博士論文（要約）

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）

若月良平

Abstract

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

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

An effect of inversion symmetry breaking also appears in transport. In inversion asymmetric systems, the resistance along the forward and backward directions can differ, and it is called nonreciprocal resistance. 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 the inversion symmetry. The nonreciprocity in crystals is called magnetochiral anisotropy (MCA), and has been investigated

in chiral materials such as Bi-helix or carbon nanotube in their normal states. However, the MCA in superconducting materials has not been discussed up to this time.

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

In the first part, we discuss magnetic structures on the surface of TIs. By integrating out the surface state electrons, we show that the DMI which twists a localized spin toward its neighboring spin appears. Remarkably, the direction of the DMI 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 and momentum 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 TIs with a domain wall of localized spins. We show that a Néel 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 indicate that the direction of the Néel wall can be reversed by electric gating. It is a great advantage in spintronics applications, for example by assuming the directions of domain walls as the information carriers.

We further discuss the possibility of skyrmion creation due to the surface DMI. Experimentally, the topological Hall effect as a signature of skyrmions has been observed in a $Cr_x(Bi_{1-y}Sb_y)_{2-x}Te_3$ (CBST) / $(Bi_{1-y}Sb_y)_2Te_3$ (BST) heterostructure. Interestingly, the topological Hall effect has been detected in neither a uniformly doped CBST sample nor an electron-doped regime. By carrying out numerical calculations on the three-dimensional tight-binding model, we show that skyrmions can be stabilized only in the hole doped regime of the CBST / BST heterostructure, 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 the *p*-orbital of Te. Skyrmions do not exist in the uniformly doped CBST because of the frustration which originates from the direction difference of the DMI between the top and bottom layers. Besides, because the DMI exists only near the surface, the relative strength between the DMI and exchange interaction becomes smaller when the CBST layer becomes thicker. From this viewpoint, investigating the magnetic / non-magnetic TI heterostructure may open a way to new functionalities of TIs.

In the latter part, we discuss the MCA in noncentrosymmetric superconductors. First, we discuss monolayer transition metal dichalcogenides (TMDs). These materials have attracted growing attention because of their two-dimensionality, valley degrees of freedom, nontrivial Berry curvature, and unique SOI. In contrast to the Rashba systems, the TMDs possess so-called Ising SOI, which splits electronic spins in the out-of-plane direction. The huge enhancement of the in-plane upper critical field beyond the Pauli limit in their superconducting states is one of the outstanding consequences of such SOI in two-dimensional materials. 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 the Ginzburg–Landau (GL) theory, we calculate the current due to the superconducting fluctuation 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 experimental results on 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 this enhancement of the MCA should be a universal feature in noncentrosymmetric superconductors.

Second, we discuss the MCA induced by the parity mixing, which is the most prominent property 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. As a prototypical model of noncentrosymmetric superconductors, we discuss the Rashba superconductor. 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 electromagnetic field angle dependence of the nonreciprocal current, which originates from symmetry constraints on the fourth-rank response tensor specific to the nonreciprocal current. It enables us to determine the sample direction by means of transport experiments.