Monte Carlo Study of Spin-Ice type Kondo Lattice Model

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Recently, metallic pyrochlore oxides $R_2T_2O_7$ (R=rare earth, T=transition metal) have attracted much interest as a typical system with both strong electron correlation and geometrical frustration. Experimentally, they are known to exhibit a variety of fascinating phenomena. For instance, unconventional anomalous Hall effect and resistivity minimum are observed in several Mo and Ir pyrochlore oxides. Metal-insulator transition are also known to take place in these compounds. These exotic phenomena have triggered intensive theoretical studies on the interplay between spin and charge in frustrated systems, but the role of the interplay is yet far from being fully understood. This is partly due to the severe phase competition under the spin-charge interplay and resulting strong fluctuations. Hence, it is highly desired to study the problem by unbiased methods that fully include the effects of competition and fluctuations.

In this study, we investigate finite-temperature magnetic phase diagrams of a simplified model for the metallic pyrochlore oxides, a Kondo lattice model on a pyrochlore lattice:

$$H = -t\sum_{\langle i,j\rangle}(c_{i\sigma}^{\dagger}c_{j\sigma} + h.c.) + J_K\sum_i S_i\cdot\sigma_i + J_S\sum_{\langle i,j\rangle} S_i\cdot S_j\ . \qquad (1)$$

Here, $c_{i\sigma}$ ($c_{i\sigma}{}^{\dagger}$) is the annihilation (creation) operator for itinerant electrons with spin σ at the ith site. S_i and σ_i is the localized spin and Pauli matrices for itinerant electrons at the ith site. Here, the localized spins are of spin-ice type, which are Ising spins with local [111] easy axes [See figure (a)]. We map out the phase diagram by using an unbiased Monte Carlo simulation on the Kondo lattice model, and classical Monte Carlo simulation for an effective Ising model derived from Eq. (1). As a consequence of the spin-charge interplay, the model exhibits many intriguing phases. For instance, in the intermediate coupling region, we find a 32-sublattice order with concomitant charge order. We demonstrate a switching of the charge order by external magnetic field. Meanwhile, in the strong coupling region, we discover a classical spin-liquid state with broken spatial inversion symmetry. This is a peculiar state which exhibits the spin-Hall effect even in the absence of spin-orbit coupling.

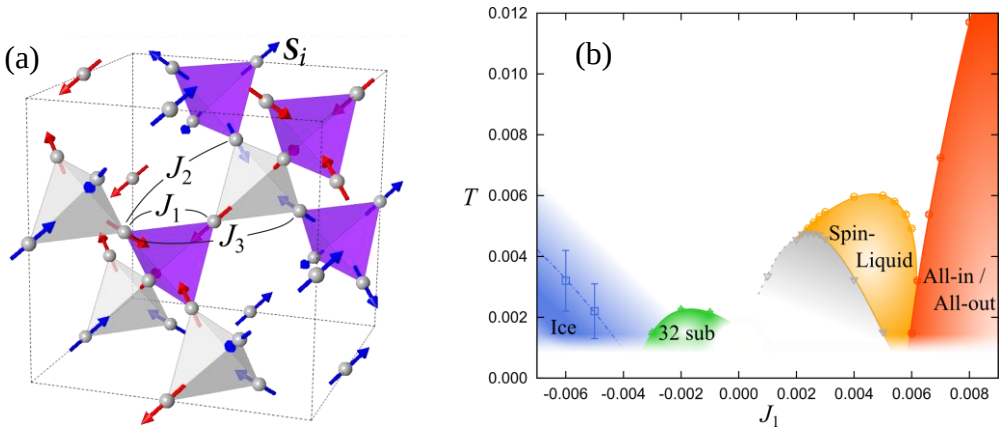

Figure: (a) Schematic picture of the spin-liquid phase in a spin-ice type Kondo lattice model on a pyrochlore lattice. The nearest, 2nd nearest, and 3rd nearest neighbour interactions we considered in the effective spin model are shown by J_1, J_2, and J_3, respectively. (b) The magnetic phase diagram for the model Eq. (1) while varying J_1 and T. J_2 and J_3 are fixed to the value obtained by perturbation theory.