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

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1. Quantum spin ice is a quantum variant of classical spin ice. In classical spin ice, Ising degrees of freedom localized at vertices of corner-sharing tetrahedra that forms the pyrochlore lattice interact with each other, so that two spins point inwards to and the other two outwards from the center in each tetrahedron. Creating "3-in, 1-out"/"1-in, 3-out" or "all-in"/"all-out" magnetic monopole defect charges costs an energy and is forbidden at low temperatures. This leaves macroscopic degeneracy of the "2-in, 2-out" spin-ice-rule ground state manifold. On the other hand, in quantum spin ice, quantum-mechanical spin exchange interactions allow a virtual hopping of monopole charges and lifts the degeneracy completely. This leads to a long-range quantum-entangled spin liquid state harboring an analogous quantum electrodynamics with emergent photons and deconfined electric and magnetic monopoles. This 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.

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,

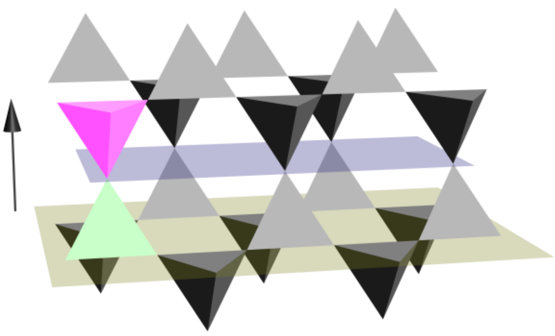

Fig.1: Pyrochlroe lattice structure composed of a corner-sharing network of tetrahedral. It contains alternately stacked triangular-lattice and kagome-lattice layers along a [111] direction (arrow).

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 b opoles 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

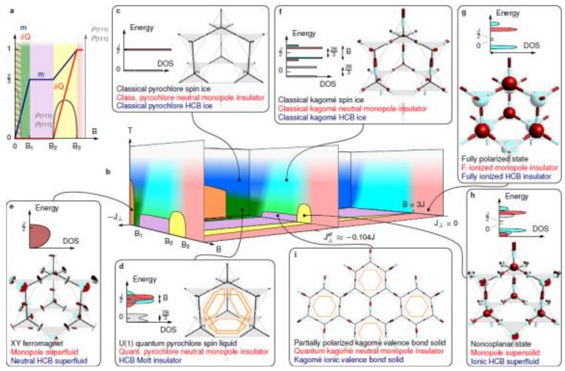

Fig.2: Quantum Monte-Carlo results on m, δQ, $\rho_{(111)}$, and $\rho_{[111]}$ for 4×10^3 spins and $J_\perp/J=-0.15$.

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.

Usage Report for Fiscal Year 2017

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

[Publications]

Troels Arnfred Bojesen, *Shigeki Onoda*, "Quantum spin ice under a [111] magnetic field: from pyrochlore to kagomé", Physical Review Letters **119**, 227204 (2017).

[Oral presentation at an international symposium]

Shigeki Onoda, "Quest to U(1) quantum spin liquids, valence bond solids, and novel ordered phases in pyrochlores and spinels: unconventional quasiparticles and interference effects", Junjiro Kanamori Memorial International Symposium (Univ. of Tokyo, Tokyo, Sep. 27-29, 2017). (Invited.)

Troels Arnfred Bojesen, *Shigeki Onoda*, "U(1) quantum spin liquid and valence bond solid ground states of quantum spin ice under a [111] magnetic field", 28th International Conference on Low Temperature Physics (Gothenburg, Sweden, Aug. 9-16, 2017). (Invited.)

Shigeki Onoda, "Quest to U(1) quantum spin liquids, valence bond solids, novel ordered phases in pyrochlores and spinels: unconventional quasiparticles and interference effects", Topological States and Phase Transitions in Strongly Correlated Systems (Kavli Institute for Theoretical Sciences, Univ. of Chinese Academy of Sciences, Jul. 3-21, 2017). (Invited.)

Shigeki Onoda, "Quantum spin ice under a [111] magnetic field: from pyrochlore to kagomé", Frustrated Magnetism: Conference (Institute of Mathematical Sciences (IMSc), Chennai, India, Apr. 10-12, 2017). (Invited.)

Shigeki Onoda, "Quantum spin ice" Part I, II, and III, Frustrated Magnetism: School (Institute of Mathematical Sciences (IMSc), Chennai, India, Apr. 3-9, 2017). (Invited.)

[Others (Press release, Science lecture for the public)]

“Monopole current offers way to control magnets”, (http://www.riken.jp/en/pr/press/2017/20171201_2/) RIKEN press release in English (December 1, 2017). See also the Japanese version (http://www.riken.jp/pr/press/2017/20171114_1/).

“Monopole current offers way to control magnets”, RIKEN RESEARCH 2018 Spring issue.