Effects of quantum lattice vibration on the spin-Peierls transitions

Hiroaki Onishi [a,b,c,1], Seiji Miyashita [a]

[a] *Department of Applied Physics, Graduate School of Engineering, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*

[b] *Advanced Science Research Center, Japan Atomic Energy Research Institute, 2-4 Shirakata Shirane, Tokai-mura, Naka-gun, Ibaraki 319-1195, Japan*

[c] *Department of Earth and Space Science, Graduate School of Science, Osaka University, 1-1 Machikaneyama-cho, Toyonaka, Osaka 560-0043, Japan*

Abstract

We investigate a one-dimensional $S = 1/2$ antiferromagnetic Heisenberg model coupled to quantum lattice vibration by a quantum Monte Carlo method. For heavy mass, the lattice fluctuation can be regarded to be adiabatic and the system dimerizes at low temperature. On the other hand, for light mass, the lattice takes a uniform configuration on the thermal average and magnetic properties coincide with those of the uniform lattice system. These phenomena can be understood from the difference of the time scale of the motion between the spin and the lattice.

Key words: spin-Peierls transition; quantum lattice fluctuation; quantum Monte Carlo method; loop algorithm

1. Introduction

The one-dimensional $S = 1/2$ Heisenberg chain shows a spontaneous lattice dimerization. When the mass of the magnetic ion is heavy, the adiabatic treatment for the lattice is valid. In this case, the dimerized state is realized in the ground state for an arbitrarily small spin-phonon coupling [1]. We have studied how the bond alternation develops at finite temperature [2]. On the other hand, for light mass, the lattice dimerization is destroyed due to quantum lattice fluctuation below a critical spin-phonon coupling [3–6].

In this paper, we study the effect of quantum lattice fluctuation in the anti-adiabatic case [7]. We investigate a spin-phonon coupled system described by

$$H = \sum_{i=1}^{N} J\left[1 + \alpha(u_i - u_{i+1})\right] \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \sum_{i=1}^{N} \left[\frac{1}{2m}p_i^2 + \frac{k}{2}(u_i - u_{i+1})^2\right]. \qquad (1)$$

We treat all degrees of freedom as quantum variables which fluctuate in the imaginary time. We use the loop algorithm for the spin [8] and the recipe introduced by Hirsch for the lattice [9]. We adopt the periodic boundary condition for both spin and lattice degrees of freedom. We fix $J = 1$, $\alpha = 1$ and $k = 1$.

2. Quantum latticefluctuation

In Figs. 1 we show the snapshot of the lattice configuration in the Monte Carlo simulation. For a heavy mass $m = 10000$, the lattice behaves adiabatically and the world-line configuration of the lattice is straight along the imaginary-time axis. The straight world lines are parallel with each other and form a dimerized configuration. As a result, we obtain the dimerized lattice configuration on the thermal average. On the other hand, for a light mass $m = 1$, quantum lattice fluctuation causes a curved world line. In this case, we obtain a uniform configuration on the thermal average, which indicates that the deviation of the world line destroys the bond-alternating order.

[1] E-mail: onishi@season.tokai.jaeri.go.jp

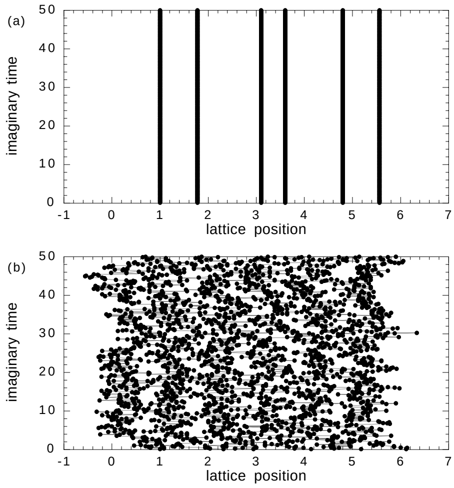

Fig. 1. The snapshot of the relative lattice displacement to the first site at the zero imaginary time for (a) $m = 10000$ and (b) $m = 1$. The data are obtained at $T = 0.02$ for the system of $N = 64$ and the Trotter number $M = 384$. Only the data from the first to sixth sites are shown in the figures.

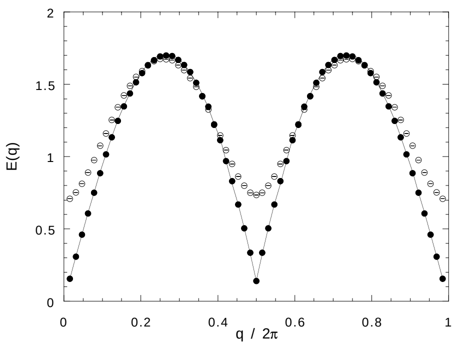

Fig. 2. The dispersion relation of the spin in the ground state of $m = 10000$ (open circle), $m = 1$ (solid circle) and the uniform lattice system (solid line). The data are calculated at $T = 0.02$ for the system of $N = 64$ and the Trotter number $M = 384$.

3. Quantum narrowing effect

In Fig. 2 we show the dispersion relation $E(q)$ of the spin in the ground state. For heavy mass, the system has an energy gap due to the bond alternation. On the other hand, for light mass, $E(q)$ coincides with the uniform lattice system.

Here we study the reason why the largely fluctuating lattice system gives the same magnetic behavior as that of the fixed uniform lattice system. In Fig. 3 we show the imaginary-time correlation functions,

$$S_{\text{spin}}(q,\tau) = \langle \mathrm{e}^{H\tau} S_q^z \mathrm{e}^{-H\tau} S_{-q}^z \rangle, \tag{2}$$

$$S_{\text{bond}}(q,\tau) = \langle \mathrm{e}^{H\tau} \Delta_q \mathrm{e}^{-H\tau} \Delta_{-q} \rangle, \tag{3}$$

where S_q and Δ_q are the Fourier components of the spin and the bond $[\Delta_i = \alpha(u_i - u_{i+1})]$, respectively. We find

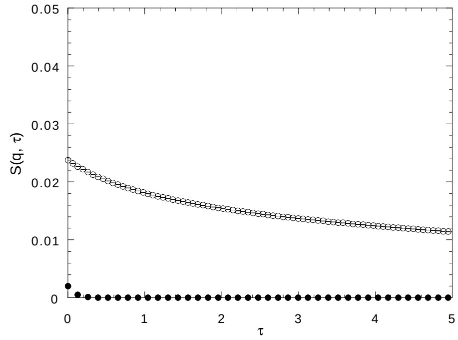

Fig. 3. The imaginary-time correlation function of the spin (open circle) and the bond (solid circle) for $m = 1$. The data are calculated at $T = 0.02$ and $q = \pi$ for the system of $N = 64$ and the Trotter number $M = 384$.

that the fluctuation of the bond along the imaginary-time axis is very rapid comparing with the relaxation of the spin. It indicates that the lattice changes much faster than the time scale of the motion of the spin. Thus we conclude that a kind of narrowing effect happens and the lattice is effectively fixed to be uniform. We call this phenomenon "quantum narrowing effect".

Acknowledgements

The authors are grateful for the use of the Supercomputer Center at the Institute for Solid State Physics, University of Tokyo. Part of the calculation has been done in the computer facility at Advanced Science Research Center, Japan Atomic Energy Research Institute. The present study is partially supported by a Grant-in-Aid from the Ministry of Education, Science, Sports and Culture of Japan.

References

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

[2] H. Onishi, S. Miyashita, J. Phys. Soc. Jpn. **69** (2000) 2634.

[3] L. G. Caron, S. Moukouri, Phys. Rev. Lett. **76** (1996) 4050.

[4] H. Zheng, Phys. Rev. B **56** (1997) 14 414.

[5] A. W. Sandvik, R. R. P. Singh, D. K. Campbell, Phys. Rev. B **56** (1997) 14 510.

[6] R. W. Kühne, U. Löw, Phys. Rev. B **60** (1999) 12 125.

[7] H. Onishi, S. Miyashita, preprint.

[8] H. G. Evertz, in *Numerical Methods for Lattice Quantum Many-Body Problems*, ed. D. J. Scalapino (Perseus books, New York, 1999).

[9] J. E. Hirsch, D. J. Scalapino, R. L. Sugar, R. Blankenbecler, Phys. Rev. Lett. **47** (1981) 1628.