論文の内容の要旨

論文題目

Effects of Electron-Electron Interaction on Dirac Fermions in Solids

（固体中のディラック電子系における電子間相互作用の効果）

氏名　金尾 太郎

In this thesis, two phenomena on electron-electron interaction in massless Dirac fermions and one related topic are theoretically investigated: the Kondo effect, charge fluctuations in the vicinity of a charge-ordered phase, and a localized state induced by a defect. The first has been experimentally observed in graphene, which is a representative of the Dirac fermion systems in solids. The second and third are related to experimentally observed anomalous behaviors in an organic conductor α-(BEDT-TTF)$_2$I$_3$ under pressure, where the massless Dirac fermions also exist at the Fermi energy. Both the first and third are caused by defects in the Dirac fermion systems.

Kondo Effect in Graphene with Defects

In the first part, we propose a theory for the Kondo effect due to point defects in graphene. We develop an effective model for this Kondo effect, where the conduction electron states and the localized magnetic moment are formed by the π electrons extending over the sample and the dangling sp^2 orbitals around the defect, respectively. Finite hybridization between them is possible owning to a lattice distortion at the defect perpendicular to the graphene plane. By analyzing this model with the numerical renormalization group (NRG) method, it is shown that the experimentally observed gate-voltage dependence of the Kondo temperature can be understood in this framework. Then, a localized state of π electrons induced by the defect is taken into account. It is shown that this state assists the Kondo screening when the density of defects is finite. The behavior of this localized state in a magnetic field is studied by using a tight-binding model with Peierls phase. It is found that the orbital motion of the π electrons in the magnetic field modulates the localized state and causes the Kondo effect which is sensitive to the magnetic field.

Localized State in α-(BEDT-TTF)$_2$I$_3$ Induced by Single Defect

In the second part, we investigate the localized state induced by a single defect in α-(BEDT-TTF)$_2$I$_3$ using a tight-binding model for this material. By diagonalizing the Hamiltonian with a single defect, it is demonstrated that the localized state is induced at the energy of Dirac points when the defect is at a certain sublattice (A or A', which correspond to A or B in graphene). This is also confirmed by using the Green's function method. This localized state enhances the local density of states in a finite region around the defect, and it shows an anisotropy. By using the Green's function method, the wave function of the localized state is evaluated in the $\boldsymbol{k}$ space. It is clarified that this state consists of both the electron and hole states near the Dirac points, and shows anisotropy around it due to the tilting of the Dirac cones. The anisotropy of the localized state in the real space is understood from this tilting of the Dirac cones in the $\boldsymbol{k}$ space. The sublattice components of the localized state are also calculated in the $\boldsymbol{k}$ space. When the defect is located at the sublattice A, the largest contribution to the induced localized state is the sublattice A' component, and vice versa, which is similar to the case of graphene. Since this localized state consists of Dirac fermions, it can be used as an experimental tool for obtaining the information of the Dirac fermions such as the tilting of the Dirac cones, the position of the Dirac points in the Brillouin zone, and the sublattice components of the Dirac fermions. Possibility of its detection in scanning tunneling microscopy (STM) and NMR experiments is discussed.

Effects of Charge Fluctuations on Dirac Fermions in α-(BEDT-TTF)$_2$I$_3$

In the third part, we investigate the effects of charge fluctuations in the vicinity of the charge-ordered phase in α-(BEDT-TTF)$_2$I$_3$, especially near the quantum critical point. First, from a minimal model which describes both the Dirac fermions and their charge ordering transition, a Landau-Ginzburg-Wilson functional is derived. This functional describes behaviors of the charge fluctuations in the Dirac fermion phase. Here, the Fermi energy is fixed at the energy of the Dirac points. We find that the charge fluctuations in Dirac fermions obey a characteristic dispersion which contains variables q and ω_l in a symmetric manner. Analyzing this functional with the perturbative renormalization group (PRG) method and the self-consistent renormalization (SCR) theory, which can take into account the coupling between several fluctuation modes, we show that the effects of the mode-mode coupling tend to be less effective in Dirac fermions compared with the case of conventional magnetic fluctuations in metals. Second, we investigate the effects of charge fluctuations on physical quantities by using the SCR theory. We show that the interaction between the electrons and the charge fluctuations causes peaks in the electron self-energy as a function of temperature and energy ω when the mode-mode coupling is strong. These peaks lead to an increase of the electron damping with decreasing temperature near the quantum critical point, which will cause an increase of resistivity as is observed in experiments. This characteristic behavior of the self-energy also causes a suppression of the density of states. Its relevance to the experimentally observed suppression of the spin susceptibility is discussed. The specific heat of the charge fluctuations is also calculated, and it is shown that the obtained temperature dependence in the case of a strong mode-mode coupling is compatible with experimental result.