Abstract

Recently, noncoplanar spin configurations with spin scalar chirality have drawn considerable attention as an origin of the anomalous Hall effect. In this mechanism, itinerant electrons acquire an internal magnetic field according to the solid angle spanning three spins through the so-called Berry phase, which can result in the anomalous Hall effect. The idea was first explored in the ferromagnetic Kondo lattice model on a kagome lattice, and extended to other lattice systems, such as a face-centered-cubic lattice and a triangular lattice. In particular, it was pointed out that in the triangular lattice system the perfect nesting of the Fermi surface at 3/4 electron filling might lead to a noncoplanar four-sublattice ordering and the anomalous Hall effect. While these previous studies have successfully revealed the nontrivial relation between the Berry phase and the anomalous Hall effect, a crucial question has been left unclear so far, i.e., when and how such noncoplanar spin order emerges and what is the role of coupling between charge and spin degrees of freedom in energetically stabilizing such ordering.

The aim of the present study is to clarify whether such noncoplanar spin ordering can occur in the spin-charge coupled systems on geometrically-frustrated lattices. In particular, our focus is on the parameter range and the stabilization mechanism of the noncoplanar ordering. For this purpose, we consider a ferromagnetic Kondo lattice model on several different frustrated lattices, such as triangular, triangular-kagome, face-centered-cubic, checkerboard, and pyrochlore lattice. We calculate the ground-state energy for various spin-ordered states up to four-sublattice orders. Using the variational calculation and the perturbation theory complementarily, we map out the ground-state phase diagram in a wide range of model parameters, i.e., electron density, Hund's-rule coupling, and antiferromagnetic superexchange interaction between localized spins.

For the triangular-lattice system, we find that a noncoplanar four-sublattice ordering with a finite scalar spin chirality emerges at and around 1/4 filling, in addition to the 3/4-filled case, which was predicted to be induced by the perfect nesting of the Fermi surface. The 1/4-filling phase is stable in a wider range of parameters than the 3/4-filling one, and includes a large region of gapped insulating state characterized by a Chern number. The chiral-ordered phases exhibit the anomalous Hall effect; in particular, the Hall conductivity takes a quantized value in the insulating regions. We also identify another noncoplanar state with an umbrella-type three-sublattice ordering in a lightly electron-doped region, while it does not lead to the anomalous Hall effect. We extend the analysis to the triangular-kagome lattice, i.e., for a continuous change of the lattice structure from the triangular lattice to the kagome lattice by modulating the transfer integrals in a periodic way. As a consequence, we find that the newly-found chiral order at 1/4 filling remains robust for such change, whereas the 3/4 filling phase is rapidly destabilized as

the nesting is lost. The result suggests that the 1/4 filling phase is stable against modifying the band structure, reflecting the fact that it is nothing to do with the nesting of the Fermi surface. We examine the origin of the noncoplanar ordering by considering the fourth-order perturbation theory in the Hund's-rule coupling. Among the derived four-spin interactions, we find that a biquadratic interaction is enhanced with a positive value near the 1/4 filling, which is potentially a cause of the noncoplanar ordering. We also argue a complementary scenario based on the level repulsion for acquiring a finite Chern number as a nonperturbative effect. We also study other frustrated lattices systematically, such as checkerboard, face-centered-cubic, and pyrochlore lattice. We clarify that similar four-sublattice order emerge near 1/4 filling also in these frustrated lattices. From the perturbation theory, we confirm that the positive biqiuadratic interaction plays a common, important role in stabilizing the noncoplanar order. Our results elucidate that the noncoplanar ordering is widely observed in frustrated Kondo lattice models, and that there is a common stabilization mechanism originating from the coupling between charge and spin degrees of freedom in these systems.