Abstract

Topology of the electronic band structure is one of the central issues in condensed matter physics. Besides the quantum Hall states and the topological insulators, which are both gapped insulators, gapless metallic states with nontrivial topology have recently attracted much attention. The Weyl semimetals (WSMs) are one of such topological gapless states which may appear in spin-orbit coupled systems with broken spatial inversion or time-reversal symmetry. The WSMs have topologically-protected nodal points in their electronic structures, called the Weyl points, where two non-degenerate bands intersect linearly. In addition, the WSMs exhibit peculiar surface states called the Fermi arcs. These topological properties are, strictly speaking, limited to bulk WSMs. Therefore, it is interesting to ask how these peculiar properties are modified when the system geometry is changed, in particular, in thin film forms. Although there have been several studies for this issue, the electronic, transport, and magnetic properties in thin film WSMs are not fully understood thus far.

In this thesis, focusing on magnetic WSMs with breaking time-reversal symmetry, we theoretically study the electronic and magnetic properties while changing the thickness of the system. Specifically, we consider several different models for magnetic WSMs, namely, a spatially uniform WSM, a magnetically-doped narrow-gap semiconductor, and a heterostructure with alternating stacking of magnetically-doped topological insulators and normal insulators. We compute the electronic band structure, the anomalous Hall conductivity, the Fermi arc surface states, and the spontaneous magnetization while systematically changing the film thickness.

First, we investigate the electronic band structures and the anomalous Hall conductivity for a model of spatially-uniform magnetic WSMs. We find that the system becomes a Chern insulator or a semimetal depending on the film thickness as well as the model parameters. In the Chern insulating states, the anomalous Hall conductivity is quantized, and the quantization value is proportional to the thickness. We show that a topological transition can take place between the Chern insulator and semimetal by tuning the interlayer hopping. We also study the Fermi arc surface states in the thin films. We find that there are two different types in the Fermi arc surface state depending on the distance from the projected Weyl points in momentum space: One exhibits a simple exponential decay as a function of the depth from the surface, but the other decays exponentially with oscillations. We show that these behaviors can be understood by the analytical solutions in the continuum limit. We also calculate the energy gap on the Fermi arc and find distinctive behaviors for the two types of the surface states. We compare these results with those for another model of a magnetic Weyl semimetal with alternative stacking of magnetically-doped topological insulators and normal insulators.

Second, we investigate the magnetic properties for a model of magnetically-doped narrow-gap semiconductors. By employing the mean-field approximation and the virtual crystal approximation, we calculate the spontaneous magnetization while changing the film thickness, doping concentration, and temperature. We find that the film systems behave differently from the bulk case in the vicinity of the Curie temperature; the system exhibits a magnetization with an oscillating component as a function of the depth from the surfaces. We also find that the behavior depends on the parity of the thickness. The peculiar magnetism might affect the topological properties of the WSMs.