§40. Computational-Science Study on Quantum Spin Systems by Numerical-Diagonalization Method

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Magnetism of insulating materials is well described by the system of an assembly of quantum spins having interactions with each other. In such a system, a nontrivial quantum wavefunction is realized due to strong quantum effect. Since they are typical many-body problems. Computational methods are very useful from a theoretical viewpoint to obtain a deep understanding of the systems, however, it is known that quantum spin systems are very difficult to be treated theoretically. The existence of frustration and higher spatial dimensionality larger than one make the investigation difficult because the quantum Monte Carlo simulations and the density matrix renormalization group calculations are not useful to systems with such conditions even though we use newly developed and modern computers. The numerical diagonalization method based on the Lanczos algorithm is an available and feasible way; but unfortunately system sizes that can be treated are limited to being very small. To overcome this disadvantage in numerical diagonalization studies, we have developed an MPI-parallelized code of Lanczos diagonalization. We carry out Lanczos-diagonalization calculations using the code to study quantum spin systems from several aspects.

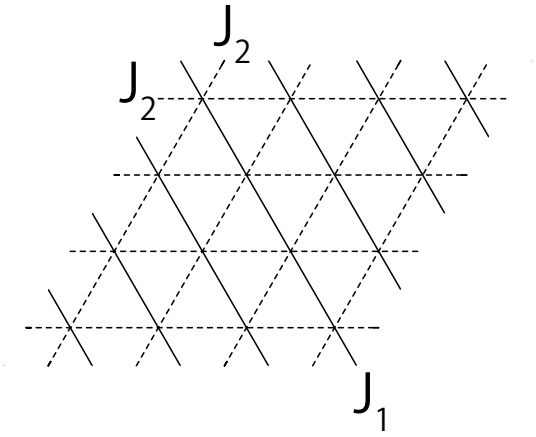

Fig. 1: Spatially anisotropic triangular lattice.

In the fiscal year of 2012, we study the $S = 1$ Heisenberg antiferromagnet on spatially anisotropic triangular lattice[1]. The Hamiltonian of this model is

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{[i,j]} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \qquad (1)$$

where the bonds of interactions with their amplitudes J_1 and J_2 are illustrated in Fig. 1. We examine the behavior of the long-range order of three-sublattice structure observed in the isotropic system between the isotropic case ($J_1 = J_2$) and the case of isolated one-dimensional chains ($J_2 = 0$). In order to extract the information of the three-sublattice magnetic order, we evaluate the quantity given by

$$m^{\mathrm{sq}}_{\mathrm{diag}} = \frac{1}{N_\alpha} \sum_{\alpha} \frac{1}{N_{\mathrm{s}}} \sum_{i} \frac{1}{N_{\mathrm{s}}/3 - 1} \sum_{j \in A_i}{}' \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle, \qquad (2)$$

where $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle$ is evaluated by $3\langle S^z_i S^z_j \rangle$ which are obtained as spin correlation functions by our Lanczos diagonalizations. Here, α denotes the label of directions concerned which is chosen as J_1 among the three directions; we take the average with respect to the direction. N_{s} denotes the number of spin sites. The maximam system size is $N_{\mathrm{s}} = 27$ in this study, which is a new world record among systems composed by $S = 1$ spins to the best of our knowledge. In the isotropic triangular lattice, our extrapolation of the three-sublattice magnetic order that we examined leads to a value which agrees well with the result from the spin-wave approximation. Our numerical data strongly suggest that the magnetic order does not disappear very quickly if the anisotropy of the interactions is switched on, does gradually decrease, and finally disappears. It is found that the region of the long-range ordered phase is much narrower than that was considered from the results by means of approximations.

We have studied quantum spin systems by several numerical approaches including MPI-parallelized calculations of Lanczos diagonalization; our results contribute to our understandings of various phenomena of the systems.

1) H. Nakano, T. Sakai, and S. Todo: J. Phys. Soc. Jpn. **82** (2013) 043715.