Abstract

Ice rule is a local constraint on the spatial configuration of Ising-type variables, originally proposed in the context of proton configurations in water ice. The local constraint induces a peculiar form of degenerate manifold at low temperatures. The physics related to the ice-rule manifold is widely observed in condensed matter physics, and has attracted increasing interest, stimulated by the discovery of many fascinating phenomena in geometrically-frustrated systems. In particular, the role of quantum fluctuations is intriguing to illuminate new aspects in the frustrated ice-rule systems.

In this thesis, we theoretically investigate the effect of quantum fluctuations on the ice-rule systems. The purpose of our study is to elucidate the effect of interplay between geometrical frustration and the quantum fluctuation on the macroscopic behavior of the system. To clarify the fundamental physics originating in both frustration and fluctuation, we employ unbiased computational methods, such as the numerical diagonalization and the qunatum Monte Carlo simulation. In particular, we focus on the two different aspects of quantum fluctuations; one is the itinerancy of electrons and the other is the transverse magnetic field.

For the former, we study a frustrated Falicov-Kimball model as a minimul model. We elucidate the remarkable effects of the ice-rule local constraint on the conduction properties and electronic structure of the itinerant electrons. The opening of energy gap at a considerably small repulsive interaction compared to the bandwidth is found universally, irrespective to the lattice structures we considered. This is a novel phase transition to a peculiar "charge-ice" insulator, which uniquely emerges in the itinerant ice-rule systems.

For the latter problem of the transverse field, we investigate the thermodynamic properties of the transverse-field Ising models on a frustrated checkerboard lattice. In the first step, we examine the order-by-disorder phenomena at low temperature in the presence of the transverse field. We find a new stripe state in the region where the ice-rule manifold becomes unstable by a longitudinal magnetic field. Next we apply the model to a hydrogen-bonded system with the ice-rule type frustration, squaric acid crystal. We map out the phase diagram of the effective model and compare the result with the experiment in applied external pressure. We successfully reproduce the presence of a peculiar locally-correlated paraelectric state down to low temperatures under the transverse field, in which the ice-rule local constraint persists but the global long-range order is destroyed. These are the direct consequences of the interplay between the geometrical frustration and quantum fluctuations.