Abstract

As *the third type of solids*, quasi-crystals have attracted much attention for more than thirty years since the discovery by D. Shechtman and his coworkers. Their peculiar electronic and transport properties have been extensively studied both experimentally and theoretically. Recently, the finding of quantum critical behavior in a magnetic quasi-crystal has gained renewed interest from the viewpoint of strong electron correlations. However, it is a theoretical challenge to elucidate the correlation effects on the quasi-periodic systems since the loss of lattice periodicity makes most of the standard techniques in solid state physics ineffective. Despite several efforts, the effects of cooperation between quasi-periodicity and electron correlations remain elusive. In order to clarify such synergetic effects, in this thesis, we theoretically investigate two models on two-dimensional Penrose lattices: the Ising model and the Falicov-Kimball model. The former is one of the simplest models in statistical mechanics and the latter is a fundamental model for the correlation effects in itinerant electron systems. We study the finite-temperature properties of these models using the replica-exchange Monte Carlo method. For the Ising model, first we study the phase transition to the Néel-type antiferromagnetic state. We find that, at low temperatures in the ordered phase, the simulation suffers from domain formation despite the use of the replica-exchange processes. We discuss the possible origin from the viewpoint of peculiar geometry of quasi-periodic clusters used in the simulation. Next, we study the effect of magnetic frustration by introducing the next-nearest neighbor coupling. Although we find the suppression of the antiferromagnetic order, the simulation becomes very hard for the frustrated cases and the complete phase diagram is left for future study. For the Falicov-Kimball model, we first study the noninteracting case and demonstrate that the system exhibits the peculiar electronic structures due to the quasi-periodicity, such as the singularity in the density of states, pseudogaps, and confined states. Then, we study the effects of electron correlations in the half-filling case with particle-hole symmetry. We find a phase transition to the Mott insulator with Néel-type ordering at low temperatures, and obtain the phase diagram while changing the electron correlation. We also study the effect of carrier doping by changing the chemical potential. We find that the model exhibits a peculiar Mott insulating state, in which the densities of itinerant and localized electrons vary with the electron correlation, while their sum is pinned at a commensurate value, half-filling. Analyzing the real-space distribution of the itinerant electrons, we elucidate that the peculiar behavior originates from the hierarchical energetics in the strongly

correlated insulator, reflecting the special geometry of the quasi-periodic lattice. Our finding suggests that the cooperation between electron correlations and quasi-periodicity leads to a new type of Mott insulating state with unusual charge fluctuations.