Lattice distortion in disordered antiferromagnetic XY models

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(Received 21 December 2011; revised manuscript received 8 January 2012)

The behavior of lattice distortion in spin 1/2 antiferromagnetic XY models with random magnetic modulation is investigated with the consideration of spin–phonon coupling in the adiabatic limit. It is found that lattice distortion relies on the strength of the random modulation. For strong or weak enough spin–phonon couplings, the average lattice distortion may decrease or increase as the random modulation is strengthened. This may be the result of competition between the random magnetic modulation and the spin–phonon coupling.

Keywords: lattice distortion, random modulation, spin–phonon coupling

PACS: 75.10.Pq, 75.50.Lk, 75.50.Ee **DOI:** 10.1088/1674-1056/21/7/077501

Magnetoelastic instability has received much attention both in experiment and in theory, since it is the foundation of the metal–insulator transition in compound $CuCO_3$.[1–9] This phenomenon may be induced by the spin–phonon coupling, which is generally characterized by a lattice distortion. In periodic low-dimensional spin systems, the lattice distortion indicates dimerized structures.[1,6] Under a quasiperiodic magnetic modulation, the lattice distortion at every site displays a self-similar character.[10] In the adiabatic limit, the lattice distortion may lower the total magnetic energy by a larger amount than the increase in the elastic energy. Then, an energy gap will be opened in the spin excitation spectrum. A number of results have been obtained for periodic Heisenberg chains coupled to phonons.[11–14] Few investigations have been performed in the case of nonperiodic structures. In many cases, the disorder turns out to play a crucial role in low-dimensional magnets.[15–21]

In this paper, we will give our investigations on the lattice distortion in spin 1/2 antiferromagnetic (AF) XY models with random magnetic modulation.

In the adiabatic approximation, the Hamiltonian of the spin 1/2 AF XY model containing lattice distortion, spin–phonon coupling, and random magnetic modulation can be written as

$$H = J\sum_i (1+\alpha u_i)(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \frac{K}{2}\sum_i u_i^2 + \sum_i W_i S_i^z, \tag{1}$$

where S_i^β is the β ($\beta = x,\ y,\ z$) component of the $S = 1/2$ operator at site i, u_i is the lattice distortion between sites i and $i+1$, K is the spring constant, α is the spin–phonon coupling, and N is the number of lattice sites. W_i represents the random magnetic modulations, which are arranged according to random number sequences. The random number sequences are generated by a computer random function. Periodic boundary conditions are imposed ($S_{N+1} = S_1$). J (> 0) is the AF coupling strength and will be taken as the unit of energy. Under the scaling $\alpha u_i \to \delta_i$, the spin–phonon coupling strength α will be absorbed in the spring constant ($K/\alpha^2 \to \eta$).

By using the Jordan–Wigner transformation,[22] the original Hamiltonian can be transformed into

$$H = \sum_i (1+\delta_i)(c_i^\dagger c_{i+1} + c_i c_{i+1}^\dagger) + \frac{\eta}{2}\sum_i \delta_i^2 + \sum_i W_i c_i^\dagger c_i, \tag{2}$$

where $c_i^\dagger$ (c_i) is the creation (annihilation) operator for a spinless electron. Hamiltonian (2) may be exactly diagonalized. We set the random number W_i in the range of $[-\lambda/2,\ \lambda/2]$, where λ represents the random modulation strength. To reveal the general properties of the infinite random chains, we study the average behavior of the physical quantities of an n-membered sequence, in which the physical quantities will be averaged over 500 different random number sequences.

The lattice distortion in Hamiltonian (2) can be obtained by using the self-consistent method intro-

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duced in Ref. [23]. In low-dimensional periodic AF Heisenberg systems, the amplitudes of lattice distortion are identical at every site, which is called dimerization. However, the random magnetic modulation destroys the translational invariance and results in different properties of the lattice distortion. In Fig. 1, we give the absolute values $|\delta_i|$ of the lattice distortion at every site for different spin–phonon coupling strengths, with $\lambda = 2.0$ and $N = 200$. It is found that the amplitudes of the lattice distortion display disordered structures. For the stronger spin–phonon coupling ($\eta = 1.0$), the amplitudes of the lattice distortion are larger than those for the weaker spin–phonon coupling ($\eta = 10.0$). So the spin–phonon coupling may aid the formation of the lattice distortion in random spin systems.

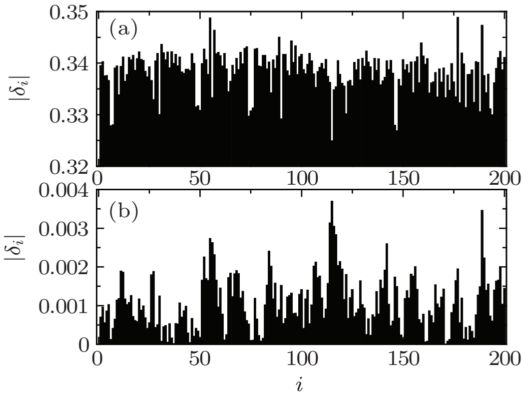

Fig. 1. Lattice distortion $|\delta_i|$ at site i for the spin–phonon couplings of (a) $\eta = 1.0$ and (b) $\eta = 10.0$ with $N = 200$. The random magnetic modulation strength is $\lambda = 2.0$.

Because of the random distribution of the lattice distortion at every site, we define the average distortion amplitude as

$$\langle \delta \rangle = \frac{1}{N} \sum_{i=1}^{N} |\delta_i|, \tag{3}$$

which is used to characterize the general distortion behavior in the random systems. In Fig. 2, the average lattice distortion as a function of random modulation strength λ is depicted for different lattice numbers N and spin–phonon couplings η. It is shown that for stronger spin–phonon couplings, the values of $\langle \delta \rangle$ decrease as λ increases from zero. But for weaker spin–phonon couplings, $\langle \delta \rangle$ will increase with the strengthening of the random modulation. When the random modulation is strong enough, $\langle \delta \rangle$ tends to a finite value for both stronger ($\eta = 1.0$) and weaker ($\eta = 10.0$) spin–phonon couplings. This indicates that for stronger spin–phonon couplings, the random modulation will obstruct the formation of the lattice distortion. However, for weaker spin–phonon couplings, the random modulation will aid the formation of the lattice distortion. Finally, as the competition between the spin–phonon coupling and the random modulation strength reaches a balance, the average lattice distortion will tend to a stabile value. The value of $\langle \delta \rangle$ for $N = 150$ is almost equal to that for $N = 200$. These results confirm that the system sizes studied are large enough and can be used to indicate the results in the thermodynamic limit.

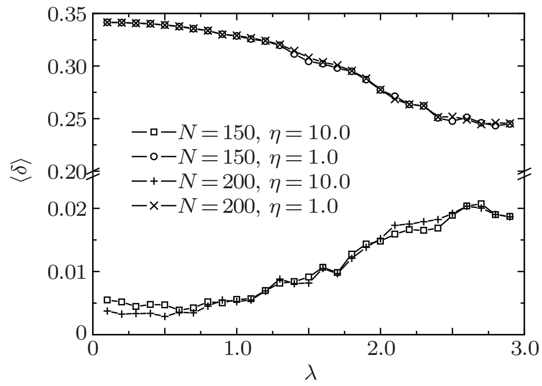

Fig. 2. Average lattice distortion $\langle \delta \rangle$ in the system as a function of random modulation strength λ for different lattice numbers N and spin–phonon couplings η.

Since for stronger or weaker spin–phonon couplings the lattice distortion varies with the disordered strength according to different laws, we are interested in the cases with moderate spin–phonon coupling strengths. In Fig. 3, the spin–phonon coupling dependences of the average lattice distortion are depicted for $\lambda = 1.0$, 2.0, and 3.0. With the increase in the spin–phonon coupling strength, the lattice distortion becomes smaller and smaller. But these curves do not meet at the same point. This indicates that there is no common critical spin–phonon coupling

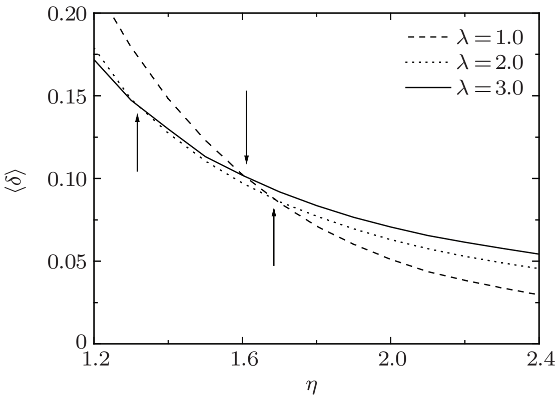

Fig. 3. Average lattice distortion $\langle \delta \rangle$ as a function of spin–phonon couplings η for $N = 150$ and $\lambda = 1.0$, 2.0, and 3.0. The arrows indicate the crossing points.

value at which $\langle\delta\rangle$ will not change with the strengthening of the random modulation. When the spin–phonon coupling lies in a certain range, the change in the lattice distortion is non-monotonic with the increase in the disordered strength.

It is well known that in periodic spin systems, lattice distortion will open an energy gap in the spin excitation spectrum. In random spin systems, the ground state energy gap is also defined as

$$\Delta E = E_0\left(\frac{N}{2}+1\right) - E_0\left(\frac{N}{2}\right), \quad (4)$$

where N is an even number, and $E_0(L)$ is the ground state energy of the system with L spins. The numerical results indicate that the ground state energy gap scales as $\ln\Delta E = -z\ln N + c$, where z is the dynamical exponent, and c is a constant. The z's do not equal zero until the random modulation is eliminated. So for an arbitrary disordered strength, metal–insulator transition will not occur.

In conclusion, the lattice distortion behavior in spin 1/2 AF XY chains is investigated by using an exact diagonalization method under random magnetic modulation in the adiabatic limit. It is shown that the lattice distortion in the random systems relies strongly on the competition between the spin–phonon coupling and the disordered strength. For strong enough spin–phonon couplings, the average lattice distortion is large and may decrease as the random modulation is strengthened. But for weak enough spin–phonon couplings, the average lattice distortion is small and will increase with the strengthening of the random modulation. As the competition reaches a balance, the average lattice distortion will tend to a stabile value.

References

[1] Cross M C and Fisher D S 1979 *Phys. Rev.* B **19** 402

[2] Aizenman M and Nachtergaele B 1994 *Commun. Math. Phys.* **164** 17

[3] Nakano T and Fukuyama H 1980 *J. Phys. Soc. Jpn* **49** 1679

[4] Feiguin A E, Riera J A, Dobry A and Ceccatto H A 1997 *Phys. Rev.* B **56** 14607

[5] Schönfeld F, Bouzerar G, Uhrig G S and Müller H E 1998 *Eur. Phys. J.* B **5** 521

[6] Hase M, Terasaki I and Uchinokura K 1993 *Phys. Rev. Lett.* **70** 3651

[7] Guo D, Kennedy T and Mazumdar S 1990 *Phys. Rev.* B **41** R9592

[8] Sandvik A W, Singh R R P and Campbell D K 1997 *Phys. Rev.* B **56** 14510

[9] Uhrig G S, Schönfeld F, Laukamp M and Dagotto E 1998 *Eur. Phys. J.* B **7** 67

[10] Li Y, Chen Y and Shi Y 2006 *Acta Phys. Sin.* **55** 2539 (in Chinese)

[11] Kouzuki A, Kawasaki K and Nakamura K 1999 *Phys. Rev.* B **60** 12874

[12] Shaz M, Smaalen S V, Palatinus L, Hoinkis M, Klemm M, Horn S and Claessen R 2005 *Phys. Rev.* B **71** 100405

[13] Hirota K, Cox D E, Lorenzo J E, Shirane G, Tranquada J M, Hase M, Uchinokura K, Kojima H, Shibuya Y and Tanaka I 1994 *Phys. Rev. Lett.* **73** 736

[14] Seidel A, Marianetti C A, Chou F C, Ceder G and Lee P A 2003 *Phys. Rev.* B **67** 020405

[15] Carlon E, Lajkó P, Rieger H and Iglói F 2004 *Phys. Rev.* B **69** 144416

[16] Lahiri D, Khalid S, Modak P, Raychaudhuri P, Dhar S K and Sharma1 S M 2010 *Phys. Rev.* B **82** 134424

[17] Lajkó P, Carlon E, Rieger H and Iglói F 2005 *Phys. Rev.* B **72** 094205

[18] Oganesyan V, Pal A and Huse D A 2009 *Phys. Rev.* B **80** 115104

[19] Roy D and Ventra M D 2010 *Phys. Rev.* B **81** 193101

[20] Shan C J, Cheng W W, Liu T K, Huang Y X, Li H and Xia Y J 2008 *Chin. Phys.* B **17** 794

[21] Yuan X J, Zhao B Y, Chen S X and Kong X M 2010 *Chin. Phys.* B **59** 1499

[22] Leib E H, Shultz T and Mattis D J 1961 *Ann. Phys.* **16** 407

[23] Fang Z, Liu Z L and Yao K L 1994 *Phys. Rev.* B **49** 3916