Numerical Study of Itinerant Electron Systems Coupled with Classical Degrees of Freedom under Geometrical Frustration

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Geometrically frustrated systems have been a matter of interest for a long time owing to their unusual features originating from macroscopic degeneracy, such as residual entropy, liquidlike behavior, and non-trivial orderings. Recently, the effect of frustration has attracted increasing interest in itinerant electron systems. For instance, some transition-metal oxides with frustrated pyrochlore structure exhibit unconventional transport properties. To elucidate the essential role of frustration in such itinerant systems, we here investigate two fundamental models in which electrons couple with classical degrees of freedom on frustrated lattices. One is a Falicov-Kimball model on various frustrated lattices with an ice-rule type local constraint on the configuration of localized particles[1,2]. By numerical diagonalization as well as an analytic solution, we clarify the peculiar nature of phase transition to a charge-ice insulator. The other model is a Kondo lattice model with Ising spins on a pyrochlore lattice[3]. By large-scale Monte Carlo simulation using the truncated polynomial expansion technique, we find a series of distinct magnetic phases and their competition while changing the electron density and coupling constant.

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[2] H. Ishizuka, M. Udagawa, and Y. Motome, Phys. Rev. B **83**, 125101 (2011).
[3] H. Ishizuka, M. Udagawa, and Y. Motome, in preparation.