Usage Report for Fiscal Year 2015

Project Title:

Numerical study on Kagome-lattice frustrated quantum spin liquids by the iDMRG method

Name: Shigeki Onoda, Hiroshi Ueda

Laboratory at RIKEN: Condensed Matter Theory Laboratory

1. The S=1/2 spins interacting antiferromagnetically with the nearest-neighbor spins on the Kagome lattice is a prototypical geometrically frustrated magnet. It does not show a long-range order magnetic order, and bears a two-dimensional quantum spin liquid without any spontaneously broken symmetry. Some candidate materials are known, although they are not ideal Kagome antiferromagnets. Of our interest in this project is the volborthite $Cu_3V_2O_7(OH)_2$·$2H_2O$. A long-range magnetic order has been observed at a low field region in a nuclear magnetic resonance experiment, while a wide plateau with the 1/3 value of the saturated magnetic moment has been observed in the magnetization curve at high fields. Recently a spatial anisotropy in the network of magnetic interactions has been recognized from first principles based on experimental findings on the crystal structure below the structural phase transition temperature. Numerical exact diagonalization study of this model on a small cluster has explained an unusually wide plateau in the magnetization curve and proposed a possibility of realizing a spin nematic state at a slightly lower field than the plateau. More serious calculations are now called for to test the proposals and further understand the properties at zero, low, and high magnetic fields.

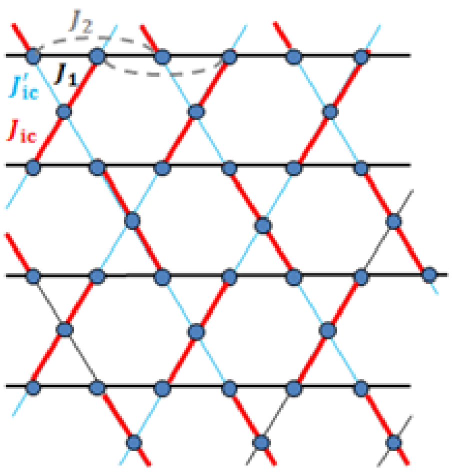

Fig.1: Network of Heisenberg spin exchange interaction in the volborthite.

The more basic project (Q15210), for resolving theoretical issues on the ground state properties of frustrated quantum spin systems candidate to quantum spin liquids, has been extended to a more case-specific study by this project since it was launched in November, 2015.

2. We adopt the density-matrix renormalization group method for infinite systems (iDMRG), and compute the ground state wavefunction by an ansatz of the matrix product state. Since November, we have spent 1.3M hours of CPU time, which is a half of the allocated usage, on the MPC system by Feb. 24.

3. The iDMRG calculations have been performed on a cylinder of the anisotropic Kagome-lattice spin-1/2 model for the volborthite (J_1, J_2, J_{ic}') = (-0.5, 0.2, -0.2) Jic with Jic = 252K, up to m=1000, where m is the number of states kept for describing the ground state. Then, only a gross feature of the magnetization (M) curve has been revealed as a function of the magnetic field (H), as shown in Fig.1, in comparison with previous exact diagonalization results (ED) on a 36-spins cluster. Although more calculations with larger m are still required to reach the convergent continuous curve in a low field region, we have already obtained a converged ground-state

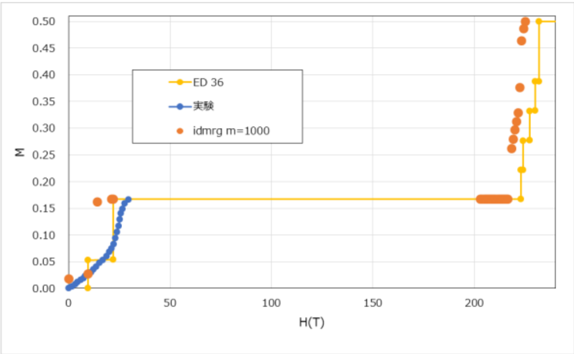

Fig.2: Magnetization M per spin versus the magnetic field H(T).

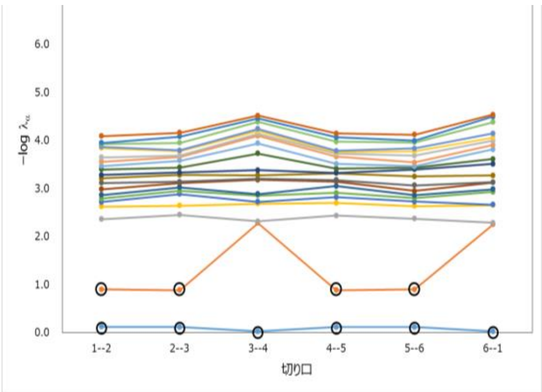

Fig.3: Entanglement spectrum at H=1.3J_{ic} in the case of splitting the whole system into two half-inifite cylinders with a special bond to be cut.

wave-function in the plateau region at intermediate field. The entanglement spectrum (Fig.2) and thus the wavefunction can be quantitatively well described as fully polarized effective spin-1/2 trimers formed by two strongest bonds with the antiferromagnetic coupling Jic. This trimer state has the spin up-down-up polarization in the plateau and does not have any degeneracy in the entanglement spectrum: it is topologically trivial. On the other hand, we found at around H=1.3J_{ic}, the entanglement spectrum at higher fields than the 1/3 plateau shows a double degeneracy in the lowest level, which is gapped from higher levels. This indicates the two possibilities: a topologically nontrivial ground state, or a symmetry broken state, for instance, with a vector-spin-chirality order or a valence bond solid order, has appeared. More calculations are required for identifying the ground states in the low- and high-field regimes.

4. The iDMRG calculations have been performed for the spin-1/2 model for a volborthite. The number of basis states kept in the ground-state wavefunction calculation was restricted to m=1000 because of the CPU time allocated so far. Nevertheless, we have clarified the topologically trivial 1/3 magnetization plateau state, and a crude result on the magnetization curve, as well as a possibly topologically nontrivial or nontrivial symmetry broken state at high fields.

5. We plan to continue the study on the model, to clarify the nature of the ground states at zero, and lower and higher fields than the 1/3 magnetization plateau regime.