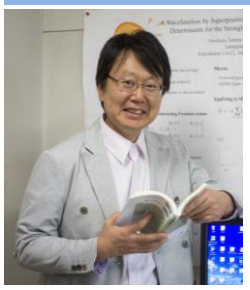
Theory on Condensed Matter Physics



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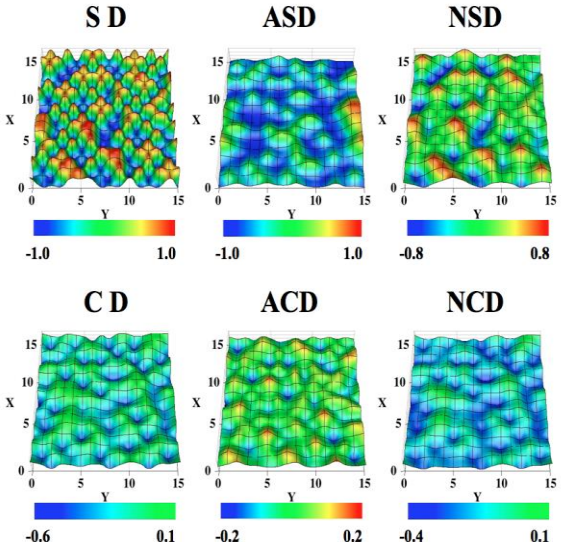
Research impact at a glance



Electronic structures of hole-doped cuprates. Polarons are formed.

We have developed a Resonating Hartree-Fock theory[1] which constructs a many-body wave function by superposition of the direct products of non-orthogonal Slater determinants $|\varphi_f\rangle$ and coherent state of phonons $|\phi_f\rangle$ such as

$$|\Psi\rangle = \sum_f C_f |\varphi_f\rangle |\phi_f\rangle .$$

The method reasonably describes the electron correlation effects and quantum fluctuations beyond the adiabatic approximation. Furthermore, we can give physics to such quantum fluctuations by analyzing the structures of the Slater determinants and coherent states. The method has been applied to high-temperature superconductors[2], conducting polymers, and charge transfer complexes. We are now planning to extend it to description of dynamics in highly correlated systems.

Detailed description of the research

Background:

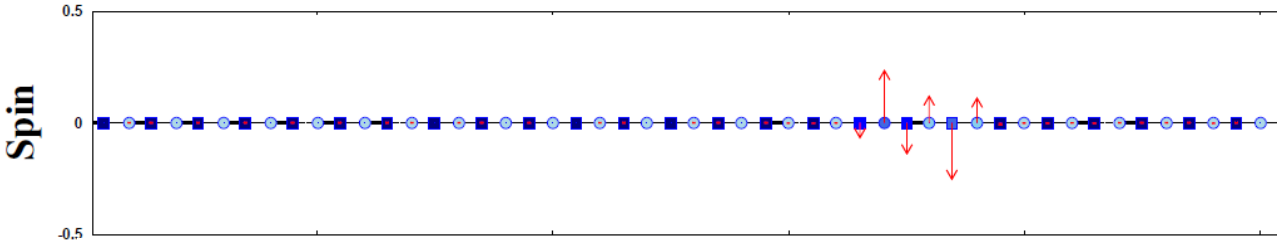
Since the discovery of high-temperature superconductors and low-dimensional materials, description of the electron correlations or quantum fluctuations has been the most challenging issue in the theoretical condensed-matter physics. In addition, as the improvement of the experimental techniques, we now need to treat the lattice or phonons beyond the adiabatic approximation, In fact, femto-second order photo-switching of one-dimensional charge transfer salts, such as TTF-CA, changes the local lattice structures as

well as the electronic structures. The main focus of our research is to describe such large quantum fluctuations including phonons beyond the adiabatic approximation.

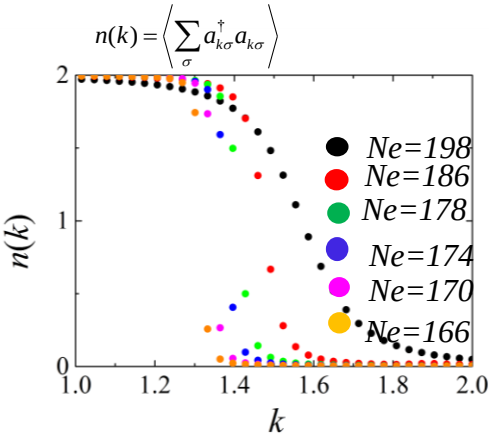
On-going research:

1. Quantum fluctuations in TTF-CA and dynamics

TTF-CA has two stable phases naturally depending on temperature. Now we can experimentally control these two phases by light. This is the photo-induced phase transition of the femto-second order. We have been trying to describe the quantum fluctuations in this TTF-CA by using the resonating Hartree-Fock theory. So far, we have clarified that quantum fluctuations due to counter-phase domains play important roles especially near the phase boundary. We believe that such counter-phase domain walls are also important in the photo-induced phase transition. We are now trying to describe dynamics in photo-excitation of the system.



Ionic phase domain (red arrows) in the neutral phase.



n_k has a large gap at heavily doped regions, which suggests the system becomes metallic.

2. Metallic states in conducting polymers

Highly doped polyacetelene has two conflicting characters, that is, pauli susceptibility and infrared absorption intensity. To satisfy these two experimental facts, we need metallic states with lattice solitons. We have applied the resonating Hartree-Fock theory and clarified that the quantum fluctuations due to lattice solitons merges soliton and valence (conduction) bands. As a result of such quantum fluctuation effects beyond the adiabatic approximation, metallic states with lattice solitons are realized.

Selected publications

Original papers:

1. J.Phys. Soci. Jpn. 84, 124803(2015)

2. Phys. Rev. Lett. 103, 116401(2009).