Abstract

It has been a challenge in condensed matter physics to find superconductors with higher critical temperatures T_c. The mechanism of high-T_c superconductivity and key factors that determine T_c have been puzzles to be solved. In strongly correlated electron systems, copper oxide (cuprate) superconductors have the highest record of T_c under ambient pressure among various types of superconductors. Cuprate superconductors share the layered perovskite structure and show anisotropic superconductivity when electrons or holes are doped into the antiferromagnetic insulating state on two-dimensional CuO_2 layers. The anisotropic superconducting gap has $d_{x^2-y^2}$ (d)-wave symmetry. In contrast to these common features of cuprates, T_c significantly depends on detailed crystal structures. Relationship between T_c and the crystal structures has attracted considerable attention as a clue to designing higher-T_c superconductors. In particular, the relationship between the number n of CuO_2 layers in a unit cell of cuprate superconductors and the optimum superconducting transition temperature $T_c^{\rm opt}$ is intriguing. As experimentally observed in Bi, Tl, and Hg based layered cuprates, $T_c^{\rm opt}$ increases when n is increased up to $n = 3$, and then, decreases for larger n. However, the mechanism behind the n dependence of $T_c^{\rm opt}$ remains elusive despite many experimental and theoretical studies

In this thesis, we focused on one of the simplest effective Hamiltonians of the multilayer cuprates, and clarified the effects of the adjacent CuO_2 layers on the stability of the superconductivity. As a method, we used a many-variable variational Monte Carlo (mVMC) method, which can flexibly and precisely describe different quantum phases by introducing 10^3 to 10^5 variational parameters. By utilizing the mVMC method, we studied a bilayer t-t'-U-V Hubbard model (t and t' are the intralayer nearest-neighbor and second-neighbor hoppings, respectively, U is the onsite Coulomb repulsion, and V represents the offsite Coulomb repulsions), in comparison with the single-layer t-t'-U-V Hubbard model. Because the direct and quantitative simulation of $T_c^{\rm opt}$ is still beyond the reach of the existing numerical algorithms, observables that correlate with $T_c^{\rm opt}$ were examined in the present thesis. Among the observables correlated with $T_c^{\rm opt}$, the superconducting correlation at long distance at zero temperature is one of the

suitable quantities for calculations with the mVMC method. The amplitude of the superconducting gap function is also estimated from the fitting of the momentum distribution obtained by the mVMC method. It was found that the in-plane superconducting correlation is not enhanced in comparison with the superconducting correlation in the single-layer t-t'-U-V Hubbard model. While the superconducting correlations at long distance both in the single-layer and bilayer models are almost the same at the optimal doping, the superconducting correlations of the bilayer Hamiltonian are significantly small in the overdoped region in comparison with those of the single-layer Hamiltonian. We showed that the stability of the superconductivity in the overdoped region is governed by the van Hove singularities in the density of states in the normal state. In addition, we found that the amplitude of the superconducting gap function is also similar in both the single-layer and bilayer t-t'-U Hubbard models at the optimal doping. Therefore, we concluded that the adjacent Hubbard layers are not relevant to the enhancement of $T_{\rm c}^{\rm opt}$ in the bilayer cuprates. Possible origins of higher $T_{\rm c}^{\rm opt}$ other than the adjacent layers are differences between the theoretical Hubbard layers and physical CuO_2 layers and effects of impurities or dopants.

To further elucidate the irrelevance of the adjacent CuO_2 layer to $T_{\rm c}^{\rm opt}$ and to study the stability of the superconductivity in multi-orbital systems including iron-based superconductors, we analyze two-body wave functions of Cooper pairs, which are called the form factors. The form factor of the Copper pairs is directly obtained from the two-particle reduced density matrix and is crucial to analyze distribution of the Copper pairs among the multiple internal degrees of freedom of the electrons, such as orbitals and layer indices. The shape of Cooper pairs is also relevant to momentum dependence of the superconducting gap. The calculations of all elements of the two-particle reduced density matrices are performed at the supercomputer Fugaku because huge computational resources (10^6 node hours) are needed. As a result of the analysis of the form factor for the bilayer t-t'-U model, first, we found that the Cooper pairs are essentially confined in each layer. Then, we also analyzed the impact of the long-range Coulomb interactions V on the Cooper pairs, which has been theoretically studied as one of the principal factors to control $T_{\rm c}^{\rm opt}$, in addition to the number of the adjacent CuO_2 layers. We found that the form factors of the single-layer and bilayer Hamiltonians show qualitatively different behaviors when we examine the dependence of the Cooper pairs on the range of the Coulomb repulsions: (a) As for the case of putting in up to the second-neighbor Coulomb repulsions V_2, the shape of the Cooper pairs becomes nematic (extended $s + d$ wave type) for the single-layer Hamiltonian, whereas it shows extended s-wave symmetry for the bilayer Hamiltonian, and (b) as for the case where up to third-neighbor interactions V_3 are introduced,

it shows d-wave symmetry for the single-layer Hamiltonian, whereas the bilayer Hamiltonian remains extended s-wave. The nematic behavior of the form factor would give insight into the experimental result of angle-resolved photoemission spectroscopy, which revealed nematicity in underdoped cuprates in the pseudogap phase above $T_{\rm c}$. The cause of the difference between the single-layer and bilayer systems is mainly attributed to the difference of the hole doping density.

To summarize, in this thesis, we have studied the ground-state properties of the bilayer t-t'-U-V Hubbard model by adopting the sophisticated mVMC method on the supercomputer Fugaku. Our main findings are that (1) adjacent Hubbard layers are not relevant to the enhancement of $T_{\rm c}^{\rm opt}$ in the bilayer model, suggesting the importance of other factors, such as differences between the Hubbard and CuO_2 layers and effects of impurities or dopants, in the stability of the superconductivity in multilayer cuprates, (2) Cooper pairs are confined within each layer in the bilayer system, which supports experimental evidences of the decoupled CuO_2 layers in five-layered or six-layered cuprates, and (3) the form factors of the Cooper pairs for the single-layer and bilayer Hamiltonians show qualitatively different behaviors for the range of the offsite Coulomb repulsions; the shape of the Cooper pairs shows extended s-wave symmetry in the bilayer case both when included up to V_2 and up to V_3, while it changes from nematic for the model up to V_2 to d-wave symmetry for that up to V_3 in the single-layer case. The analysis of the form factors in the underdoped region is desired to clarify the nematicity in the present Hamiltonians in future.