論文の内容の要旨

論文題目

Novel properties of the optical conductivity due to electric-dipole-induced magnetic transitions in the Hubbard model

(電気双極子に由来する磁気遷移による新規な光学伝導度)

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In this thesis, we study the electron spin resonance (ESR) induced by an AC electric field in the Hubbard model, and its effects on the optical conductivity. The weakly correlated and strongly correlated regimes are both considered, but with different approaches which effectively split the thesis into two parts.

In the weak coupling regime, the electric dipole moment is described in terms of the current $\mathbf{j}$ of nearly free electrons. In the Hubbard model, the operator is written as a hopping operator between neighboring sites, as shown in Figure 1, in terms of the electron creation (annihilation) operators $c^{\dagger}_{i,\alpha}(c_{i,\alpha})$ with spin α and position $\mathbf{r}_i$. A spin-dependent hopping $t_{\alpha\beta}$ can result in electric-dipole-induced spin-flip transitions.

In contrast, in the Mott insulating phase of the Hubbard model, the electrons are localized at each site due to the Coulomb repulsion U. Treating t as a perturbation, effective magnetic interactions emerge from virtual hopping of the electrons to neighboring sites. In addition, a finite local electric polarization operator $\mathbf{P}$ can emerge even at low energies, i.e., with matrix elements between magnetic states in the low-energy manifold. The resulting effective operator $\mathbf{P}_{\text{eff}}$, written in terms of local spin operators, scales as t^n/U^n for virtual hopping around loops of n sites. This magnetoelectric (ME) effect results in intricate electric-dipole-induced magnetic transitions in the effective spin model, below the optical gap. Besides, we also consider the ME effect originating form the overlap of the electronic wave functions on neighboring sites.

In both limits, spin-orbit coupling (SOC), which explicitly couples the spin of the electrons to their motional degree of freedom, plays a central role.

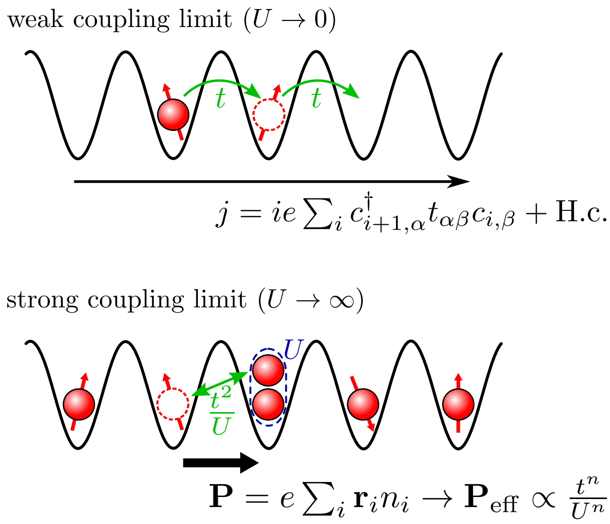

Figure 1: Origin of the spin-dependent electric dipole moment in the weak and strong coupling regimes (at half-filling).

The first chapter introduces the motivation for the research and the outline of the main contributions of the thesis. In this thesis, we extensively consider the coupling of the spin and charge degrees of freedom of electrons in the Hubbard model, and how it affects the optical conductivity through electric-dipole-induced magnetic transitions.

In Chapter 2, we first investigate spin-flip transitions in one-dimensional (1D) and two-dimensional (2D) tight-binding models, in the non-interacting limit. The synergetic effect of strong SOC and Zeeman splitting (ZS) on the spin resonance is studied using the Kubo formula. With both SOC and ZS, the spin flip can be induced by an AC electric field: the so-called electric dipole spin resonance (EDSR). The resulting contribution to the optical conductivity is analyzed analytically. We show that the electromagnetic absorption spectrum is considerably influenced by the interplay of SOC and ZS, and depends on the relative angle between the SOC vector and the magnetic field direction. In particular, the EDSR is dominant over the traditional magnetic-dipole-induced ESR. Additionally, the spectrum depends on the lattice, the band structure, and the Fermi energy. In 2D systems, we show that the resonance spectrum becomes continuous with unexpected Van Hove-like singularities.

The effect of the Coulomb repulsion U on the spin resonance is also studied numerically in the 1D model. We find that at half-filling, the resonance is first enhanced for small U but vanishes when the optical gap becomes larger than the kinetic hopping amplitude t.

In the $U \to \infty$ limit of the same model at half-filling, we also investigate the resonance between the lower and upper Hubbard bands appearing at $\hbar\omega \sim U$, above the optical gap. A large magnetic field tends to suppress the resonance while it is recovered thanks to SOC depending on the relative angle of the magnetic field.

In the second part of the thesis, we study the low-energy electric-dipole-induced magnetic transitions in the Mott insulating phase, below the optical gap. By treating the inter-site hopping as a perturbation, we show in Chapter 3 how the electric polarization operator can have non-trivial matrix elements between different low-energy magnetic states through virtual hopping of the electrons. This effective spin-polarization coupling is generally allowed in trimers for the single-band Hubbard model. In addition, we exhaustively derive the possible two-spin effective polarization operators emerging from spin-dependent hopping.

Motivated by terahertz spectroscopy measurements in α-$RuCl_3$, a so-called Kitaev material, multi-orbital Hubbard models are then considered. In Chapter 4, we develop a theory for electronic ME effects in Mott insulators of d^5 transition metal ions in an octahedral crystal field. For $4d$ and $5d$ compounds, the extended orbitals favor charge fluctuations of the localized electrons to neighboring ions and a significant ME effect from electronic mechanisms is expected. The electric polarization originating from two-spin operators on bonds of nearest-neighbor magnetic sites is considered. The allowed coupling is first derived using a symmetry approach. Then, the effective polarization operator in the ground state manifold is evaluated using perturbation theory. We show in particular that the involved lattice structure of Kitaev materials results in a new type of electronic ME coupling.

Finally, in Chapter 5 we calculate the optical conductivity of ideal Kitaev materials originating from the derived ME coupling. Using exact analytical results of the Kitaev honeycomb spin model, we calculate the continuous terahertz spectrum of the quantum spin liquid originating from Majorana excitations.