Monte Carlo Study of Spin-Peierls Transition in Quasi-One-Dimensional Heisenberg Model with Finite-Frequency Phonons

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A quasi-one-dimensional spin-1/2 Heisenberg antiferromagnet coupled with quantum phonons is numerically studied by the quantum Monte Carlo method. We have implemented the stochastic series expansion method for the spin part and the path-integral quantization method for the phonon part. In this way, we have calculated the spin-Peierls transition temperature as a function of the frequency of optical phonons. It is found that the transition temperature decreases as the phonon frequency increases. Above critical frequency, the spin-Peierls transition does not occur all the way down to zero temperature due to quantum fluctuations.[1]

The phase diagram is topologically equivalent to that of the two-dimensional Blume-Capel(BC) model with a tricritical point separating the first- and second-order lines. We have determined the universality class of the spin-Peierls transition by the phenomenological finite-size scaling analysis. The transition at lower frequency region belongs to the universality class of the two-dimensional Ising model while the transition at a larger frequency is characterized by the tricritical exponents of the two-dimensional spin-1 BC model. Thus we can conclude that the quantum phase transition from the spin-Peierls to antiferromagnetic state at zero temperature is of the first order.

[1] Y. Matsumoto and A. Terai, submitted to J. Phys. Soc. Jpn.