§26. Study of Quantum Spin Systems by Largescale Parallel Calculatios

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Magnetism of insulating materials is well described by an assembly of interacting quantum spins. Strong quantum effect often induces a nontrivial wavefunction in such a system. To analyze such systems precisely is, however, difficult because the systems are typical many-body problems. To understand the systems more deeply, under circumstances, computational methods are very useful. Each method has not only merits but also demerits at the same time. Therefore, to treat frustrated systems in dimensions that are larger than one by such a method is quite difficult. When one uses the quantum Monte Carlo simulations to study frustrated systems, one suffers from a so-called negative sign problem. The density matrix renormalization group method, on the other hand, is powerful for one-dimensional cases although the effective applications to systems in dimensions larger than one are now being developed. The numerical diagonalization method based on the Lanczos algorithm is an available and feasible way to apply to two-dimensional frustrated systems. Unfortunately, available system sizes are limited to being quite small. To overcome this disadvantage in numerical-diagonalization studies and to succeed in calculating frustrated systems in two dimensions, we have developed an MPI-parallelized code of Lanczos diagonalization. We carry out calculations of the Lanczos diagonalization with this code.

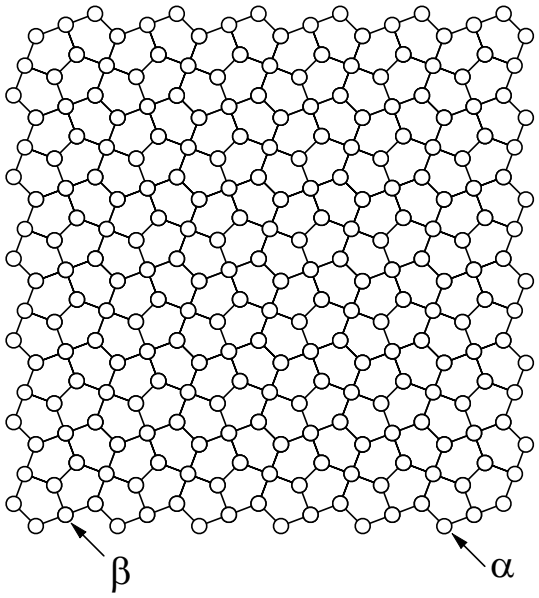

Fig. 1: Cairo-pentagon lattice. There are two types of vertices illustrated by α and β.

In the fiscal year of 2014, we study the magnetization process of the $S = 1/2$ Heisenberg antiferromagnet on the Cairo-pentagon lattice[1, 2]. This lattice is illustrated in Fig. 1. Note here that the lattice includes α and β sites. Thus, the Hamiltonian of this model is

$$\mathcal{H} = J_{\alpha\alpha} \sum_{\langle i,j\rangle, i,j\in\alpha} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_{\alpha\beta} \sum_{\langle i,j\rangle, i\in\alpha, j\in\beta} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \quad (1)$$

where $\langle i, j\rangle$ denotes the summation running over all the nearest-neighbor pairs on the Cairo-pentagon lattice. We examine the magnetization process of this system. We find in the magnetization process that a magnetization plateau appears at the one-third height of the saturation in its magnetization process; the plateau is accompanied by a magnetization jump at one of the edges. The side of the edges with the appearance of the jump depends on the ratio of $J_{\alpha\alpha}$ and $J_{\alpha\beta}$. The jump appears owing to the spin-flop phenomenon which occurs in spite of the fact that the system is isotropic in spin space, where the spin-flop phenomenon is widely known to be a phenomenon that occurs when the system includes some anisotropy. The same behavior was originally observed in the Heisenberg antiferromagnet on the square-kagome lattice. Similar jumps are also observed in the Heisenberg antiferromagnets on the distorted kagome lattice and the *shuriken*-bonded honeycomb lattice[3, 4].

We have also studied other quantum spin systems by MPI-parallelized calculations of Lanczos diagonalization [5, 6, 7, 8]. Our results contribute much to our understandings of several frustrated systems.

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