論文の内容の要旨

論文題目　Quantum Monte Carlo Study of Superfluidity and Supersolidity in Bosonic Lattice Systems
（量子モンテカルロ法を用いた格子ボーズ系における超流動及び超固体の研究）

氏名　大越　孝洋

Since the pioneering work by Greiner *et al.* in 2002, there has been great experimental development on cold atoms and molecules trapped in optical lattices. Such systems are well described by the Bose-Hubbard models. Owing to the high controllability and cleanness, such a system offers an opportunity to realize fascinating phenomena that are predicted theoretically. Recently, multi-component systems or dipolar systems have attracted great attention, because it may produce new physics due to the multiple degree-of-freedom or long-range anisotropic interactions. Indeed, it is expected that exotic superfluidity appears such as super-counter-fluidity in two-component system and supersolidity —coexistence of superfluidity and solidity— in dipolar system, respectively. Motivated by this background, we have investigated super-counter-fluidity in the previous work (Chapter 3). Then, for this thesis, we have investigated supersolidity and other fascinating quantum phases mainly by using the improved QMC method (Chapter 2,4,5).

In Chapter 2, we review the QMC method based on the path-integral (world-line) representation, and, then, present a new improved algorithm especially for simulations of systems with long-range interactions. The QMC method we adopt is the directed-loop algorithm where efficient global updates are performed. This algorithm is widely used for simulations for spin models. With some modifications, it also works well for soft-core bosonic models. However, it still suffers from severe slowing down when it is applied to systems with long-range interactions. Therefore, we present an improved algorithm to overcome it. The improved algorithm enables us to perform efficient simulation of systems with long-range (but integrable) interactions in $O(N)$ time (N is the system size).

In Chapter 3, we review our previous study on super-counter-fluidity in the two-component hard-core Bose-Hubbard model on a square lattice.

Super-counter-fluidity is characterized by development of pair-correlation and suppression of one-body correlations. However, the conventional algorithm for the grand-canonical ensemble has difficulty in measuring two-body correlations function like the pair-correlation function. In this study, we have proposed a simple modification of the algorithm to measure the pair-correlation of the super-counter-fluidity. By obtained pair-correlation function, we have studied the properties of the super-counter-fluidity. Furthermore, we show that the modified algorithm overcomes slowing down which occurs in the super-counter-fluid phase.

In Chapter 4, we investigate supersolid phases in the soft-core Bose-Hubbard model with the nearest-neighbor repulsion on a square and cubic lattice. This model is one of the simplest models to support the existence of supersolid phase, and can be realized by cold dipolar bosons in two-dimensional(2D) optical lattices where all dipoles are polarized perpendicular to the 2D plane by an external field. Most supersolid states are known to appear at incommensurate filling factors when particles or holes are doped into a commensurate perfect solid. However, we present direct evidence of supersolid at commensurate filling factor 1/2 for two-dimensions as well as three-dimensions. In addition, we find a novel double-peak structure in the momentum distribution of bosons, which may be observed by time-of-flight measurement in the future experiments.

In Chapter 5, we study the Bose-Hubbard model with the dipole-dipole interaction on a square lattice. Owing to the long-range and/or anisotropic nature of the dipole-dipole interaction, the phase diagram contains rich quantum phases -- various solids with different periodicities, their associated supersolid phases, and appearance of numerous completing ground-states. By our QMC simulations, we explore novel quantum phases in the ground-state phase diagram. As a result, we find a phase where numerous striped solid states are competing for hard-core bosons with anisotropic interaction, and a solid phase with nested-solid structure and its associated supersolid phase for soft-core bosons with isotropic interaction. We also provide a strong-coupling argument to understand why long-range interactions stabilize a supersolid state for hard-core bosons with isotropic interaction.

Finally, in Chapter 6, we summarize our results. We believe that our improved algorithm enables us to perform simulations of large systems comparable with future experiments on 2D dipolar Bose gases. Not only the experimental realization of supersolid and observation of our new findings but also such a direct comparison are hopeful and they will have a great impact on the field of cold atoms and molecules in the future works.