博士論文（要約）

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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Acknowledgement

I would like to express my sincere gratitude to Prof. Masatoshi Imada for his supervision, encouragement and stimulating discussions. His daily attitude to physics also enlightened me. I would like to thank Dr. Youhei Yamaji and Dr. Satoshi Morita for his advices and fruitful discussions. This work could not be accomplished without their supervision and advice. I wish to thank Dr. Takahiro Misawa, Dr. Yasuhiro Yamada, Dr. Huihai Zhao, Dr. Motoaki Hirayama, Dr. Ryui Kaneko, Mr. Kensaku Takai, Mr. Kosuke Miyatani, Mr. Kota Ido and Mr. Dai Kubota for daily discussions. I am very grateful to Ms. Mamiko Horii for her continual help. Finally, I would like to appreciate my family for their warm-hearted encouragement and support.

Abstract

We study quantum phases and their phase transitions emergent from the interplay of spin-orbit interactions and strong electron correlation. Strong electron correlation has long been one of the central issues of the condensed matter physics because of the following reasons. First, it has constantly generated rich physical concepts such as those in magnetism and superconductivity. Second, we can not solve many particle problems exactly and therefore understanding strong correlations has always been challenges.

Compared to the electron correlation, the spin orbit interaction has recently attracted revived interest because topological characters of electrons have newly drawn attention. For example, recent studies have established topological classifications of the time-reversal-invariant band insulators in two and three spatial dimensions and it is revealed that spin-orbit interactions play a crucial role for the emergence of the topologically nontrivial phase.

Here we focus on their interplay, for which a theoretical scheme to treat both the spin-orbit interactions and the electron correlations is necessary. Therefore the aim of the present thesis is twofold. One is to develop a numerical method which is able to reliably treat the interplay of the electron correlation and the spin orbit interaction. The other is of course to clarify physics emerging from the interplay of the electron correlations and the spin orbit interaction by applying the numerical method.

The first half of this thesis is devoted to a review for the recent improvement of the numerical method, multi-variable variational Monte Carlo method(MVMC). Our variational wave function is a combination of generalized Pfaffian-Slater wave function, Jastrow-Gutzwiller-type projections, and quantum number projections. In our study, we have generalized previous wave functions that already allow any type of symmetry broken 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 then detail our new optimization scheme developed for the generalized Pfaffian-Slater wave functions with complex-

number variational parameters. Generalized quantum number projections are also introduced, which impose the conservation of not only spin and momentum quantum numbers but also local conserved quantities related to the system and Wilson loops. As a demonstration of the capability of the present variational Monte Carlo method, the accuracy and efficiency of the present method are 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 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 energies. Our framework offers accurate solutions for the systems with the strong electron correlation and spin-orbit interaction.

In the second part of the thesis we study the possibility of the topological insulator emerging from electron correlations (called topological Mott insulator) on the honeycomb lattice. By seriously considering the stability of charge density wave, we found that the topological Mott insulator claimed in the literature to be stable in a region of the parameter space are destabilized and replaced by the charge density wave even by the mean-field approximation. However we show that the topological Mott insulator becomes stable 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 also critically analyze the problem by using the newly developed MVMC. By taking the extrapolation to the thermodynamic and weak field limit, we present the realistic criteria for the existence of the topological Mott insulator. Gaining insights from this theoretical analysis, we pursue the possibility of realizing a topological Mott insulator in bilayer graphene and clarify that it is in the range of realistic experimental effort.