§29. Study of Quantum Spin Systems by Largescale Parallel Calculations

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Magnetic materials are well described by an assembly of interacting quantum spins. In such a system, a nontrivial wavefunction is often induced by a strong quantum effect. Since the systems are typical many-body problems, however, it is difficult to capture the behavior of such systems. Under circumstances, for a deeper understanding of the systems, computational methods become more and more useful. Each method has both merits and demerits at the same time; therefore, it is quite difficult to treat frustrated systems in dimensions that are larger than one by such a method. When one studies frustrated systems by the quantum Monte Carlo simulations, a so-called negative sign problem happens. The density matrix renormalization group method can be applied to one-dimensional systems but the effective applications to systems in dimensions larger than one are now being developed. Only the numerical diagonalization method is an available and feasible way to apply to two-dimensional frustrated systems even now. Available system sizes, unfortunately, are limited to being quite small. To overcome this disadvantage in this method and to succeed in calculating frustrated systems in two dimensions, we have developed an MPI-parallelized code of nuemrical diagonalization based on the Lanczos algorithm. We use this code to carry out calculations of the Lanczos diagonalization.

In the fiscal year of 2015, we study the magnetization process of the $S = 1/2$ Heisenberg antiferromagnet on the square-kagome lattice with a distortion[1]. The magnetization jump was observed in the case without the distortion[2] originally. However, within this study examining the finite-size systems up to 36 sites, the skip of the jump δM in a finite-size system is detected up to $\delta M = 2$. Only the skip $\delta M = 2$ cannot deny the possibility that this jump appears owing to the formation of the spin-nematic state. The reason is that this state is a two-magnon bound state. We attack, then, calculations for a system with larger size of 42 sites. We successfully obtain the magnetization processes of this model with and without a distortion. In our result for the undistorted system of 42 sites, the same skip of $\delta M = 2$ is detected. When a small distortion is switched on in the square-kagome lattice (see Fig.1), on the other hand, we successfully find the skip of $\delta M = 3$ in the 42-site system. This result means the exclusion of the possibility that this jump occurs owing to the formation of a two-magnon bound state. At the same time, this result suggests that the magnetization jump is a macroscopic phenomenon which survives in the thermodynamic limit. Previously, the same behaviors of the jump were reported for the Heisenberg antiferromagnets on the Cairo-pentagon-lattice[3, 4], the $\sqrt{3}\times\sqrt{3}$-distorted kagome lattice[5, 6], and the *Shuriken*-bonded honeycomb lattice[5]. However, only the finite-size jump of $\delta M = 2$ are detected in these systems. To clarify the behavior of the magnetization jump in the thermodynamic limit, further studies by calculations of larger sizes on these lattices will be required. Such studies will contribute to our understandings of this magnetization jump.

We have also studied the general-S Heisenberg antiferromagnet on the kagome lattice by MPI-parallelized calculations of Lanczos diagonalization [7]. Our results contribute much to our deeper understandings of the nontrivial effect of frustration in magnetic materials.

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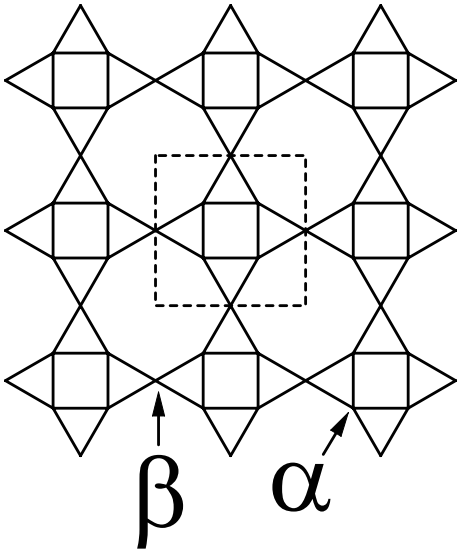

Fig. 1: Square-kagome lattice. Spin sites at vertices are divided into two groups α and β. We consider the distortion when interaction between α-α sites and interaction α-β sites become different.