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# The effect of antiferromagnetic interchain coupling on multipolar phases in quasi-1D quantum helimagnets

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**Abstract.** Coupled $s = 1/2$ frustrated Heisenberg chains with ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor exchange interactions in high magnetic field are studied by density-matrix renormalization group (DMRG) and hard-core boson (HCB) approaches at $T = 0$. First, we propose an appropriate one-dimensional array for the construction of a 3D system to be studied with the DMRG method and demonstrate the performance by comparing the ground-state energy to the exact solution. Next, the binding energy of multimagnon bound state is calculated as a function of interchain coupling. We find that the multimagnon bound state is easily destroyed by weak interchain coupling. In the 2-magnon phase the DMRG results are supported by the HCB approach.

## 1. Introduction

For a long time, the exotic phenomena emerged by magnetic frustration have been fascinating and challenging subjects of research in condensed matter physics [1]. Nowadays, the one-dimensional (1D) frustrated Heisenberg chain is a standard model for edge-shared chain cuprates [2] and it has been intensively studied. Recently, some theoretical studies have indicated that the 1D frustrated Heisenberg system exhibits nematic quasi-long-range order in high magnetic field [3, 4, 5]. This nematic state might be thought to be a condensate of 2-magnon bound states [6]. However, to establish whether such multimagnon bound states can be realized in real materials it is essential to determine their robustness against finite interchain couplings. Thus, we study coupled $s = 1/2$ frustrated Heisenberg chains in high magnetic field by using density-matrix renormalization group (DMRG) [7] and hard-core boson (HCB) [8] approaches.

## 2. Model and method

### *2.1. Hamiltonian*

The Hamiltonian of the coupled $s = \frac{1}{2}$ frustrated Heisenberg chains is given by

$$H = J_1 \sum_{\beta,i} \vec{S}_{\beta,i} \cdot \vec{S}_{\beta,i+1} + J_2 \sum_{\beta,i} \vec{S}_{\beta,i} \cdot \vec{S}_{\beta,i+2} + J_{\rm ic} \sum_{\beta,\beta',i} \vec{S}_{\beta,i} \cdot \vec{S}_{\beta',i}, \quad (1)$$

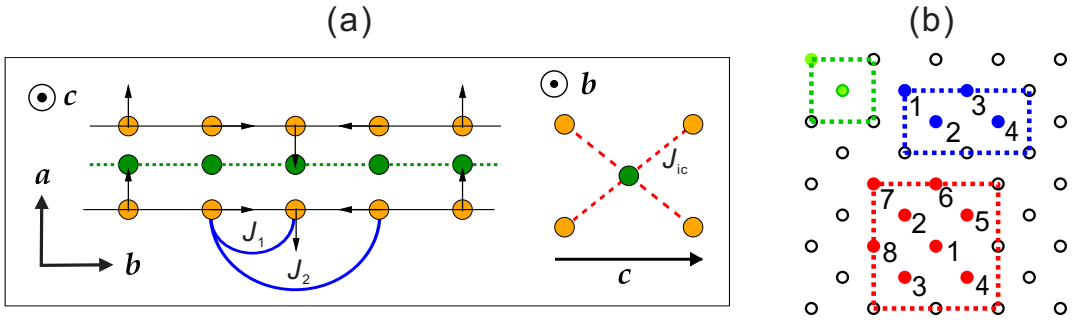


**Figure 1.** (a) Lattice structure of the coupled frustrated Heisenberg chains. (b) The 3D arrangement of chains used for the DMRG calculation.

where $\vec{S}_{\beta,i}$ is a spin-$\frac{1}{2}$ operator at site $i$ on chain $\beta$. $J_1$ ($J_2$) is nearest-neighbor ferromagnetic (next-nearest-neighbor antiferromagnetic) exchange interaction in the chain direction and $J_{\rm ic}$ is antiferromagnetic interchain exchange interaction in the perpendicular direction. The lattice structure is shown in Fig. 1(a). We use $\alpha = J_2/|J_1|$ as a frustration parameter afterwards.

*2.2. DMRG and HCB methods*

We apply the DMRG method with periodic boundary conditions (PBC) in all directions. In general, this method is much less favorable for $D > 1$; however, on current workstations, spin systems with up to about $\sqrt{10} \times \sqrt{10} \times \sqrt{50}$ sites, i.e. 10 coupled chains of length $L \sim 50$, can be studied without difficulty. Thus, by taking a proper arrangement of the chains 3D lattices can be simulated. Let us now describe how the block states are constructed: in the $N_{\rm c} \times L$ cluster, where $N_{\rm c}$ denotes the number of chains. If we regard $N_{\rm c}$ sites in the ac-plane as a "unit cell", the system can be treated as an effective 1D chain with $L$ sites. This enables us to use an appropriate 1D array for the construction of the PBC (see Fig. 1 of Ref.[9]). Then, the sites within each "unit cell" are arranged into numeric order as shown in the inset of Fig. 1(b). Since the exchange interactions run spatially throughout the system, the wave function converges very slowly with DMRG sweep but without getting trapped in a 'false' ground state. We typically keep $m = 800 - 4000$ density-matrix eigenstates in the DMRG procedure and the discarded weight in the renormalization is less than $10^{-6}$. About $20 - 40$ sweeps are necessary to obtain the ground-state energy within a convergence of $10^{-7}|J_1|$ for each $m$ value. For high-spin states $[S_z \geq (N_{\rm c}L - 10)/2)]$ the ground-state energy can be obtained with an error less than $10^{-12}$ by carrying out several thousands sweeps even with small $m \approx 100 - 800$. Furthermore, we use the HCB approach to support the DMRG results. With the HCB method the one- and two-magnon excitation spectrum for fully-polarized state can be found exactly at $T = 0$.

## 3. Results

*3.1. Accuracy check of the DMRG method*

In the DMRG calculation of the model (1) the most difficult case is for uncoupled chains, namely, at $J_{\rm ic} = 0$ and $N_{\rm c} > 1$. Since the DMRG can provide an almost exact solution for single chain ($N_{\rm c} = 1$) and the ground-state energy should scale with $N_{\rm c}$ for a fixed $L$ in the case of $J_{\rm ic} = 0$, we can check the accuracy of our results for $N_{\rm c} > 1$ by comparing them to the single-chain result. Here, we choose three parameters $\alpha = 0.3$, 0.5, and 1 for the check. It is known that in high magnetic field the 2-magnon (3-magnon) bound state is the most stable for $\alpha = 0.5$ and 1 (0.3) for the single chain. Thus, the $z$-component of the total spin is fixed at $S_z = N_{\rm c}(L - 2n)/2$ for the $n$-magnon phase and the ground-state energy is calculated. When this is done, the ground state of all chains is assumed to be the same, i.e., *one* $n$-magnon quasiparticle is flipped from

**Table 1.** Ground-state energy per site for various values of $N_c$ and $\alpha$ at $L = 48$ (in unit of $|J_1|$).

| $N_{\rm chain}$ | $\alpha = 0.3$ | $\alpha = 0.5$ | $\alpha = 1$ |
|---|---|---|---|
| 1 | -0.176866 | -0.138889 | -0.052083 |
| 2 | -0.176863 | -0.138889 | -0.052083 |
| 4 | -0.176860 | -0.138876 | -0.052037 |
| 8 | -0.176822 | -0.138855 | -0.051927 |

the fully-polarized state in each chain. In Table 1 the ground-state energy per site is shown for $N_c = 1$, 2, 4, and 8 at $L = 48$. For an appropriate comparison, we fix $m = 1600$ through the calculations. We can see that for all $\alpha$ values the results at $N_c > 1$ are in good agreement with those at $N_c = 1$. Although the accuracy becomes worse as $N_c$ increases, the maximum error is only $10^{-4}|J_1|$ in the hardest case ($N_c = 8$, $\alpha = 1$). However, we strongly argue that the accuracy for $N_c > 1$ is rapidly improved with increasing $J_{\rm ic}$. It is because that an improper localization of spins, which is one of the most serious problem in the DMRG calculation, can be resolved by dense network of the exchange interactions.

*3.2. Binding energy of the magnon bound state*

Near the saturation field, the binding energy for an $n$-magnon bound state is defined as

$$E_{\rm b}(n) = \frac{1}{n}[E(S_z = S_{\rm max} - n) - E(S_z = S_{\rm max})] - [E(S_z = S_{\rm max} - 1) - E(S_z = S_{\rm max})], \qquad (2)$$

where $E(S_z = S)$ is the ground-state energy with the z-component of total spin $S_z = S$, and $S_z = S_{\rm max}$ corresponds to the fully-polarized state. When the largest value of $E_{\rm b}(n)(> 0)$ is given by $n = n_{\rm max}$, we can prove that the $n_{\rm max}$-magnon bound state is the most stable; whereas, if $E_{\rm b}(n) < 0$ for all $n$ values no low-energy magnon bound state exists.

First, we calculate $E_{\rm b}(n)$ for single chain ($N_c = 1$). In Fig. 2 (a) and (b), the binding energy for $N_c = 1$ is plotted as a function of $\alpha$. The transition between $n$- and $n'$-magnon phases can be estimated from the crossing point of $E_{\rm b}(n)$ and $E_{\rm b}(n')$. We find that the system is in the 4-, 3-, and 2-magnon phases at $0.2662 \le \alpha \le 0.2845$, $0.2845 \le \alpha \le 0.3676$, and $\alpha \ge 0.3676$, respectively. For the 2-magnon phase the HCB solution is available and the binding energy is exactly obtained as $E_{\rm b}(2) = (3\alpha - 1)/[8\alpha(\alpha + 1)]$.

Next, let us take into account the interchain coupling $J_{\rm ic}$. In Fig. 2 (c)-(e) the binding energy for $N_c = 8$ is plotted as a function of $J_{\rm ic}$ for $\alpha = 11/40$, $1/3$, and $1/2$, where the 4-, 3-, and 2-magnon bound states are stabilized at $J_{\rm ic} = 0$, respectively. The HCB result is also shown by the dotted line in Fig. 2 (e) in perfect agreement with the DMRG result. For all the $\alpha$ values, the binding energy is reduced with increasing $J_{\rm ic}$ and reaches zero at some value $J_{\rm ic}(\equiv J_{\rm ic,cr})$. It means that the multimagnon bound state is no longer present in the ground state for $J_{\rm ic} > J_{\rm ic,cr}$. No crossing of $E_{\rm b}(n)$ with different $n$ values is seen in the $n$-magnon phase, so that this is a direct transition from the $n$-magnon to 1-magnon (dipolar) phases. Note, however, that such a crossing could be possible in the immediate vicinity of the phase boundary between different multimagnon phases. Moreover, we find that the qualitative behavior of $E_{\rm b}(n)$ with $J_{\rm ic}$ is almost independent of $N_c$ and a relation $J_{\rm ic,cr}/N_c \sim$ const. is fulfilled for a fixed $\alpha$. It implies that the critical strength of interchain coupling to destroy a multimagnon bound state is determined merely by the total amount of interchain couplings. And, the estimated values of $J_{\rm ic,cr}$ are essentially equivalent to those from a kink position of the saturation field [10, 11]. It is also worth noting that the behavior of $E_b(n)$ with $\alpha$ is fairly similar to that of $J_{\rm ic,cr}$ (see Fig. 2 in [11]). It would be a rather natural consequence of the fact that the critical interchain coupling $J_{\rm ic,cr}$ is roughly proportional to the binding energy of the multimagnon bound state at $J_{\rm ic} = 0$.

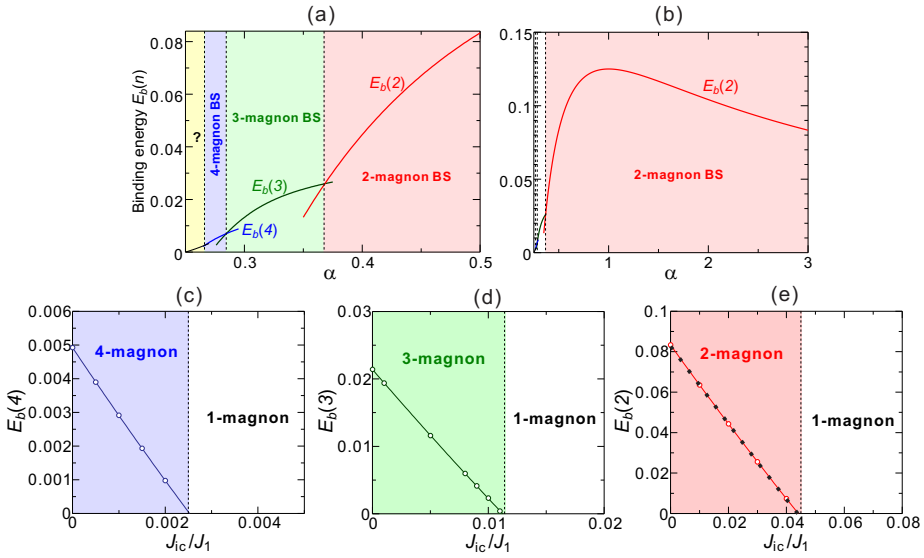


**Figure 2.** (Top) DMRG results of $E_{\rm b}(n)$ for a single chain at (a) $0.25 \leq \alpha \leq 0.5$ and (b) $0.25 \leq \alpha \leq 3$. (Bottom) DMRG results of $E_{\rm b}(n)$ for $N_{\rm c} = 8$ as a function of $J_{\rm ic}$ at (c) $\alpha = 11/40$, (d) 1/3, and (e) 1/2. The HCB result: thick dotted line in (e).

## 4. Summary

We considered coupled $s = 1/2$ frustrated Heisenberg chains in high magnetic field by the DMRG method. We compare the ground-state energy of uncoupled chains, which is the most difficult case for the DMRG calculation, with that of a single chain and confirm that the 3D Heisenberg system can be studied by the DMRG method. Then, by calculating the binding energy of multimagnon bound state we find that the multimagnon bound state is destroyed by weak antiferromagnetic interchain coupling. For the 2-magnon phase the DMRG results are supported by the HCB approach. Finally, we mention that possible materials for quantum spin nematics or multipolar phases are $LiVCuO_4$ and $PbCuSO_4(OH)_2$.

## Acknowledgments

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