論 文 の 内 容 の 要 旨

論文題目

Chiral magnetism and quantum transport phenomena in noncentrosymmetric metals
（空間反転対称性の破れた金属におけるカイラル磁性と量子輸送現象）

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Chirality, which is also termed handedness, often plays a decisive role in condensed matter physics. Among many chiral materials, chiral magnets have attracted considerable attention due to the topological characteristics arising from their noncolinear and noncoplanar magnetic textures, such as helices and vortices. The chiral magnetism has been studied theoretically for a long time since the pioneering work by Dzyaloshinskii in 1960s. An archetypical example of the chiral magnetic texture is a chiral helimagnetic state (CHM) in monoaxial chiral magnets, which looks like a twisted ribbon in a quasi-one-dimensional system. The CHM turns into other chiral magnetic states in a magnetic field; it changes to a chiral soliton lattice (CSL) and a chiral conical magnetic state (CCM) in the field perpendicular and parallel to the helical axis, respectively. Such chiral magnetic textures lead to peculiar transport phenomena, such as a nonlinear negative magnetoresistance in the CSL and nonreciprocal transport in the CCM. On the other hand, cubic chiral magnets show superpositions of several helices, which are called multiple-Q states. A typical one is a triple-Q skyrmion lattice (3Q-SkL), which is a periodic array of swirling magnetic textures like quasi-two-dimensional vortices. The noncoplanar spin texture in the 3Q-SkL yields an emergent magnetic field through the spin Berry phase and leads to an unconventional anomalous Hall response, called the topological Hall effect (THE). Furthermore, three-dimensional chiral magnetic textures, which are called the magnetic hedgehog lattices (HLs), have also attracted much attentions due to their peculiar emergent magnetic field regarded as a periodic array of magnetic monopoles and antimonopoles. In such HLs, large THE and topological thermoelectric transport were experimentally observed, whose origin was discussed in relation with fluctuations of the emergent field. Theoretically, most of the previous studies for the chiral magnets have been done for effective spin models with an antisymmetric exchange interaction, which is called the Dzyaloshinskii-Moriya (DM) interaction. Although such models successfully explain many interesting magnetic properties, there still remain a lot of open issues, especially on the electronic state, quantum transport phenomena, and the role of the interplay between the chiral magnetic textures and itinerant electrons. It is highly desired to clarify these issues beyond the previous studies based on the spin-only models.

The purpose of this thesis is to theoretically investigate the magnetic, electric, and transport properties of the chiral magnets by taking into account the effects of itinerant electrons. For this purpose, we study minimal models describing the interplay between the magnetic textures and itinerant electrons: some extensions of the spin-charge coupled model with the antisymmetric interactions and the effective spin models derived from them. The recent studies have reported that such models potentially stabilize the magnetic SkLs due to effective long-range interactions mediated by a kinetic motion of itinerant electrons. In this thesis, in particular, we focus on monoaxial and cubic chiral magnets, which exhibit the quasi-one- and three-dimensional chiral magnetic textures, respectively. We study the ground state and thermodynamic properties of the extended spin-charge coupled models and the effective spin models by using variational calculations, simulated annealing, and Monte Carlo simulations. We also investigate the charge and spin transport in the chiral magnetic states by using the linear and nonlinear response theory and the Landauer method based on Green's functions.

First, we discuss the magnetic and electric properties of the CSL which appears in the monoaxial chiral magnets, such as $CrNb_3S_6$ and $Yb(Ni_{1-x}Cu_x)_3Al_9$. These compounds exhibit the CHM in the absence of an external magnetic field. Once a magnetic field is applied perpendicular to the chiral axis, the CHM turns into the CSL, whose period increases with the magnetic field, and finally relaxes into a forced ferromagnetic state (FFM). The CSL exhibits a unique negative magnetoresistance which is nonlinear to the applied field. In addition, a peculiar lock-in of the CSL was discovered in the $Yb(Ni_{1-x}Cu_x)_3Al_9$; the period is locked at a particular value while changing the magnetic field. These behaviors remain elusive in the previous studies for the spin-only models. We here study these magnetic and transport properties in the CSL by including the itinerant electrons in the model. In the absence of the magnetic field, we show that the one-dimensional spin-charge coupled model with the DM interaction exhibits the CHM whose period depends on the spin-charge interaction, the DM interaction, and electron filling. In an external magnetic field, we show that the itinerant electrons modify the development of the CSL from that in the spin-only models used in the previous studies. In particular, we find that the period of the CSL can be locked at a set of particular values dictated by the Fermi wave number. The lock-in is explained by the gap opening in the electronic states due to the scattering of itinerant electrons by the chiral solitons. We also find the same mechanism can lead to a spontaneous formation of the CSL even in the absence of the magnetic field. We discuss our findings as a possible mechanism for the lock-in observed in $Yb(Ni_{1-x}Cu_x)_3Al_9$. We also investigate the finite-temperature properties of the model by Monte Carlo simulations. Using this unbiased method beyond the variational study, we clarify how the model develops the CHM and CSL at low temperature by calculating the spin structure factor. Furthermore, by computing the optical conductivity and the winding number of the CSL, we find that the coherent part of the optical conductivity increases with the decrease of the chiral solitons; namely, the system exhibits a peculiar negative magnetoresistance proportional to the soliton density. While raising temperature, the CSL is melted by thermal fluctuations and the coherent conduction is suppressed. These results clearly indicate that the electrical transport in the CSL is governed by the spin scattering of itinerant electrons by the chiral solitons. We also discuss that our results are qualitatively consistent with the experimental data for the monoaxial chiral magnets such as $CrNb_3S_6$.

Next, we discuss nonlinear and nonreciprocal transport in the CCM state. The CCM is experimentally found in not only monoaxial chiral magnets, such as $CrNb_3S_6$ and $Yb(Ni_{1-x}Cu_x)_3Al_9$, but also cubic chiral magnets like *B*20-type compounds. The CHM turns into the CCM under the magnetic field parallel to the chiral axis. As the field increases, the umbrella-like spin structure is gradually closed and finally relaxed into the FFM. The CCM has attracted much interest as a possible origin of nonreciprocal transport since it breaks both spatial inversion and time reversal symmetries. For instance, a nonreciprocal electric current, which can be switched by the chirality and the direction of the external magnetic field, has been reported and dubbed as the electrical magnetochiral effect (EMCE). The previous study showed that the EMCE in the paramagnetic state originates from peculiar magnetic fluctuations proportional to the product of the magnetization and vector spin chirality. However, the EMCE in the CCM has not been fully understood. In addition, the spin transport is less studied in both experimentally and theoretically for not only the CCM in the magnetic field but also the CHM in the absence of the external field. In order to clarify these issues, we here study the one-dimensional spin-charge coupled model with the DM interaction by variational calculations and nonlinear response theory. We show that the EMCE appears in the CCM as a ground state due to the asymmetric distortion of the energy dispersion of the itinerant electrons originating from the breaking of spatial inversion and time reversal symmetries. We also investigate the effect of thermal fluctuations on the EMCE by Monte Carlo simulations. In the temperature region where the spin correlations develop rapidly while decreasing temperature, we find a large EMCE which is not explained by the product of the magnetization and vector spin chirality, suggesting additional contributions from thermal fluctuations in the development of the CCM. In addition, we calculate the nonlinear optical responses with finite frequency for two interesting cases: the shift current and the second-harmonic generation. We find that these second-order optical responses in the CCM change in not only the magnitude but also the sign depending on the external field and frequency of light. Although similar second-order optical responses have been reported in Weyl semimetals, the sign change is a unique property owing to the tunable magnetism in the CCM. We also explore the nonreciprocal spin transport in the monoaxial chiral magnets by using the Landauer method based on Green's functions. We show that a nonreciprocal spin current can be generated in both CHM and CCM by reflecting the spin states of the itinerant electrons near the leads. The nonreciprocity depends on the chirality, period, cone angle, and polarization of the spin current. Our results indicate that the chiral magnetic conductors are useful as spin-current diodes.

Finally, we discuss the stabilization mechanism and topological properties of the HLs in noncentrosymmetric metals. Recently, the HL characterized by three wave numbers (3Q-HL) was discovered in a B20-type compound MnGe. In addition, a different chiral spin texture characterized by four wave numbers, the 4Q-HL, was also found in $MnSi_{1-x}Ge_x$. These two HLs have different types of periodic arrays of magnetic monopoles and antimonopoles. In these materials, large THE and topological thermal transport were observed in a magnetic field, which are presumably related to the motions of the monopoles and antimonopoles. However, the stabilization mechanism of the HLs has not been fully understood thus far. Furthermore, the motions of monopoles and antimonopoles in an applied magnetic field also remain elusive despite the possible relevance to the peculiar transport phenomena. To clarify these unsolved issues, we here investigate the ground state of an effective spin model with long-range interactions arising from the itinerant nature of electrons, by variational calculations and simulated annealing. Our model includes the Ruderman-Kittel-Kasuya-Yosida interaction, the DM-type interaction originating from the antisymmetric spin-orbit coupling, and a four-spin interaction from the spin-charge coupling, all of which are specified by wave numbers determined by the nesting property of the Fermi surface. We find that both 3Q- and 4Q-HLs are stabilized at zero field by the synergetic effect of the DM-type and four-spin interactions. We also clarify the full phase diagram in the magnetic field along the [001], [110], and [111] directions. The model exhibits multiple phase transitions, some of which are associated with changes in the number of monopoles and antimonopoles. By tracing the positions of monopoles and antimonopoles by calculating the monopole charge, we find multiple topological transitions driven by pair annihilation of the monopoles and antimonopoles in the magnetic field. We find that the spin scalar chirality drastically changes in such topological transitions, which implies the importance of the pair annihilation for the topological transport phenomena originating from the emergent magnetic field.

To summarize, in this thesis, we have theoretically unveiled nontrivial magnetic and transport properties of the chiral magnetic textures in noncentrosymmetric metals arising from the interplay between itinerant electrons and localized magnetic moments. In these systems, the chiral magnetic texture is not merely an internal magnetic field to the itinerant electrons: There is an interplay between the magnetic texture and the itinerant electrons, and the magnetic and electronic states are determined in a self-consistent manner by optimizing the total free energy of the system. Our studies by the variational calculations, the simulated annealing, and the Monte Carlo simulations have revealed that the interplay is crucially important for the peculiar magnetic, electric, and transport properties that have not been obtained in the spin-only models in the previous studies. Our findings indicate a new direction to design the candidate materials by clarifying the contributions of itinerant electrons to the stability of the chiral magnetic textures. Moreover, our results for the linear and nonlinear transport phenomena in the chiral magnets provide a foundation for next-generation electronic devices. Therefore, we believe that our results pave the way for further exploration of the spin-charge interplay in the chiral magnets.