a,i+2} + J_3 \vec{S}_{1,i} \cdot \vec{S}_{2,i},$$

(1)

where $a = 1, 2$ are the zigzag ladder indices. $\vec{S}_{a,i}$ is the spin operator at reference site $i$ on zigzag ladder $a$. We set the FM $J_1 = -1$ and treat the AFM $J_2$ and $J_3$ as variable quantities. We use periodic boundary condition along the rungs, whereas it is open along the legs of the system.

We use the exact diagonalization (ED) method for small systems and density matrix renormalization group (DMRG) method to handle the large degrees of freedom for large systems. The DMRG is a state of art numerical technique for 1D or quasi-1D system, and it is based on the systematic truncation of irrelevant degrees of freedom at every step of growth of the chain [28–30]. We use recently developed DMRG method where four new sites are added at every DMRG steps [31]. For the renormalization of operators, we keep $m$ eigenvectors corresponding to largest eigenvalues of the density matrix of the system in the ground state of the Hamiltonian in Eq. (1). We have kept $m$ up to 300 to constraint the truncation error less than $10^{-10}$. We have used system sizes up to $N = 400$ to minimize the finite size effect.

3. Results

It is well known that the zigzag spin-1/2 ladder has a FM ordered ground state for FM $J_1$ and AFM $J_2 \leq |J_1|/4$ [12]. The AFM coupling, i.e., the rung interaction $J_3$ between two isolated zigzag spin-1/2 ladders retains the FM arrangement in each zigzag ladder; however, the spins on two zigzag ladders are in AFM arrangement to each other, as depicted in the schematic Fig. 1. In other words, the effective ground state of the whole system is in $S^z = 0$ manifold, though the spins on each zigzag ladder are arranged ferromagnetically. The ground state forms singlet dimer along the rung in the large $J_3$ limit, and ground state wave function can be represented as the product of singlet dimers. However, to study the effect of $J_3$ on the ground state, we analyze longitudinal correlation function, longitudinal bond order and spin gap.

In this paper we focus $J_2/|J_1| < \frac{1}{4}$ limit where each zigzag ladder have the FM order in the ground state for $J_3 = 0$. For a finite $J_3$, we calculate the longitudinal spin-spin correlations $C(r) = \langle S^z_i S^z_{i+r} \rangle$, where $S^z_i$ and $S^z_{i+r}$ are the $z$-component of the spin operators at the reference site $i$ and the site at a distance $r$ from $i$, respectively. In 1. We have shown the distance $r$ along the same zigzag ladder with bold numerics, and otherwise in normal numerics, where the reference site is at the 0th position. We note that in $J_2/|J_1| < \frac{1}{4}$ limit all the spins are aligned in parallel on each zigzag ladder and have short range longitudinal correlation for finite $J_3$. As we increase the strength of $J_3$, $C(r)$ shows an exponential behavior as shown in the main Fig. 2 for $J_2 = 0.15$. We notice that each zigzag

![Figure 2: The longitudinal spin-spin correlation C(r) shown for N = 122. J_2 = 0.15 and different J_3 as indicated adjacent the respective curves. The solid lines represent respective exponential fits. The inset shows the correlation length \( \xi \) vs. \( J_3 \) plots for \( J_2 = 0.1 \) and 0.15 in log-log scale.](image-url)
ladder shows FM arrangement as $C(r) > 0$, but it decays exponentially with $r$, i.e. $C(r) \propto \exp(-r/\xi)$. The correlation length $\xi$ follows an algebraic decay with $J_3$, as shown in the inset of Fig. 2. $\xi$ for $J_3 = 0.1$ is approximately 28.5, however it decrease to 1.58 for $J_3 = 0.6$. $\xi$ becomes less than 1 for $J_3 > 0.9$ for $J_2 = 0.15$, and in this parameter regime the system is completely dimerized along the rung.

To study the effect of $J_3$ on the bonds along the rung, diagonal and leg directions, we calculate correlations $C^R$, $C^D$ and $C^L$, respectively as shown in Fig. 3. The calculations of these three correlations are confined to the first neighbor along the respective directions. $|C^R|$ increases exponentially with $J_3$ and follows $|C^R| = 0.25(1 - 0.60\exp(-1.48J_3))$. $C^D$ and $C^L$ are represented by square and diamond symbols, respectively, and both these bond orders exponentially decrease with $J_3$. The exponent of the $C^D$ and $C^L$ are 0.42 and 1.50 respectively. $C^L$ decays faster than $C^D$, because $J_2$ allows the magnon to deconfine along the leg of the zigzag ladder; therefore weaker $J_2$ reduces $C^L$.

The correlation function $C(r)$ of the system shows the short range spin order. Therefore, we explore the excitations energy or spin gap in the system. The rung interaction dominates other interactions; thus we expect the opening of the spin gap $\Delta$. We calculate $\Delta$ for various $J_3 = 0.1, 0.3, 0.4$ and 0.5. The main Fig. 4 shows the extrapolation of the spin gap $\Delta$, from which we obtain the spin gap $\Delta_\infty$ in the thermodynamic limit. $\Delta_\infty$ increases algebraically with $J_3$, as shown in the inset of Fig. 4 for $J_2 = 0.1$ and 0.15. The algebraic exponent $\gamma$ for $J_2 = 0.1$ and 0.15 are 3.33 and 3.13, respectively. We notice that $\gamma$ decreases with increasing $J_2$. This may be due to the delocalization of magnon along the leg of zigzag ladder. The large $J_2/|J_1|$ enhances the interaction of spin along each leg of zigzag ladder and the each leg of the system can have quasi-long range correlation like a normal Heisenberg chain, in $J_2/|J_1| >> 1$ limit. In this limit, system behaves as three non-interacting spin-1/2 Heisenberg chains with gapless spectrum [32].

4. Discussion and Conclusions

In this paper the effect of $J_3$ on FM order in each zigzag ladder of a trellis ladder with FM $J_1$ and AFM $J_2 < |J_1|$ is studied. We show that even a small $J_3$ induces spin gap in the system. The correlation between spins on a zigzag ladder decays exponentially with distance. It may be because of the confinement of magnon along the rungs. As shown in Fig. 4 the gap increases rapidly with $J_3$ for $J_2 = 0.1$. The correlation length of the system reduced less than a unit lattice for $J_3 > 0.9$ at $J_2 \approx 0.15$. This implies the setting of the dimerized state.

This model can also be mapped to a two interacting $J_1 - J_2$ Heisenberg spin-1/2 chains. This system is studied recently by Ronald et al. [21]. They have mostly studied the effect of inter-chain coupling on the spiral nature of the ground state in large $J_2$ and low $J_3$ limit. There are many compounds like CaV$_2$O$_5$ [33], SrCu$_2$O$_3$ [16, 22] etc, which have both strong $J_3$ and $J_2$. However, our prediction are confined to the $J_2 < |J_1|/4$ and large $J_3$ limit.

In summary, this model system goes from a FM ordered ground state along a zigzag ladder in the $J_3 = 0$ limit to a rung dimer state in large $J_3$ limit. The correlation length $\xi$ of the system decreases algebraically and spin gap $\Delta_\infty$ increases algebraically with exponent higher than $\gamma > 3$, on increase in $J_3$ for a given $J_2$.

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