Eur. Phys. J. B **51**, 473–476 (2006)
DOI: 10.1140/epjb/e2006-00255-1

THE EUROPEAN PHYSICAL JOURNAL B

Second- to first-order transition in two coupled antiferromagnetic rings

P.F. Li[a], Y.G. Chen, and H. Chen

Pohl Institute of Solid State Physics, Tongji University, Shanghai 200092, P.R. China

Received 25 November 2005 / Received in final form 9 February 2006
Published online 28 June 2006 –

Abstract. We numerically investigate an $S = 1/2$ spin model, in which two dimerized antiferromagnetic rings interact with each other ferromagnetically. It is shown that the order of the magnetoelastic transition is strongly affected by the interring coupling $J_\perp$ and there may exist a critical $J_\perp^*$ dividing the first-order transition and the continuous transition.

PACS. 75.10.Jm Quantized spin models – 75.10.Pq Spin chain models – 75.30.Kz Magnetic phase boundaries (including magnetic transitions, metamagnetism, etc.)

1 Introduction

In low-dimensional spin systems, magnetoelastic (ME) instability, generally characterized by a lattice dimerization, has attracted extensively attention [1–9]. This phenomenon may be induced by spin-phonon interaction which is often considered in the context of spin-Peierls (SP) transition. In adiabatic limit, the lattice dimerization may lower the total magnetic energy by a greater amount than the increase in elastic energy due to lattice deformation. Then the system will open an energy gap in the spin excitation spectrum. Such a transition was first predicted to occur in the infinite $S = 1/2$ Heisenberg antiferromagnetic (AF) chain [1] and it was indeed observed experimentally in the quasi-one-dimensional $S = 1/2$ compound $CuGeO_3$ [5]. Recently, in the mesoscopic magnetic molecule Cu_8 rings, the ^{63}Cu NQR (nuclear quadrupole resonance) spectrum shows four structurally nonequivalent Cu ions [10], which is perhaps related to the appearance of dimerization. In theory, the ME transition is strongly affected by the spin value and system size. In finite ring-shaped systems, there exists a critical spring constant beyond which the symmetric phase is unstable. The most interesting result is that there is a first order transition for the system with spin larger than one-half case (exactly speaking, the ME transition in finite system is not a real phase transition which is possible only in a infinite system [11]), while for spin one-half system, the transition is continuous, as the spring constant is reduced [6]. But in infinite systems, the ME transition is possible for all half-integer spins for arbitrarily large spring constant, and it is absent for integer spins [7].

The spin systems with interchain coupling have been intensively considered in many theoretical works [12–22]. In the two-leg Heisenberg AF spin-ladder model (two coupling AF spin chains with AF rung), it is shown the evidence of a nonzero singlet-triplet energy gap for all finite interchain coupling [12]. But for single spin-1/2 AF chain, according to Haldane's conjecture, the excitation spectrum is gapless [23]. For two-dimensional XY model, there may exist a first order transition from dimerized phase to uniform phase as the interchain coupling is larger than zero [14]. The effects of interchain coupling on the spin chains in quasi-one-dimensional system are intensively studied because there are true materials with spin ladder structure [24–28]. Also considering spin ladder systems provides a way to study the two dimensional systems [29]. Very recently, the studies of ferromagnetic (FM) interchain coupling are becoming vive because such kinds of materials are synthesized [26–28]. These materials display some novel properties. A weak FM interchain coupling may stabilize the long range AF order [26]. In external magnetic field, such kind of materials may have unusual properties [27]. Theoretically, the two-leg AF spin-ladder model with FM rung has been investigated and found that the ground state is the Haldane state with an excitation gap for $J_\perp > 0$ ($J_\perp$ is the interchain coupling) [18].

With above consideration for the spin systems, one question may be raised: if the interchain and spin-phonon interaction are all embodied in a finite size spin system, what will happen? This is our main motivation of present paper. We will study an $S = 1/2$ spin model, in which two dimerized AF rings interact each other by a FM interring coupling. We have found a nonzero critical interring coupling, beyond which the ME transition is first order and below which the transition is second order.

[a] e-mail: 0310103008@smail.tongji.edu.cn

2 Models and methods

In adiabatic approximation, the model studied in this paper can be given as:

$$H = J \sum_{i=1,j=1,2}^{N} [1+\delta_{i,j}]\, \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} - J_\perp \sum_{i=1}^{N} \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} + \frac{K}{2} \sum_{i=1,j=1,2}^{N} \delta_{i,j}^2, \quad (1)$$

where $\mathbf{S}_{i,j}$ (respectively, $\delta_{i,j}$) represents the spin-1/2 operator at site i (respectively, the lattice distortion between site i and $i+1$) in the jth ring. K is the spring constant, and N is lattice number in each ring. J and $J_\perp$ (>0) are the coupling strength of intraring and interring, respectively. J will be taken as the unit of energy. Periodic boundary condition is considered. The spin-lattice coupling strength has been absorbed in the spring constant [6].

The lattice distortion of Hamiltonian (1) with minimal ground state energy is obtained by the following iterative procedure. First, by the Lanczos diagonalization technique, we determine the lowest energy eigenvalue of (1) with a random initial distortion pattern $\{\delta_{i,j}\}$ which satisfies the constraint $\sum_{i=1,j=1,2}^{N} \delta_{i,j} = 0$. Then, according to the equilibrium condition derived from the Hellman-Feynman theorem [6],

$$K\delta_{i,j} + J \langle \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} \rangle - \frac{J}{N} \sum_{i=1,j=1,2}^{N} \langle \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} \rangle = 0, \quad (2)$$

we update the lattice distortion until the iteration converge. As already obtained in reference [6], in the system we examined, we found either an undistorted or a dimerized configuration (represented by δ^*) along the rings.

3 Results and discussion

The ground state properties of above model without interring interaction ($J_\perp = 0$) has been well studied in reference [6], in which the authors have calculated the order parameter: the lattice dimerization δ^* and found a ME phase transition from uniform phase (U) ($\delta^* = 0$) to dimerized phase (D) ($\delta^* \neq 0$). The phase transition order depends on the value of spin S. In our model, dimerization δ^* is still a proper order parameter. Without loss of generality, we only systematically study the model with $N = 6$.

In the following we will present our results. Since the order parameter δ^* should be determined by ground state energy, we first show the ground energy per site E_g as a function of lattice distortion in Figure 1. By this figure, one can find that there are two kinds of case. For small $J_\perp$, as shown in Figure 1a, the ground state energy has only one stable point for a given K. By this stable point, one

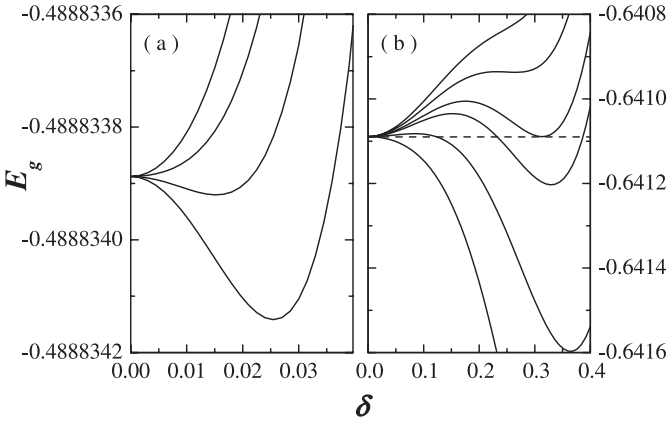

Fig. 1. The δ dependence of the ground-state energy per site for various values of K. (a) $J_\perp = 0.5$, from bottom to top, $K = 0.991$, 0.992, 0.993, 0.994. (b) $J_\perp = 2.0$, from bottom to top, $K = 0.5500$, 0.5625, 0.5705, 0.5712, 0.5751, 0.5780.

can obtain the dimerization δ^*. With increasing the spring constant K to a finite value, δ^* will be monotonously reduced to zero. That is to say, there is a critical value of K_c, which is the transition point from D phase to U phase. The transition is continuous. For large $J_\perp$ case, the situation is quite different. In Figure 1b, one may find that there are two minimal points in the ground state energy as the spring constant is larger than a critical value K_c^1. At these two minimal points, one is $\delta^* = 0$ and another one is $\delta^* \neq 0$. They are corresponding to U phase and D phase, respectively. At the lowest energy point, $\delta^* \neq 0$ and the D phase is a stable phase. And the U phase is a metastable phase. With increasing K, the energy of minimal point with non-zero value of δ^* will be increased. At a critical value of K_c^2, the two minimal points have equal ground state energy. That is to say, the D phase and U phase coexist at this point. As K is increased from K_c^2, the D phase will become unstable (metastable dimerized phase), and U phase turns into stable phase. When K reaches to the third critical value K_c^3, the minimal point with $\delta^* \neq 0$ will totally disappear. So in the case of larger interring coupling, at the K_c^2 the order parameter δ^* will change to zero from a finite value suddenly. Similar behaviors are still found in dimerized $S = 1$ Heisenberg model [30]. This phenomenon clearly implies a first order transition from D phase to U phase.

With above analysis, we can give the spring constant dependence of dimerization displacement under different interring coupling in Figure 2. From this figure, one can clearly find that, as $J_\perp = 0$, the dimerization displacement may be continuously decreased to zero value with increasing K. This result is consistent with the result for single spin one-half AF ring [6]. In this case, the transition is second order or continuous. For small finite $J_\perp$ (in Fig. 2, $J_\perp = 0.5$), the order of transition from D phase to U phase is same as that of $J_\perp = 0$. For large $J_\perp$ (in Fig. 2, $J_\perp = 2.0$ and 3.0), as the spring constant K is increased, firstly the dimerization is reduced, then the lattice dimerization δ^* will jump to zero abruptly as K equals to a

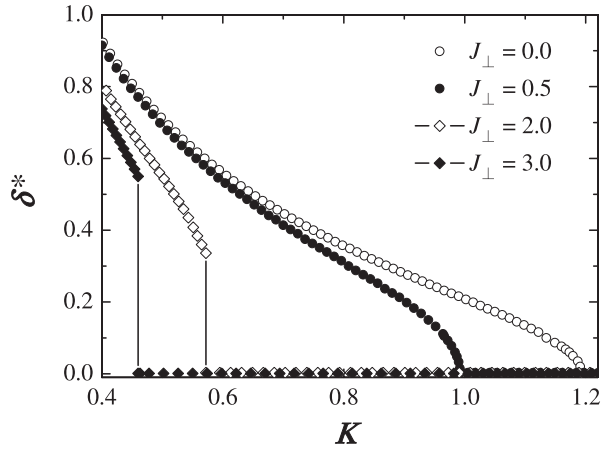

Fig. 2. The spring constant dependence of dimerization with different interring coupling.

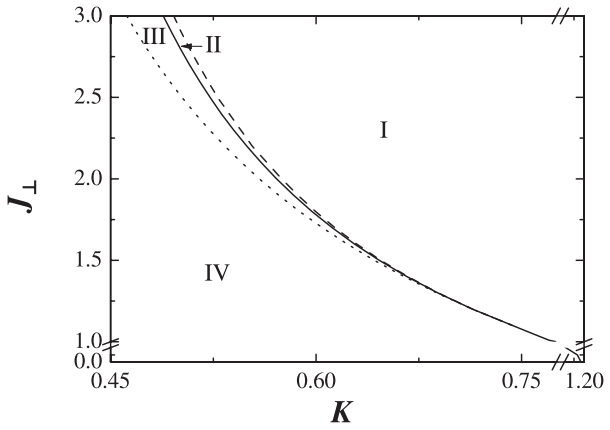

Fig. 3. Phase diagram for the spin-ladder model in the parameter space of interring coupling and spring constant. For $J_\perp > J_\perp^*$, the dot, solid, and dash line correspond to $K = K_c^1$, K_c^2 and K_c^3, respectively. For $J_\perp < J_\perp^*$, the solid line corresponds to $K = K_c$.

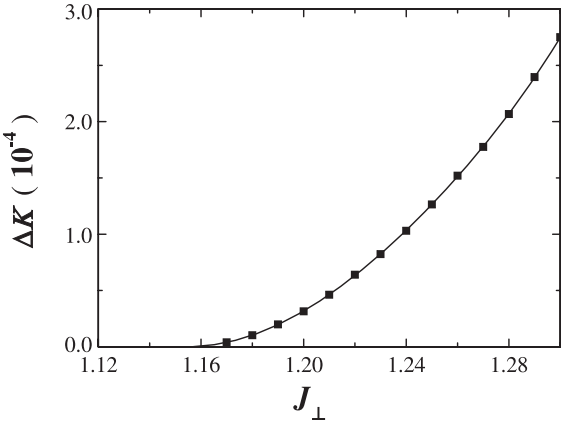

Fig. 4. The $J_\perp$ dependence of $\Delta K = K_c^3 - K_c^1$. The solid squares are numerical data and the solid lines are polynomial fit with the sixth order.

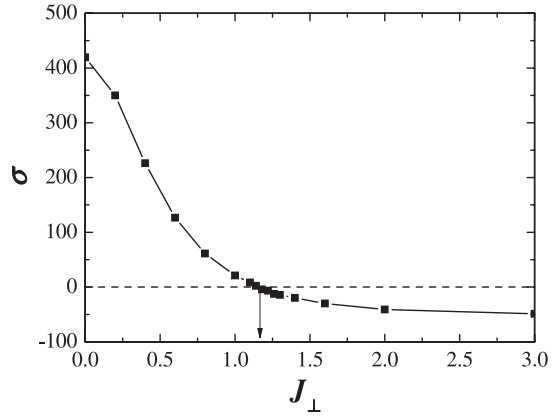

Fig. 5. Fourth derivative of ground state energy with respect to δ at $\delta = 0$ as a function of interring coupling. The arrow points to the critical interring coupling which divides the continuous transition and first order transition. For the dash line, $\sigma = 0$.

critical value K_c^2. It may imply that it will occur a first order transition, which also be found in single finite AF ring for $S > 1/2$. Although there may exist a critical interring coupling $J_\perp^*$, where the transition order changes from second to first order, it is hard to identify $J_\perp^*$ only by Figures 1 and 2. Thus we will try to find $J_\perp^*$ by other ways.

Summarizing above results, a full phase diagram is given in Figure 3. For clearly showing the phase transition order, we plot K_c, K_c^1, K_c^2 and K_c^3 dependence on interring coupling $J_\perp$. The phase diagram in parameter space (K, $J_\perp$) can be divided into four regions. The phase in I and II region is U phase. But in the region II there exists a metastable dimerized phase. In region III and IV, the system locates in D phase. In region III, the metastable uniform phase will appear. In this phase diagram, there is a very special point, at which the line of K_c^1, K_c^2 and K_c^3 will end and K_c will begin. This point can be denoted by the critical value $J_\perp^*$. For $J_\perp > J_\perp^*$, the transition from D phase to U phase is first order and $J_\perp < J_\perp^*$, the transition is continuous. For identifying the value of $J_\perp^*$, we give the $J_\perp$ dependence of $\Delta K = K_c^3 - K_c^1$ in Figure 4. The solid squares are numerical results and the solid lines are polynomial fit with the sixth order. With decreasing the value of $J_\perp$, ΔK will be reduced. At $J_\perp = J_\perp^*$, $\Delta K = 0$. This phenomenon means that the metastable phases totally disappear and the transition order is changed. By this figure, one can find that $J_\perp^* \approx 1.16$.

For confirming the value of $J_\perp^*$, we compute the fourth derivative of ground state energy with respect to δ at $\delta = 0$, $\sigma = 2N\partial^4 E_g/\partial\delta^4\big|_{\delta=0}$, which can be used to identify the order of transition. According to the standard Landau-Ginzburg approach, for continuous phase transition, $\sigma > 0$. For the first order transition, $\sigma < 0$ [6]. In Figure 5, we give σ as a function of interring coupling $J_\perp$. As $J_\perp = 0$, $\sigma = 419.6$, which well agrees with the result in reference [6] ($\sigma = 423.3$). For small nonzero $J_\perp$, $\sigma > 0$, the transition is continuous. With increasing $J_\perp$, σ become smaller and smaller. At $J_\perp^* \approx 1.16$, the sign of σ changes from positive to negative. So the transition order may be changed from second to first at $J_\perp^* = 1.16$, which is consistent with the

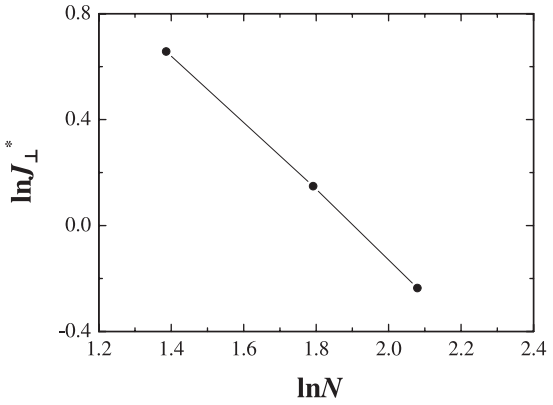

Fig. 6. The ln$N$ dependence of ln$J_\perp^*$ for $N = 4$, 6 and 8.

result obtained from Figure 4. One can also find that, as $J_\perp \to \infty$, σ may approach to the value in $S = 1$ single AF ring [6].

Further, we investigate the size effect of the critical interring coupling $J_\perp^*$. In Figure 6, the values of ln$J_\perp^*$ against ln$N$ is plotted for $N = 4$, 6 and 8, in which the linearity of ln$J_\perp^*$ to ln$N$ is fairly good. This means that $J_\perp^*$ may approach to zero according to power law as $N \to \infty$. That is to say, in thermodynamic limit, any nonzero FM interring coupling will induce a first order ME transition in two-leg spin ladder model. The effects of interchain coupling in infinite system may give us some hints to understand our results. In an infinite system, the properties of $S = 1$ Heisenberg chain can be understand by representing the $S = 1$ model as two coupled $S = 1/2$ model [31]. This fact may help us to explain the first order transition in our results. That is to say, as the interring coupling is strong enough, the behavior of the coupled rings belongs to the class of $S = 1$ dimerized Heisenberg model, in which there is a first order transition [30]. As the interring coupling is small enough, the behavior of the coupled rings belongs to the class of $S = 1/2$.

4 Conclusions

In conclusion, we numerically investigate an $S = 1/2$ spin model where two dimerized AF rings interact with each other by a FM interring coupling. It is shown that the ME instabilities would be strongly affected by the interring coupling. In this system, there exists a critical interring coupling $J_\perp^*$ to divide the continuous transition and first order transition and the critical value may depend on the lattice number.

This work is supported by Natural Science Foundation of China under Grants No. 10304014 and Foundations from Sci. & Tech. Committee of Shanghai Municipality (Grant Nos. 03QA14054 and 0452nm077). We also express our gratitude to Prof. H. Nishimori at Department of Physics, Tokyo Institute of Technology for approving the use of the computer program.

References

1. M.C. Cross, D.S. Fisher, Phys. Rev. B **19**, 402 (1979); M. Aizenman, B. Nachtergaele, Commun. Math. Phys. **164**, 17 (1994)
2. T. Nakano, H. Fukuyama, J. Phys. Soc. Jpn **49**, 1679 (1980)
3. A.E. Feiguin, J.A. Riera, A. Dobry, H.A. Ceccatto, Phys. Rev. B **56**, 14607 (1997)
4. F. Schönfeld, G. Bouzerar, G.S. Uhrig, E. Müller-Hartmann, Eur. Phys. J. B **5**, 521 (1998)
5. M. Hase, I. Terasaki, K. Uchinokura, Phys. Rev. Lett. **70**, 3651 (1993)
6. L. Spanu, A. Parola, Phys. Rev. Lett. **92**, 197202 (2004)
7. D. Guo, T. Kennedy, S. Mazumdar, Phys. Rev. B **41**, R9592 (1990)
8. A.W. Sandvik, R.R.P. Singh, D.K. Campbell, Phys. Rev. B **56**, 14510 (1997)
9. G.S. Uhrig, F. Schönfeld, M. Laukamp, E. Dagotto, Eur. Phys. J. B **7**, 67 (1998)
10. A. Lascialfari, Z.H. Jang, F. Borsa, D. Gatteschi, A. Cornia, D. Rovai, A. Caneschi, P. Carretta, Phys. Rev. B **61**, 6839 (2000)
11. C.N. Yang, T.D. Lee, Phys. Rev. **87**,404 (1952)
12. T. Barnes, E. Dagotto, J. Riera, E.S. Swanson, Phys. Rev. B **47**, 3196 (1993)
13. M. Greven, R.J. Birgeneau, Phys. Rev. Lett. **81**, 1945 (1998)
14. Q. Yuan, Y. Zhang, H. Chen, Phys. Rev. B **64**, 012414 (2001)
15. G. Fáth, Ö. Ligeza, J. Sólyom, Phys. Rev. B **63**, 134403 (2001)
16. D.N. Aristov, M.N. Kiselev, Phys. Rev. B **70**, 224402 (2004)
17. N. Haga, S.I. Suga, Phys. Rev. B **66**, 132415 (2002)
18. H. Watanabe, K. Nomura, S. Takada, J. Phys. Soc. Jpn **62**, 2845 (1993)
19. C. Itoi, S. Qin, Phys. Rev. B **63**, 224423 (2001)
20. J. Sznajd, Phys. Rev. B **68**, 174420 (2003)
21. Y. Ji, J. Qi, J. Li, C. Gong, J. Phys.: Condens. Matter **9**, 2259 (1997)
22. D. Schmeltzer, P. Sun, J. Phys.: Condens. Matter **10**, 4435 (1998)
23. F.D.M. Haldane, Phys. Lett. **93A**, 464 (1983)
24. T. Vuletić, B. Korin-Hamzić, S. Tomić, B. Gorshunov, P. Haas, T. Rõõm, M. Dressel, J. Akimitsu, T. Sasaki, T. Nagata, Phys. Rev. Lett. **90**, 257002 (2003)
25. N. Fujiwara, N. Môri, Y. Uwatoko, T. Matsumoto, N. Motoyama, S. Uchida, Phys. Rev. Lett. **90**, 137001 (2003)
26. M.D. Lumsden, G.E. Granroth, D. Mandrus, S.E. Nagler, J.R. Thompson, J.P. Castellan, B.D. Gaulin, Phys. Rev. B **62**, R9244 (2000)
27. M. Köppen, M. Lang, R. Helfrich, F. Steglich, P. Thalmeier, B. Schmidt, B. Wand, D. Pankert, H. Benner, H. Aoki, A. Ochiai, Phys. Rev. Lett. **82**, 4548 (1999)
28. P. Gegenwarte, H. Aoki, T. Cichorek, J. Custers, N. Harrison, M. Jaime, M. Lang, A. Ochiai, F. Steglich, Physica B **312–313**, 315 (2002)
29. E. Dagotto, T.M. Rice, Science **271**, 618 (1996)
30. H. Onishi, S. Miyashita, Phys. Rev. B **64**, 014405 (2001)
31. H.J. Schulz, Phys. Rev. B **34**, 6372 (1986)