Usage Report for Fiscal Year 2016

Project Title: Quantum Monte-Carlo study on quantum spin ice under the magnetic field

Name: Shigeki Onoda, Troels Bojesen, Hiroshi Ueda

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

1. Frustrated quantum magnets provide an intriguing laboratory for realizing novel states of condensed matter. In particular, quantum spin liquids are postulated as Mott-insulating states with electron spins being disordered and fractionalized into so-called spinons. Among many candidates are magnetic rare-earth pyrochlores modeled as quantum spin ice. It has attracted great interest for hosting a U(1) quantum spin liquid, which involves spin-ice monopoles as gapped deconfined spinons as well as gapless excitations analogous to photons, as indeed evidenced by our previous unbiased quantum Monte-Carlo simulations. However, the fate of these monopoles and photons under a [111] magnetic field remains unanswered. In the classical case, a weak field aligns the spins on triangular-lattice layers, producing kagome spin ice with a 2/3 magnetization plateau. An increase in the field induces a direct discontinuous transition to a fully polarized state through a perfect ionization and crystallization of monopoles. Now unbiased numerical simulations on quantum spin ice under the [111] magnetic field have been called for.

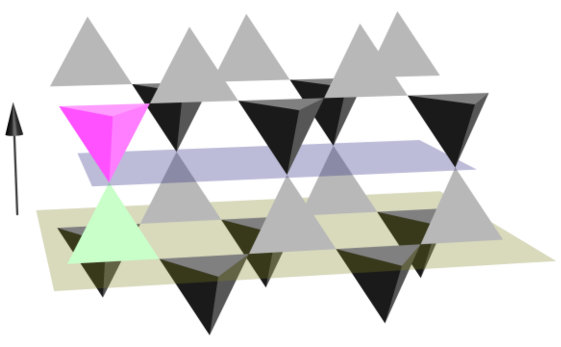

Fig.1: Pyrochlroe lattice structure composed of a corner-sharing network of tetrahedral. It contains alternately stacked triangular-lattice and kagome-lattice layers along a [111] direction (arrow).

2. We have performed extensive numerical simulations on the minimal nearest-neighbor quantum spin ice model,

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

where $J_\perp$ and $J(>0)$ represent the nearest-neighbor transverse and longitudinal exchange couplings, respectively, and B a magnetic field applied along the [111] direction. We have defined a set of spin-1/2 operators (S_r^x, S_r^y, S_r^z) on a pyrochlore lattice site r in such a set of local coordinate frames that the local z direction points to a center of the tetrahedron. In particular, the inner product c_r of the [111] applied field and the local z directions takes 1 at the triangular-lattice sites and -1/3 at the kagome-lattice sites. We have adopted a quantum Monte-Carlo method with a modified directed loop algorithm in a continuous imaginary time. CPU times of 0.64M hours and 54k hours have been consumed on the MPC and ACSG systems, respectively, by February 21st.

3. We have computed a [111] magnetization $m = \sum_{r\in T_R} c_r S_r^z$ and an ionized monopole charge $\delta Q = \left|\sum_{r\in T_R} S_r^z\right|$ per each tetrahedron as well as two components of the transverse spin stiffness, which is equivalent to one fourth of the monopole superfluid stiffness, $\rho_{(111)}$ and $\rho_{[111]}$ being normal and parallel to the [111] field direction. The results for $J_\perp/J = -0.15$ are shown in Fig.2. Increasing B from 0 up to $\sim 0.1J$ at the lowest value of temperature T, m arises from 0 with a

finite slope, while both $\rho_{(111)}$ and $\rho_{[111]}$ steeply decay to zero, pointing that the monopole superfluid at the zero magnetic field dies out quickly. Further increasing B up to $B_1 \sim 0.4J$, m increases up to 2/3 and is pinned at the 2/3 plateau up to $B_2 \sim 1.4J$. In these low-field ranges, monopoles are prevented from living on a long-time scale, so $\delta Q = 0$, as in kagome spin ice. With further increasing B above B_2, m restarts increasing from 2/3 and simultaneously, δQ, $\rho_{(111)}$, and $\rho_{[111]}$ also start increasing from zero. This defines a monopole supersolid showing a partial ionization $0 < \delta Q < 1$ of monopoles and a long-range transverse spin order. The spin stiffness is strongly anisotropic with $\rho_{(111)}$ being an order of magnitude larger than $\rho_{[111]}$, indicating that the transverse spin order is triggered by correlations within kagome layers. A further increase in B drives a phase transition to the inonic monopole insulator with $\rho_{(111)} = \rho_{[111]} = 0$. It has also been found that with increasing $J_\perp/J$, B_1 and B_3 increase while B_2 decreases.

4. Our extensive quantum Monte-Carlo simulations have uncovered the global phase diagram of a minimal quantum spin ice model in the space of $J_\perp/J$, T, and B. Two-step discontinuous transitions from pyrochlore spin ice through kagome spin ice to the fully polarized 3-in, 1-out state in classical spin ice under the [111] magnetic field is replaced with successive transitions from a U(1) quantum spin liquid though a quantum variant of kagome spin ice showing the 2/3 magnetization plateau state to the monopole supersolid, and then to the fully polarized state in the case of quantum spin ice. The nature of the kagome spin ice plateau state is studied in another project Q16210.

5. We request a renewal of the project in the FY2016, to complete calculations beyond $J_\perp/J = -0.15$ probably up to $J_\perp/J \sim -0.5$ to observe that the kagome spin ice plateau shrinks. It is also crucial to perform $T = 0$ calculations in order to directly tackle the topological properties of the U(1) quantum spin liquid ground state and the kagome plateau state.

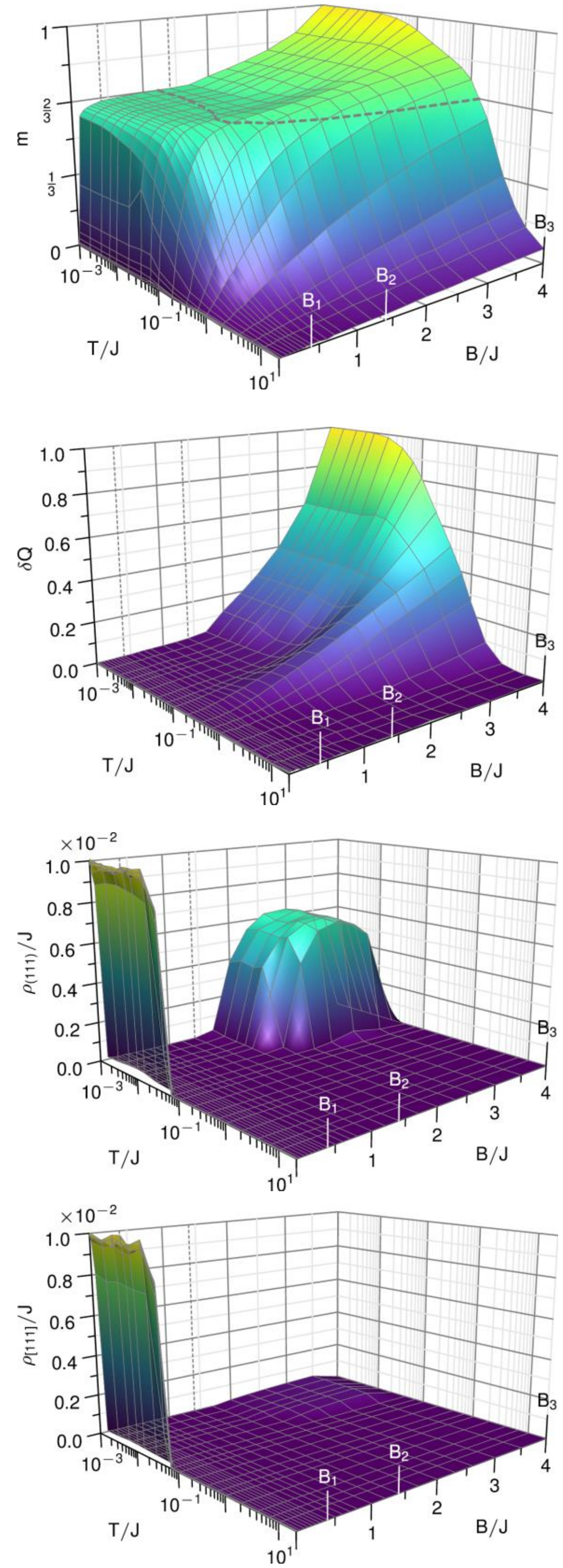

Fig.2: Quantum Monte-Carlo results on m, δQ, $\rho_{(111)}$, and $\rho_{[111]}$ for 4×10^3 spins and $J_\perp/J = -0.15$.

Fiscal Year 2016 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).