博士論文（要約）

Theoretical Study on Electron Correlation Effects in Topological Matters

(トポロジカル物質における電子相関効果の理論的研究)

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Topological matters have been the focus of intensive study in condensed matter physics since the theoretical prediction and the experimental observation of topological insulators. The salient feature of topological matters is the nontrivial topology of electron wave function in the bulk, which is characterized by a topological invariant. The nontrivial topology gives rise to a twist at the boundary of the material, exhibiting a gapless state localized on the boundary. This gapless state is described by massless Dirac electrons with its linear energy dispersion. For a nontrivial topological wave function, the relativistic spin-orbit interaction (SOI) plays a key role. The SOI induces an inverted band to create a nontrivial ground state. The topological insulator phase is adiabatically separated from a topologically trivial phase under time-reversal symmetry, whereas they are smoothly connected in the absence of time-reversal symmetry. In this respect, the topological insulator phase is also called a symmetry-protected topological (SPT) phase. Since topological phase transition requires bulk gap closing and hence the topological properties are robust to small perturbations, many studies heretofore have been carried out under the noninteracting regime.

In contrast, to study materials consisting of a large number of electrons, electron correlation effect has been one of the most important elements of condensed matter physics. Electron correlation provides rich physics beyond independent electron approximation. It gives not only just correction to a noninteracting ground state, but strong enough electron correlation might cause a phase transition. Understanding of electron correlation has improved immensely over years, including Mott transition in transition metal oxides, heavy fermions in $4f$ or $5f$ materials, and high-T_c superconductivity realized in cuprates. As for topological electronic states, an electron correlation driven topological phase transition and a collapse of noninteracting classification are theoretically predicted. Electron correlation effects in topological matters have taken growing interest in recent years.

The aim of this dissertation is to theoretically study effects of electron correlation in topological matters. To this end, we adopt three approaches. We study the electromagnetic interaction in Dirac electron systems, the interplay between electron correlation and the SOI in a microscopic model, and the classification of interacting topological crystalline insulators (TCIs).

First, we investigate the quantum critical phenomenon at the phase transition between topological and trivial insulator phases in (3+1) dimensions. It is modeled by a sign change of the Dirac mass in the Dirac Hamiltonian, consisting of a four-component fermion field. At the critical point, the Dirac mass vanishes and the energy gap closes, which gives a Dirac cone energy spectrum. When the Fermi energy lies at the apex of the Dirac cone, the density of states vanishes and hence the electromagnetic force is unscreened and long-ranged. Therefore the long-range electron-electron interaction is relevant at the critical point of the topological phase transition.

The situation is similar to Weyl semimetals, which exhibit gapless two-component fermions. Weyl semimetals are realized in three-dimensional materials with either inversion or time-reversal symmetry broken. The lack of either symmetry makes a four-component massless Dirac fermion split into two two-component massless Weyl fermions with oppo-

site chiralities. Since right-handed and left-handed Weyl fermions appear in pairs, Weyl semimetals can also be described by the massless Dirac model. The chirality of a Weyl node is considered as a topological number. Its topological nature yields the Fermi arc surface states.

The renormalization group (RG) analysis is performed to study the electromagnetic interaction in a massless Dirac system with N Dirac nodes. The analysis bears a similarity to quantum electrodynamics (QED), but in contrast to QED, the speed of light c and electrons v are different in materials, violating the Lorentz invariance. We derive the RG equations for c, v, and the running coupling constant α. Our RG analysis reveals that c and v approach to the common value in the infrared limit. It concludes that the Lorentz in variance is recovered in the long-wavelength and low-energy limit. There are two momentum/energy scales separating three regions of different scaling behaviors. The running coupling constant α shows a logarithmic decrease just as in QED. We also find a reasonably accurate approximate solution for generic N, indicating c^2v^N being almost unrenormalized. Physical consequences are discussed from the viewpoint of RG analysis, such as the temperature dependence of the dielectric constant, magnetic susceptibility, spectral function, DC conductivity, and mass gap.

We also consider electron correlation effects in a two-dimensional (2D) Dirac material. α-(BEDT-TTF)$_2$I$_3$ [BEDT-TTF: bis(ethylenedithio)tetrathiafulvalene] is a quasi-2D organic semiconductor. Under hydrostatic pressure above 1.5 GPa, it exhibits the gapless Dirac fermion phase. It has linear dispersion with anisotropic velocities, called anisotropic Dirac cones. Since the Fermi level lies at the point where the density of states vanishes, the long-range Coulomb interaction is relevant. Our RG analysis deals with the long-range Coulomb interaction and the low-energy and long-wavelength behavior is studied. By a perturbative RG analysis at one-loop level, we find a nearly logarithmic enhancement of the velocities whereas the tilt of the Dirac cone remains unrenormalized, which describes the reshaped tilted Dirac cones. The reshaped energy dispersion alters the properties in low temperature. The theoretical calculation of the site-dependent spin susceptibility shows a reduction in low temperature, which can be observed in an NMR measurement.

Second, we study the interplay between the SOI and electron correlation. The SOI brings about novel effects, such as the anomalous Hall effect and spin Hall effect as well as topological insulators. Usually, strong SOI is needed to realize these novel effects, which requires heavy elements such as Ir, Pt, Hg, and Bi. Considering applications, lighter and common elements are highly desirable instead of these heavy elements. If we look at d electrons, electron correlation becomes stronger when we trace the Periodic Table from $5d$ to $4d$ and $3d$ elements, whereas the SOI is weaker for lighter elements. In this respect, it would be favorable if the SOI is effectively enhanced by electron correlation.

There are theoretical proposals that the spontaneous symmetry breaking of the spin rotational symmetry by electron correlation generates the topological insulator phase at mean field level. The symmetry breaking generates electron hopping with spin flip, which has the same effect as the SOI in the noninteracting models for topological insulators. One could say that interatomic SOI is induced by electron correlation. It suggests the

possibility that electron correlation replaces the role of SOI in a certain situation.

Looking at the electron correlation physics at atomic level, Hund's rule determines the ground state multiplet. On the other hand, the band theory is suitable in the opposite limit for nearly free electron systems, with electron hopping among atoms. In the crossover between the two limits, we expect effectively enhanced SOI, and aim to generalize Hund's rule including itinerant electrons.

For a better understanding of the interplay between the SOI and electron correlation, we study a two-site system consisting of three t_{2g} orbitals for each site and see how Hund's rule is modified by electron hopping between the two atoms. The two-site system includes electron hopping, which gives qualitative differences from a single-site problem. This system can accommodate electrons up to 12. Due to the complementary relation between electrons and holes, we study the cases of one to six electrons.

The model is analyzed by exactly diagonalizing the Hamiltonian and the eigenstates are obtained numerically. It is found that the competition between the Hund's coupling J and transfer integral t describes the crossover from the itinerant, molecular orbital limit to the localized, strong coupling limit. The total spin of the system S well represents the ground state. It grows as the ratio J/t increases, except for the half-filled case. The half-filled system resembles the quantum antiferromagnetic Heisenberg model, and the total spin is vanishingly small regardless of the Hund's coupling. Especially the focus is on the effective on-site and interatomic SOIs in the presence of electron correlation. The remarkable result is that the effective SOIs are enhanced in the intermediate spin states, where neither spin nor orbital angular momentum is polarized or quenched and both have moderate values. The conditions for the enhancement are intermediate Hund's coupling and filling of four or five electrons, namely $t_{2g}^{2-2.5}$ configurations.

Finally, we examine the effect of electron interactions in TCIs protected by mirror symmetry. In TCIs, topological surface states are protected by crystalline symmetry, instead of time-reversal symmetry for TIs. The study of TCIs has gained broad interest since the theoretical prediction followed by the experimental observation of TCIs in the SnTe material class. The class of materials has the rocksalt structure and hence possesses mirror symmetry. Thin films of SnTe realize 2D TCIs, which can also be considered as $U(1) \times \mathbb{Z}_2$ SPT phase. The topological invariant for TCIs with mirror symmetry is the mirror Chern number according to the band theory. The noninteracting TCIs with mirror symmetry are classified by integers both in two and three dimensions.

In general, topological invariants are defined depending on symmetry and spatial dimension. The tenfold way classification is a remarkable success in the study of topological electronic states before the finding of TCIs. The classification table provides information about the existence of topological states for a given symmetry in a given dimension, and if exist, the kind of topological invariants. The tenfold way classification includes three symmetries: time-reversal, particle-hole, and chiral (or sublattice) symmetry.

Recently, theoretical works have revealed that the classification for interacting systems is different from that for noninteracting cases for a variety of symmetry classes in different dimensions. Then one may question whether the classification of TCIs with mirror

symmetry breaks down in the presence of electron interactions.

We show the reduction of the noninteracting classification of TCIs by analyzing the stability of edge states. The analysis of the effective edge Lagrangian obtained from the Chern-Simons theory reveals that the classification reduces from $\mathbb{Z}$ to $\mathbb{Z}_4$ for 2D TCIs. $\mathbb{Z}_4$ classification means four pairs of helical edge modes can be gapped out by interactions, and a 2D TCI with the mirror Chern number four can be adiabatically connected to a trivial phase. Also we find a novel type of protected edge states with a spin gap in the presence of interactions. It can be detected by an STM measurement from a pinning of charge density wave at boundaries and impurities. In addition, geometric consideration provides an unusual approach to the classification of 3D TCIs with mirror symmetry. Interactions reduces the classification from $\mathbb{Z}$ to $\mathbb{Z}_8$.

We investigate electron correlation physics in topological insulators as well as quantum criticality of topological phase transition and Dirac materials. Studies of these fields have gained interest in recent years, providing unprecedented consequences beyond noninteracting approximations. In addition, topological matters involve novel gapless modes and spin structures, which can be utilized for applications such as electronics and spintronics devices. We expect our researches on the interplay between topological matters and electron correlation contribute to condensed matter physics and also applications.