Magnetoelastic instability in the XXZ rings with next-nearest neighbour coupling

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This paper numerically investigates the magnetoelastic instability in the $S = 1/2$ XXZ rings containing finite spins N with antiferromagnetic nearest-neighbour (NN) and next-nearest neighbour (NNN) coupling. It finds that, as the NN anisotropy Δ_1 equals the NNN anisotropy Δ_2, there exists a critical NNN coupling strength J_2^c (≈ 0.5), at which the systems always locate in dimerized phase for arbitrary large spring constant. As $\Delta_1 \neq \Delta_2$, the values of J_2^c are dependent on N and the difference of $(\Delta_1 - \Delta_2)$.

Keywords: single molecular magnets, anisotropy, magnetoelastic instability

PACC: 7550X, 7550E

1. Introduction

Single molecule magnets (SMMs) have become extensively investigated topics in recent years, which are nanostructured materials and formed by a finite number of exchange-coupled transition-metal ions. Experimentally, plenty of SMMs have been synthesized.[1−7] Almost at the same time, theoretical interests have been aroused to study them by using numerical and analytical methods.[8−14] Recently, in the nanostructured magnetic Cu8 ring, the ^{3}Cu nuclear quadrupole resonance spectrum shows four structurally nonequivalent Cu ions,[3] which is perhaps related to the appearance of lattice dimerization. The lattice dimerization is a magnetoelastic (ME) instability, which may originate from the spin–phonon interaction. Such a phenomenon, which is often considered in the context of spin-Peierls transition, was first predicted to occur in the infinite $S = 1/2$ Heisenberg antiferromagnetic (AF) chain[15] and it was indeed observed experimentally in the quasi-one-dimensional $S = 1/2$ compound $CuGeO_3$.[16] For nanostructured magnetic systems, the spin-phonon interaction indicates stronger effects on the ME instability.[8]

In condensed matter physics, the studies on spin anisotropy have attracted extensive attention in the past years.[17−22] For XXZ model with nearest-neighbour (NN) coupling easy-axis anisotropy (Δ), as $\Delta < -1$, the system is in the ferromagnetic phase, while as $\Delta > 1$, it indicates the Néel phase. In the case of XY–type anisotropy ($-1 < \Delta < 1$), the ground state is characterized by gapless excitations and algebraic decay of spin correlations (spin-fluid).[17] On the other hand, in real physics systems, there often exists next-nearest neighbour (NNN) coupling J_2 besides NN coupling J_1.[23−25] The NNN couplings can introduce frustration and this is known to lead to new physics and phase in the one-dimensional spin systems. It is known that in the case of a spin-1/2 chain with NN and NNN couplings, there are two different phases depending on the ratio between J_1 and J_2. As $J_2/J_1 \geq 0.24$, the ground state is spontaneously dimerized and opens an energy gap in the excitation spectrum.[26] Recently, some compounds containing CuO chains with edge-sharing CuO_4 plaquette have been expected to be described by the XXZ model with NNN interaction.[27]

In finite spin systems, the ME instability indicates different characterization from that in the thermodynamic limit.[8] For XXZ rings only with NN coupling and even number spins, in the region $-1 < \Delta \leq 1$, there may exist a critical Δ_c dividing the first order transition and the continuous transition.[14] But in the previous studies, the effects of NNN coupling anisotropy on the ME instability under the spin-phonon interaction were not reported. In this paper, we have investigated this problem and found that the systems indicate novel behaviour of ME instability.

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2. Models and results

In adiabatic approximation, the Hamiltonian describing lattice distortion and NNN anisotropic exchange interactions (exchange anisotropy) can be written as:

$$H = J_1 \sum_{i=1}^{N} (1+\alpha u_i)\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta_1 S_i^z S_{i+1}^z\right) + J_2 \sum_{i=1}^{N}\left(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + \Delta_2 S_i^z S_{i+2}^z\right) + \frac{K}{2}\sum_{i=1}^{N} u_i^2, \quad (1)$$

where S_i^β represents the β ($\beta = x$, y, z) component of the $S = 1/2$ operator at site i. The u_i is the lattice distortion between site i and $i+1$, K is the lattice spring constant, J_1 (> 0) and J_2 (> 0) are the NN and NNN couplings and the corresponding easy-axis anisotropies are defined by Δ_1 and Δ_2 (in this paper, $0 < \Delta_1$ (Δ_2) ≤ 1), respectively. J_1 will be taken as the unit of energy. Periodic boundary condition is considered. Under the scaling $\alpha u_i \to \delta_i$, the spin–phonon coupling strength α has been absorbed in the spring constant ($K/\alpha^2 \to K$). In this paper, the Lanczos diagonalization technique is used in $S^z_{\rm total} = 0$ space.

For finite spin systems with even number spins, the ground state locates either in dimerized (D) phase or in uniform (U) phase. The transition from D phase to U phase (not the thermodynamic transition) is a first-order or second-order transition.[8,14] It is reasonable that in this paper we have taken $\delta_i = (-1)^i\delta$. So the ground state energy is the function of δ. As $\delta = \delta^*$ (dimerization displacement), the ground state energy equals a minimum value, which corresponds to a stable state. Firstly, we investigate the lattice distortion as $\Delta_1 = \Delta_2$. In Fig. 1, the K dependence of δ^* is given for $\Delta_1 = \Delta_2 = 0.4$ and $N = 8$. The open squares, circles and triangles correspond to $J_2 = 0.0$, 0.3 and 1.0, respectively. It is found that, for all cases we have considered, the phase transition from D phase to U phase is continuous (second order transition) with increasing K. Corresponding to $J_2 = 0.0$, 0.3 and 1.0, the critical values of $K_{\rm c}$ (the value of K at the transition point) are 1.11, 3.78 and 2.91, respectively. This indicates that there must exist a critical NNN coupling $J_2^{\rm c}$, as $J_2 < J_2^{\rm c}$, the values of $K_{\rm c}$ are increased with strengthening the NNN coupling. But as $J_2 > J_2^{\rm c}$, $K_{\rm c}$'s are decreased with increasing the NNN coupling. That is to say, the NNN coupling favors (respectively, holds back) the formation of D phase for $J_2 < J_2^{\rm c}$ (respectively, $J_2 > J_2^{\rm c}$). But from Fig. 1, it is difficult to decide the precise $J_2^{\rm c}$.

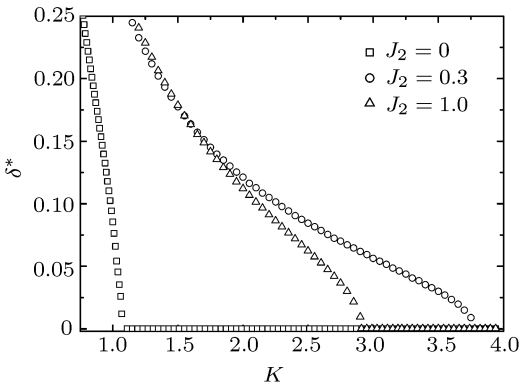


Fig. 1. The spring constant K dependence of dimerization δ^* with different NNN coupling.

In order to confirm the existence of $J_2^{\rm c}$, we calculate the fourth derivative of ground state energy with respect to the lattice distortion δ at $\delta = 0$,

$$\sigma = \left.\frac{\partial^4 E_g}{\partial \delta^4}\right|_{\delta=0}, \quad (2)$$

where $E_{\rm g}$ is the ground state energy. For continuous transition, $\sigma > 0$ and for the first order transition, $\sigma < 0$.[8] In Fig. 2, the function relations between J_2 and σ are given for $\Delta_1 = \Delta_2 = 0.4$ and $N = 8$. The lines are the guide to the eyes. As the NNN couplings are strengthened from zero, the values of σ are increased monotonously. At $J_2 \approx 0.5$, $\sigma \to +\infty$. After that, the values of σ become smaller and smaller with increasing J_2. So $J_2 \approx 0.5$ may be the critical value $J_2^{\rm c}$. One can also see that, for all the values of J_2, σ's are always larger than zero. So the phase transition from D phase to U phase is always continuous.

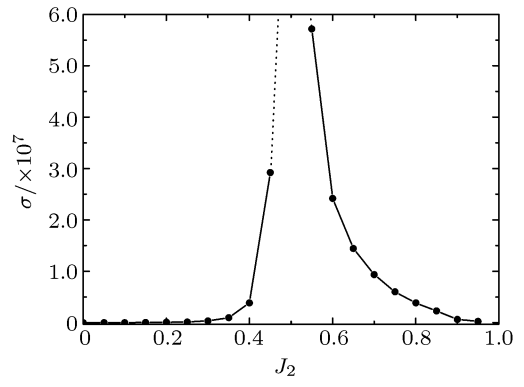


Fig. 2. The fourth derivative of ground state energy with respect to δ at $\delta = 0$ as a function of NNN coupling. The lines are the guide to the eyes.

In Fig. 3, the J_2 dependence of $1/K_c$ is given for $\Delta_1 = \Delta_2 = 0.4$ and different N. The open squares, circles and triangles are the numerical results corresponding to $N = 6$, 8 and 10, respectively, and the solid lines are polynomial fit with the third order. These results indicate that, as J_2 is increased from zero, the values of $1/K_c$ become smaller and smaller. At $J_2 \approx 0.5$, $1/K_c \to 0$. Correspondingly, the values of $K_c \to +\infty$. That is to say, at this point, the systems may always locate in D phase for arbitrary large K. Another interesting result is that, the values of J_2^c are irrelevant to the lattice number N.

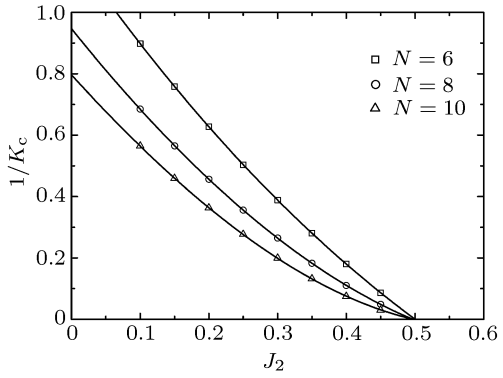


Fig. 3. The NNN coupling J_2 dependence of $1/K_c$ with $\Delta_1 = \Delta_2 = 0.4$. The open squares, circles and triangles are the numerical results and the solid lines are polynomial fit with the third order.

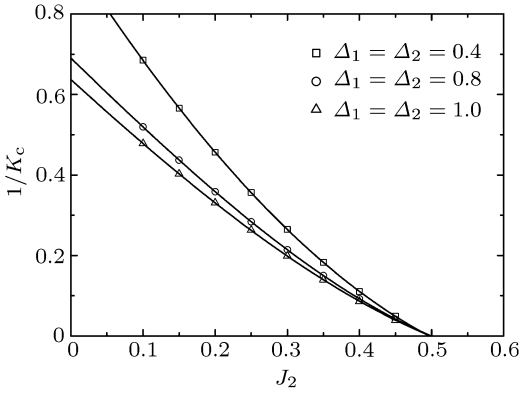


Fig. 4. The NNN coupling J_2 dependence of $1/K_c$ with $N = 8$. The open squares, circles and triangles are the numerical results corresponding to $\Delta_1 = \Delta_2 = 0.4$, 0.8 and 1.0, respectively, and the solid lines are polynomial fit with the third order.

Furthermore, the J_2 dependence of $1/K_c$ is depicted in Fig. 4 for $N = 8$ and $\Delta_1 = \Delta_2 = 0.4$ (open squares), 0.8 (open circles) and 1.0 (open triangles). The solid lines are polynomial fit with the third order. It is found that, as $J_2 \approx 0.5$, the values of $1/K_c$ for all cases approach zero. So, these results indicate that the critical value J_2^c is not dependent on Δ_1 and Δ_2 as $\Delta_1 = \Delta_2$.

In the following, we consider the critical behaviour of the NNN coupling for different Δ_1 and Δ_2. In the inset of Fig. 5, the function relations between $(\Delta_1 - \Delta_2)$ and J_2^c are given with $N = 8$. It is found that, for $\Delta_1 > \Delta_2$, J_2^c is larger than 0.5. But for $\Delta_1 < \Delta_2$, the critical value J_2^c is smaller than 0.5. J_2^c is also dependent on the difference of $(\Delta_1 - \Delta_2)$. With decreasing the values of $|\Delta_1 - \Delta_2|$, the corresponding J_2^c approaches 0.5. In Fig. 5, the scaling behaviours of J_2^c are plotted for $\Delta_1 \neq \Delta_2$. The open squares ($\Delta_1 = 0.4$, $\Delta_2 = 0.8$), solid squares ($\Delta_1 = 0.5$, $\Delta_2 = 0.7$), open circles ($\Delta_1 = 0.8$, $\Delta_2 = 0.4$) and solid circles ($\Delta_1 = 0.7$, $\Delta_2 = 0.5$) are numerical results and the solid lines are linear fit. The results indicate that, with increasing the lattice numbers, the values of J_2^c decrease monotonously. In the thermodynamic limit, J_2^c approaches a finite value which is larger (respectively, smaller) than 0.5 as $\Delta_1 > \Delta_2$ (respectively, $\Delta_1 < \Delta_2$).

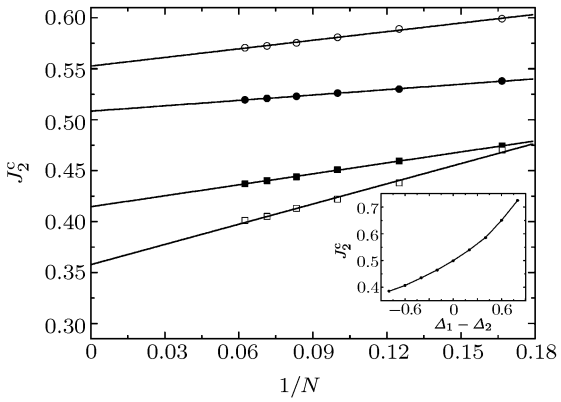


Fig. 5. The scaling behaviours of J_2^c for different Δ_1 and Δ_2. The open squares ($\Delta_1 = 0.4$, $\Delta_2 = 0.8$), solid squares ($\Delta_1 = 0.5$, $\Delta_2 = 0.7$), open circles ($\Delta_1 = 0.8$, $\Delta_2 = 0.4$) and solid circles ($\Delta_1 = 0.7$, $\Delta_2 = 0.5$) are numerical results and the solid lines are linear fit. In the inset: the function relations between $(\Delta_1 - \Delta_2)$ and J_2^c with $N = 8$. The corresponding values of Δ_1 (Δ_2) from the left to right points are: 0.2 (1.0), 0.3 (0.9), 0.4 (0.8), 0.5 (0.7), 0.6 (0.6), 0.7 (0.5), 0.8 (0.4), 0.9 (0.3), 1.0 (0.2).

The novel ME instability in finite spin systems may originate from the competition between NN and NNN coupling. In the thermodynamic limit, for the $S = 1/2$ AF XXZ chain with AF NNN couplings, in the case of $\Delta_1 = \Delta_2 = 1.0$, the competition between J_1 and J_2 induces the existence of the so-called Majumdar–Ghosh point ($J_2 = 0.5$), at which the ground state is twofold degenerate and it is irrelevant

to the spin numbers.[28] In the region $0 \leq \Delta_1\ (\Delta_2) < 1$, the ordering tendency of the NN coupling is frustrated by the NNN coupling and the interplay of the two competing terms in the presence of quantum fluctuations produces the dimmer phase as J_2 is larger than a critical value.[29] In finite spin systems, the frustration effect of the NNN coupling is stronger than that in the thermodynamic limit. So the NNN couplings indicate more evident effects on the ME transition behaviour in finite systems.

3. Conclusions

In conclusion, the ME instability in $S = 1/2$ XXZ model with finite spins has been investigated under the consideration of the NN and NNN couplings for easy-axis anisotropy Δ_1 and Δ_2 in the region $0 < \Delta_1\ (\Delta_2) \leq 1$. As $\Delta_1 = \Delta_2$, there may exist a critical NNN coupling strength $J_2^{\rm c}$ (≈ 0.5), at which the systems always locate in D phase for arbitrary large K. As $J_2 < J_2^{\rm c}$, the values of $K_{\rm c}$ are increased with strengthening NNN coupling. As $J_2 > J_2^{\rm c}$, $K_{\rm c}$ is decreased with increasing the values of J_2. For $\Delta_1 \neq \Delta_2$, the critical values of $J_2^{\rm c}$ are dependent on the lattice number and the difference of $(\Delta_1 - \Delta_2)$.

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