Usage Report for Fiscal Year 2016

Project Title:

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

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1. Frustrated quantum spin-1/2 systems provide intriguing possibilities of hosting unconventional nontrivial ground states that do not have classical counterparts. It may happen that instead of showing any classical long-range order whose ground state can be described by a direct product of local states, spins show a quantum entanglement over a long distance in a stable phase. Such quantum ground states are called quantum spin liquids. On the other hand, it is also possible that only a finite-size cluster of spins are entangled and the ground state can be described by their direct product states. Such short-range entangled states are categorized into valence bond solids. It has been found that a kagome-lattice antiferromagnet is a promising candidate to host a quantum spin-liquid ground state at zero magnetic field and a valence bond solid ground state at finite magnetic fields. However, the nature of the spin liquid and valence bond solid ground states remain elusive. To tackle this issue, the density-matrix renormalization group method for infinite systems (iDMRG) or tensor-network methods are powerful, since they provides a numerically exact or variational ground-state wavefunction, without a negative sign problem as in the quantum Monte-Carlo method. Last year, we performed extensive iDMRG calculations on a simple nearest-neighbor spin-1/2 XXZ model,

$$H = \sum_{<r,r'>}^{n.n.} \left(J_{xy}\left(S_r^x S_{r'}^x + S_r^y S_{r'}^y\right) + J S_r^z S_{r'}^z\right) - B \sum_r S_r^z$$

for $J_{xy} < 0$ and $J > 0$ on the kagome lattice in a cylindrical geometry with an extremely large aspect ratio. Although we successfully obtained a magnetization curve (Fig.1), it has been required to check the validity by comparing the results with those of the quantum Monte-Carlo (QMC) simulations. Especially, the ground-state properties at the magnetization plateau remain open to date.

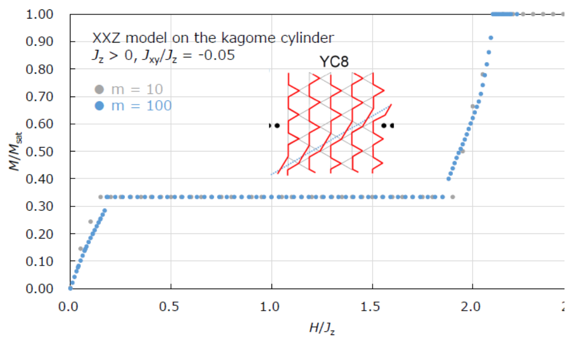

Fig.1: Magntization curve of the spin-1/2 kagome XXZ model with ferromagnetic J_{xy} and antiferromagnetic $J = J_z$.

2. We have implemented an efficient numerical code for QMC simulations based on the modified directed loop algorithm in a continuous imaginary time. Using this QMC code, we studied a relevant model of a minimal quantum spin ice on the pyrochlore lattice, as in another project Q16343. The relevance to the kagome problem is clear. The pyrochlore lattice is comprised of alternately stacked triangular-lattice and kagome-lattice layers. We have spent 1.26M hours and 58k hours of CPU time on the MPC and ASCG systems, respectively, by February 24.

3. As reported in the project Q16343, quantum

spin ice under a [111] magnetic field shows a 2/3 magnetization plateau, where all the spins on the triangular-lattice layers are aligned by the field, leaving almost decoupled kagome-lattice layers, each of which corresponds to the above spin-1/2 XXZ model on the kagome lattice. We have focused on this magnetization plateau region of the prochlore problem. The QMC results on the neutron-scattering cross-section in this plateau regime are shown in Fig.2. On cooling, we have observed a rapid increase of superlattice peaks associated with the enlarged unit cell by $\sqrt{3}\times\sqrt{3}$ on each kagome layer. (Compare Fig.2a for a higher temperature with Fig.2b for a lower temperature and see Fig.2e). The spatial profile (Fig.2b) at the lowest temperature is consistent with the valence bond solid depicted in Fig.3. We have also tried to extend the iDMRG code to correctly describe this valence bond solid. However, it has turned out that because the unit cell is enlarged, it is required to take a much larger translation unit for the matrix product state representation of the ground state by the iDMRG method than we intended last year. This must be treated in the near future.

4. We have revealed that the magnetization plateau state of the spin-1/2 XXZ model on the pyrochlore lattice under the [111] magnetic field has a valence bond solid order enlarging the unit cell by $\sqrt{3}\times\sqrt{3}$. This is consistent with the previous QMC calculations on the relevant kagome-lattice model.

5. Now that the $\sqrt{3}\times\sqrt{3}$ enlarged unit cell is confirmed, we plan to perform iDMRG calculations on the plateau regime by taking into account this enlarged unit cell in the next fiscal year. Then, we will tackle more generic and controversial cases including the kagome Heisenberg antiferromagnet at zero magnetic field.

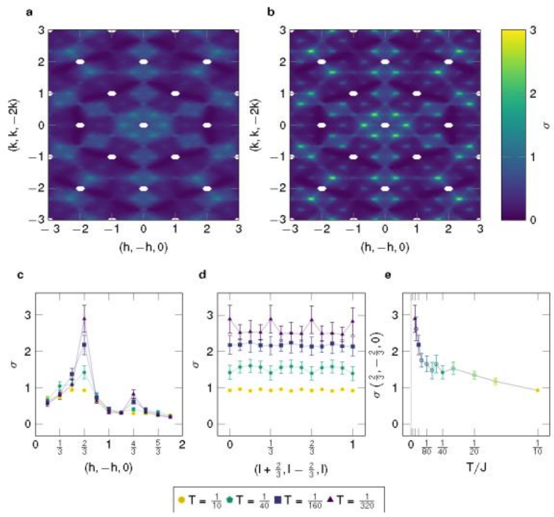

Fig.2: QMC results on the neutron-scattering cross-section σ for $J_{xy}/J = -0.15$. a: $T/J = 1/20$. b: $T/J = 1/320$.

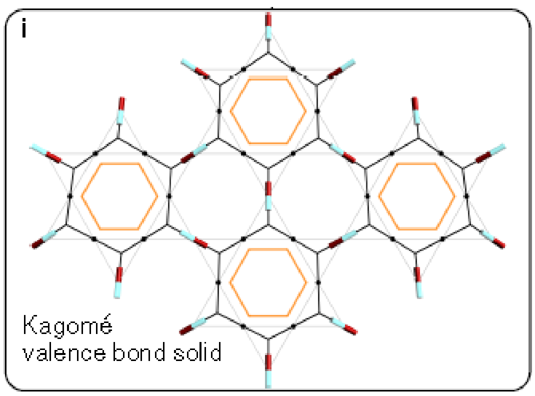

Fig.3: Pictorial representation of a candidate ground state of a kagome valence

Fiscal Year 2015 List of Publications Resulting from the Use of the supercomputer

[Oral presentation at an international symposium]

Shigeki Onoda, “Resolving controversies on quantum spin ice: $Yb_2Ti_2O_7$ and $Tb_2Ti_2O_7$”, International Conference on Highly Frustrated Magnetism 2016 (Taipei, Taiwan, September 7, 2016).

Troels Arnfred Bojesen and Shigeki Onoda, “Quantum spin ice under a [111] magnetic field: from pyrochlore to kagome”, 2017 American Physical Society March Meeting (New Orleans, USA, March 15, 2017).