論 文 の 内 容 の 要 旨

論文題目
Numerical Studies on Quantum Phases Emergent from Interplay of Spin-Orbit Interactions and Strong Electron Correlations
（スピン軌道相互作用と電子相関の協奏が生む量子相の数値的研究）

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We have studied emergent quantum phases where spin-orbit interaction and strong electron correlations become the driving force.

In recent studies on condensed matter physics, topological properties of the time-reversal-invariant band insulators in two and three dimensions have been extensively studied. The insulators under time reversal symmetry with non-trivial topological invariant are called "topological insulators" and intensively studied because of the existence of robust surface metallic states. Both in two and three dimensions, the topological phases are typically realized in the systems with strong spin-orbit interaction.

On the other hand, it is suggested that the extended Hubbard model on the honeycomb lattice can generate an effective spin-orbit interaction from a spontaneous symmetry breaking at the Hartree-Fock mean-field level leading to a topologically non-trivial phase. Since the system, which are semimetals in the non-interacting limit, becomes topologically a nontrivial insulator phase driven by the Coulomb interaction, this phase is often called "topological Mott insulator". This phenomenon is quite unusual not only because the electron correlation effectively acts as spin-orbit interaction, but also it shows universality class that depends on the electron band dispersion near the Fermi point.

However, this is not the only example where the electron correlation and the spin-orbit interaction play a crucial role for the emergence of exotic topological phases. Recent theoretical prediction shows that, under the strong electron correlation and spin-orbit interaction, the Iridium compounds are a potential candidate for the realization of the Kitaev model, where a quantum spin liquid described by a Majorana fermion state becomes the ground state. This prediction was made by taking the limit of strong electron correlation in the presence of the spin-orbit interaction.

Theoretically, the existence of electron correlation in many-body system makes the problem unsolvable in exact way and the spin-orbit interaction makes the problem further complex. In the first part of this thesis, we report our contribution to the numerical method to handle quantum phases where strong electron correlation and spin-orbit interaction coexists. There we develop and test the accuracy of a multi-variable variational Monte-Carlo method (MVMC). This method has a wide applicability to the strongly correlated electron systems while it has a limitation arising from the given variational form of the wave function. In particular, it is not clear whether this method can describe the correct critical exponents beyond the mean field theory. By calculating the anti-ferromagnetic transition of the Hubbard model on the honeycomb lattice, we show that the MVMC largely improves the universality and critical point of the mean field result toward the accurate quantum Monte Carlo result.

In the next section, we propose an accurate MVMC applicable in the presence of the strong spin-orbit interaction. Our variational wave functions consist of generalized Pfaffian-Slater wave functions that involve mixtures of singlet and triplet Cooper pairs, Jastrow-Gutzwiller-type projections, and quantum number projections. The generalized wave functions allow any type of symmetry breaking states, ranging from magnetic and/or charge ordered states to superconducting states and their fluctuations, on equal footing without any ad hoc ansatz for the type of the symmetry breaking. We detail our optimization scheme for the generalized Pfaffian-Slater wave functions with complex-number variational parameters. Generalized quantum number projections are also introduced, which imposes the conservation of not only spin and momentum quantum numbers but also Wilson loops. As a demonstration of the capability of the present variational Monte Carlo method, the accuracy and efficiency of the present method is tested for the Kitaev and Kitaev-Heisenberg models. The Kitaev model serves as a critical benchmark of the present method: The exact ground state of the model is a typical gapless quantum spin liquid far beyond the applicability range of simple mean-field wave functions. The newly introduced quantum number projections precisely reproduce the ground state degeneracy of the Kitaev spin liquids, in addition to their ground state energy. Our framework offers accurate solutions for the systems where strong electron correlation and spin-orbit interaction coexist.

In the second part of the thesis we study the possibility of the topological insulator induced by electron correlation (topological Mott insulator) on the honeycomb lattice. By seriously considering the effect of charge density wave, we found that the region where the topological Mott insulator claimed to be stable in the previous study disappears. However we show that this region recovers by controlling the Fermi velocity of the Dirac point. Since the mean-field calculation cannot satisfactorily treat the correlation effect and overestimates the ordered phase, we use the newly developed MVMC for the calculation. By taking the extrapolation to the thermodynamic and weak field limit, we present the realistic criteria for the existence of the topological Mott insulator. By using the result we discuss the relation to the graphene and discuss the possibility of realizing the topological Mott insulator in bilayer graphene.