Usage Report for Fiscal Year 2015

Project Title:

Numerical studies on two-dimensional frustrated quantum spin systems by the DMRG and tensor-network methods

Name: Shigeki Onoda, Hiroshi Ueda, Troels Bojesen

Laboratory at RIKEN: Condensed Matter Theory Laboratory
Quantum Matter Theory Research Team, Center for Emergent Matter Science

1. Two-dimensional frustrated spin-1/2 systems provide intriguing possibilities of realizing quantum spin liquids without any spontaneously broken symmetry. The Kagome lattice antiferromagnet is a promising candidate to host a quantum spin liquid ground state, although the nature of the spin liquid ground state, including the issue of the presence or absence of the spin gap, remains controversial to date. The density-matrix renormalization group (DMRG) method has been widely applied to attack the problem. However, because of the two-dimensionality, the geometry is usually restricted to a cylindrical geometry with a short length around the cylinder, making an aspect ratio very large. The DMRG method with a sine square deformation has been applied to the problem, but it may also contains a bias depending on the choice of the center. Now it is highly required to check the validity of the DMRG method in the case where the quantum Monte-Carlo (QMC) simulations do not suffer from the negative sign problem and can provide statistically exact results to be compared to DMRG results and then to recently developed variational results based on tensor networks. This will increase the credibility and efficiency of the new numerical algorithms of both the DMRG and tensor-network calculations, on even more nontrivial cases including the Kagome Heisenberg antiferromagnet.

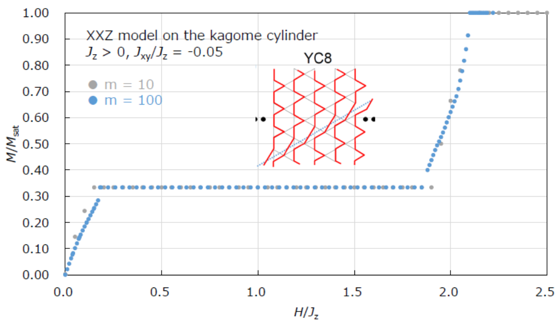

Fig.1: Magntization curve of spin-1/2 Kagome XXZ model with ferromagnetic Jxy and antiferromagnetic Jz.

2. We first adopt the density-matrix renormalization group method for infinite systems (iDMRG), to compute the ground-state wavefunction by an ansatz of the matrix product state with a certain translational unit. The tensor-network method has just been perfoemd just for tests, since it is much more costly in may aspects. Since May, 2015 when the project was launched, 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. At the moment, we have succeeded in implementing an efficient iDMRG algorithm so that it can provide a continuous magnetization curve in the nearest-neighbor spin-1/2 Kagome XXZ model with a ferromagnetic Jxy and antiferromagnetic Jz, as shown in Fig.1. There is a previous report on QMC calculations in the same model, in which the region of the 1/3 magnetization plateau was numerically clarified. Our results approach to the QMC results within the error bars if we increase the number of basis states kept in the iDMRG method from m=10 to m=100, although this number for the iDMRG method to work will depend on models.

Systematic iDMRG and QMC calculations on this particular model for a benchmark of the algorithm are underway. Once we almost finish this comparison, we plan to embark on the tensor-network calculations and compare the results with the QMC and iDMRG calculations, which will enable us to examine the dependence on the aspect ratio of the kagome lattice geometry.

4. The iDMRG calculations have been performed for the spin-1/2 XXZ model on the kagome lattice with a ferromagnetic Jxy and an antiferromagnetic Jz. With the number of basis states kept in the ground-state wavefunction calculation up to m=100, it was possible to reproduce the magnetization curve obtained with the QMC simulations.

5. We request a renewal of the project in the FY2016, to complete a comparison of results of the iDMRG and tensor-network calculations with the QMC. The nature of the 1/3 magnetization plateau state will also be clarified from viewpoints of the entanglement spectrum.