

Contents

1 Introduction	11
1.1 Superconductivity in strongly correlated electron system	11
1.2 Empirical correlation between T_c and number of CuO ₂ layers	13
1.3 Overview of cuprate superconductors	14
1.3.1 Common physical properties of high- T_c superconductors	14
1.3.2 Crystal structure	16
1.3.3 Previous theoretical studies for the single-layer cuprate superconductors	19
1.4 Multi-layered cuprates	25
1.4.1 Experimental results for the multi-layered cuprates	25
1.4.2 Previous theoretical studies for multi-layered cuprate superconductors	28
1.5 Off-diagonal long-range order and shape of Cooper pairs	30
1.6 Purpose of this thesis	32
2 Models	35
2.1 Effective Hamiltonian for Bilayer Cuprates	35
2.2 Single-particle picture: Bonding and antibonding bands	37
3 Methods	39
3.1 Variational wave function	39
3.1.1 Pair-product state	40
3.1.2 Correlation factors	40
3.1.3 Quantum-number projections	41
3.1.4 Initial wave functions	41
3.2 Optimization method	44
3.3 Observables	44
3.3.1 Monte Carlo samplings	44

3.3.2 Spin structure factor	45
3.3.3 Superconducting correlation function	45
3.3.4 Momentum distribution function	46
3.3.5 Many-body chemical potential	46
3.3.6 Form factor	47
3.4 Parameters for convergence	48
3.4.1 System size	48
3.4.2 Number of Monte Carlo samples	49
3.4.3 Variance	49
3.5 Numerical details	49
4 Results	51
4.1 Bilayer t - t' - U Hubbard model	51
4.1.1 Spin and superconducting correlations	52
4.1.2 Momentum distribution	53
4.1.3 Charge fluctuations	62
4.1.4 Structure of Cooper pairs	63
4.2 Effect of intralayer long-range Coulomb interaction	76
4.2.1 Superconducting correlation	77
4.2.2 Impact on structure of Cooper pairs	79
5 Discussion	93
5.1 Superconducting correlations	93
5.2 Behavior of form factor	95
5.2.1 Intralayer component	95
5.2.2 Bilayer case	97
5.2.3 Effect of long-range Coulomb interactions	98
5.2.4 Insights from form factors	99
6 Conclusion	101
Appendix	105
A Benchmarking	105
B Effect of the spin quantum-number projection on the superconductivity	106
C Form factors for bonding band and antibonding band	106

CONTENTS

5

D <i>U/t</i> -dependence of superconducting correlations	108
--	-----