Project Title:

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

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1. Conventional magnetic materials show a spontaneous symmetry breaking by the formation of a magnetic order at low temperatures. However, there exist some materials, where a long-range ordering is prevented by quantum spin fluctuations due to a low dimensionality and by a geometrical frustration of magnetic interactions. They are so-called quantum spin liquids and have attracted great interest for hosting a long-range entanglement and fractionalized quasiparticle excitations. The spin-1/2 antiferromagnetic Heisenberg (HB) model on the kagome lattice [Fig. 1 (a)] is a prototypical model for Mott-insulating frustrated magnets.

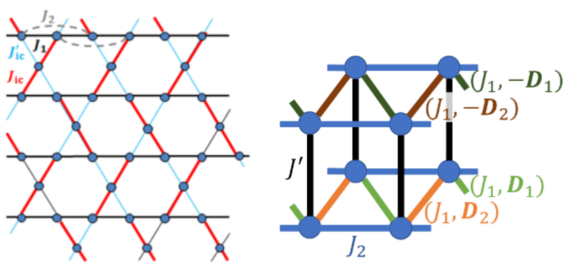

Fig.1: Left: Distorted kagome lattice network of spin exchange interactions proposed for the volborthite. Right: Coupled ferromagnetic-J_1 antiferromagnetic-J_2 frustrated spin ladder for $Rb_2Cu_2Mo_3O_{12}$. The Dzyaloshinski-Moriya vectors are taken as $\boldsymbol{D}_1 = J_1(D_s^x, 0, D_u^z)$ and $\boldsymbol{D}_{1'} = J_1(-D_s^x, 0, D_u^z)$ in one spin chain, and by $-\boldsymbol{D}_1$ and $-\boldsymbol{D}_{1'}$ in the other chain.

A main goal of this project is to understand the magnetic property of not only the ground state but also the low-energy excitations of frustrated kagome antiferromagnets on the kagome lattice in the magnetic field. Of our particular interest is the volborthite $Cu_3V_2O_7(OH)_2$-$2H_2O$, which contains a significant level of distortions of the network of exchange interactions from the ideal kagome lattice, as shown in the left panel of Fig.1. Last year, we successfully obtained the ground-state wavefunction for this candidate model for the volborthite under the magnetic field as well as the magnetization curve compared to the experimental results. However, the magnetization curve is actually not very much sensitive to the details of the model. To explain more experimental results than the magnetization curve, it is important to include effects of magnetic anisotropy, including Dzyaloshinski-Moriya interactions. It is also necessary to compute the excited states for explaining spectroscopic properties. For this purpose, we have planned to include Dzyaloshinski-Moriya interaction into the density-matrix renormalization group method for infinite systems (iDMRG) and then compute excited states. To test the new implementation, we have worked on a simpler system of the one-dimensional frustrated spin-1/2 ladder material $Rb_2Cu_2Mo_3O_{12}$, which has been experimentally uncovered as a spin-gapped ferroelectric system.

2. We apply the real-space parallelized iDMRG method to compute the ground state and several low-energy excited states of the model explained in the right panel of Fig.1. We have spent 1.3M hours and 59k hours of CPU time on the MPC and ACSG systems, respectively, by February 22, 2017.

3. We have established an algorithm for calculating low-energy excited-state wavefunctions from the ground state and its implementation into the iDMRG code, as far as the first excitation energy from the ground state is finite. First, an impurity structure was introduced into the otherwise periodic matrix product state describing the ground state. Then, a periodicity of the excited states, which are orthogonal to the ground state, was approximately recovered through an update procedure of the iDMRG. Finally, a convergence was checked with respect to the number of states kept in the iDMRG. These excited-state wavefunctions have then been used to compute various experimental observables, including inelastic neutron-scattering spectra and the electron spin resonance spectra.

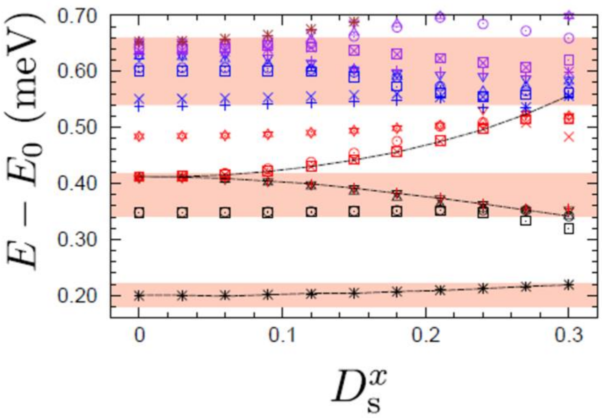

Fig.2: Energy spectrum for $D_u^z = 0.12$, $J_1/J_2 = -3.1$, $J'/J_2 = 0.47$, $J_2 = 37.5$ (K). Excited levels from the ground state are depicted by the symbols +, ×, □, ○, △, and ▽. Three shaded bands represent the areas for the first three low-energy peaks in inelastic neutron-scattering spectra of $Rb_2Cu_2Mo_3O_{12}$.

We have successfully obtained the low-lying energies and checked the validity by comparison with the exact diagonalization results on a small cluster of 28 spins. The exchange coupling parameters that reproduce neutron-scattering experiments in $Rb_2Cu_2Mo_3O_{12}$ have also been found. Using these excited state wavefunctions, electron spin resonance spectra are now under investigation.

4. We can reasonably obtain the low-lying energy spectra by slightly modification of the matrix product state given by the density matrix renormalization group for infinite one-dimensional systems, especially the spin-gapped frustrated spin-1/2 ladder system $Rb_2Cu_2Mo_3O_{12}$.

5. In the next fiscal year, we plan to continue this project. In particular, as a smoking gun of the current framework, we compute the electron resonance spectra in the same frustrated spin-1/2 ladder system describing the magnetic property of $Rb_2Cu_2Mo_3O_{12}$. After that, we apply the framework to the volborthite of our main interest, and then resolve controversies over experimental results on this material.

Usage Report for Fiscal Year 2016

Fiscal Year 2016 List of Publications Resulting from the Use of the supercomputer

Hiroshi Ueda and Shigeki Onoda, "Frustrated spin-1/2 zigzag chains with alternating exchange coupling and anisotropy", 8th International Conference on Highly Frustrated Magnetism (Taipei, Taiwan, September 8, 2016).