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

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An assembly of quantum spins with interactions is a system that describes well magnetism of insulating materials. Due to strong quantum effect, nontrivial quantum wavefunctions are realized. It is, however, known that such quantum spin systems are very difficult to investigate because they are typical many-body problems. Computational methods are very useful from a theoretical viewpoint to obtain a deep understanding of the systems. Even though we use newly developed and modern computers, 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. The numerical diagonalization method based on the Lanczos algorithm is available; but system sizes that we can treat are limited to being very small. To overcome this disadvantage we have developed an MPI-parallelized code of Lanczos diagonalization. Using this Lanczos-diagonalization calculation as a primary approach and other numerical methods as supplementary ones, we study quantum spin systems from several aspects.

The kagome lattice and triangular lattice are typical cases of the systems mentioned in the above; we study these systems from various aspects [1, 2, 3, 4, 5]. We clarify that the kagome-lattice Heisenberg antiferromagnet shows a "magnetization ramp," which is anomalous behavior of its magnetization process at the one-third height of the saturation while the triangular-lattice antiferromagnet clearly reveals the magnetization plateau at the same height. Whether or not the kagome-lattice Heisenberg antiferromagnet has nonzero energy gap in its spin excitation is is known as a unresolved and fundamental issue. We successfully calculate the finite-size energy gap of the kagome-lattice Heisenberg antiferromagnet with system size of $N = 42$; our analysis of a system-size extrapolation indicates that the spin excitation is gapless. Specific heat and magnetic susceptibility of the kagome-lattice antiferromagnet with Ising-like anisotropy are also investigated[6]. We study the triangulated-kagome-lattice antiferromagnet; the system reveals three magnetization plateaux[7, 8]. We find in several systems that an intermediate ferrimagnetic phase appears between nonmagnetic state and a known ferrimagnetic state which occurs as a consequence of the Marshal-Lieb-Mattis (MLM) theorem[9, 10, 11, 12]. The ferrimagnetism in the intermediate phase cannot be understood within the MLM theorem. Our findings suggest that frustration plays an important role in the occurrence of ferrimagnetism.

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.

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