論 文 の 内 容 の 要 旨

論文題目

Theoretical study on electronic states
in noncentrosymmetric metals and superconductors
（空間反転非対称な金属・超伝導体の電子状態に関する理論的研究）

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Inversion symmetry is one of the most fundamental symmetries in condensed matter physics. Typical examples related to the inversion symmetry breaking are ferroelectric and Weyl semimetals, which have been highlighted in these decades. The inversion symmetry relates electrons with the opposite momenta and the same spins. Therefore, several nontrivial band structures require the inversion symmetry breaking. A spin-split band due to the Rashba effect, which originates from the combination of the relativistic spin–orbit interaction and the inversion symmetry breaking, is a representative consequence of the inversion symmetry breaking.

The surface state of a topological insulator can be considered as a limit of strong Rashba spin–orbit interaction because it consists of a single Weyl cone with the helical spin texture in the momentum space. A remarkable consequence of this peculiar surface state is the quantized anomalous Hall effect in magnetically doped topological insulators without an external magnetic field. The inversion symmetry breaking also plays an important role in spin systems in the real space. A prominent example is the emergence of skyrmions in chiral magnets with the Dzyaloshinskii–Moriya (DM) interaction, which twists neighboring spins along a particular direction. Up to now, the main focus on magnetic topological insulators has been the uniformly aligned spin configuration. In reality, there should be a modulation in a real space such as domain walls or skyrmions. Moreover, electronics or spintronics application of such magnetic structure have taken growing interests.

An effect of inversion symmetry breaking also appears in transport. In inversion asymmetric systems, the resistivity along the forward and backward directions can differ. It is called nonreciprocal current. The classical example is the p-n junction, whose inversion symmetry is broken by its device structure. However, even a crystal, which has translational symmetry, can possess nonreciprocal response if it lacks inversion symmetry. The nonreciprocity in crystals is called magnetochiral anisotropy (MCA). There have been several experiments on the MCA in chiral materials such as Bi-helix or carbon nanotube in the normal state. However, the MCA in superconducting materials has not been discussed.

The aim of this dissertation is to investigate the two effects in inversion asymmetric systems. (1) The interplay between the surface state of topological insulators and localized spins, or, the spin structures in the momentum and real spaces. (2) The MCA in noncentrosymmetric superconductors.

In the first part, we discuss magnetic structures on the surface of topological insulators. By integrating out the surface state electrons, we show that the DM interaction which twists a localized spin toward its neighboring spin appears. Remarkably, the direction of the DM interaction reverses depending on the Fermi energy (valence or conduction) and the layer (top or bottom). It is reflected by the fact that the helicity of spin in the Weyl cone depends on both the electron–hole and layer degrees of freedom.

In order to confirm this scenario, we first analyze domain wall structure. We perform numerical calculations on a tight-binding model of three-dimensional topological insulators with a domain wall of localized spins. We show that a Neel type domain wall is the most stable when carriers are doped in the surface state, and its direction depends on the Fermi energy. Hence, the numerical calculations are consistent with the analytical expectations. The results mean that the direction of the Neel wall can be reversed by electric gating. It is a great advantage in spintronics application, for example by accumulating information on the direction of domain walls.

We further discuss the possibility of skyrmion creation due to the DM interaction. Experimentally, the topological Hall effect, which is an evidence of the existence of skyrmions, has been observed in a Cr-doped Bi_2Te_3 (CBST) / Bi_2Te_3 (BST) heterostructure. Interestingly, the topological Hall effect has been detected in neither a uniformly doped CBST system nor an electron-doped case. By using the tight-binding model, we show that skyrmions can be stabilized only in the CBST / BST heterostructure in the hole doped regime, which is consistent with the experimental results. The reason why hole doping is essential is that the coupling strength with the magnetic atom Cr differs between Bi and Te, namely, in CBST, because Bi is replaced with Cr, Cr strongly couples with Te, and the hole band mainly consists of *p*-orbital of Te. Skyrmions do not exist in the uniformly doped CBST because the direction of the DM interaction differs between the top and bottom layers, and the frustration occurs. Besides, the relative strength between the DM and exchange interactions becomes smaller when the CBST layer becomes thicker.

In the latter part, we discuss the MCA in noncentrosymmetric superconductors. First, we treat monolayer transition metal dichalcogenides (TMDs). These materials have gathered growing attention because of their two-dimensionality, valley degrees of freedom, nontrivial Berry curvature, and unique spin–orbit interaction. In contrast to the Rashba systems, the TMDs possess so-called Ising spin–orbit interaction, which splits electronic spins in the out-of-plane direction. An outstanding consequence is the huge enhancement of the upper critical field beyond the Pauli limit in the superconducting state. We consider the MCA in the TMD, especially in its superconducting fluctuation regime, where the current is carried by the thermal fluctuation of the superconducting order parameter. By employing Ginzburg–Landau (GL) theory, we calculate the fluctuation current up to the second order of the electric field, and evaluate the amplitude of the MCA. We show that the MCA is drastically enhanced in the superconducting fluctuation regime compared with its normal state value, and the ratio of the enhancement is about 10^6. The result is consistent with the experiment for superconducting MoS_2. This radical enhancement of the MCA originates from the energy scale difference between the Fermi energy and superconducting gap. Therefore, we expect that the enhancement of the MCA should be a universal feature in noncentrosymmetric superconductors.

Second, we discuss the effect of parity mixing, which is the most prominent characteristics of noncentrosymmetric superconductors. Due to the absence of inversion symmetry, the parity is not preserved any more. Accordingly, the even-parity spin-singlet and odd-parity spin-triplet order parameters are mixed. We treat the Rashba superconductor, which is the textbook example of noncentrosymmetric superconductors. In order to deal with the two-component nature of the order parameter appropriately, we employ the two-component GL theory. We show that the MCA becomes larger if the mixing amplitude is stronger, and vanishes when the mixing is absent. The MCA is extremely larger than its normal state value as in the case of TMDs. We also show a unique electric and magnetic fields angle dependence of the nonreciprocal current, which originates from symmetry constraints on the higher rank response tensor specific to the nonreciprocal current.