Contents

| 1 | Introduction | | | | | |
|---|---|---|----|--|--|--|
| | 1.1 | Strongly Correlated Materials | 1 | | | |
| | 1.2 | Basic Models in Strongly Correlated Systems Theory | 4 | | | |
| | 1.3 | Methods for Models Investigation | 6 | | | |
| | 1.4 | Ab-initio Electronic Structure Calculation Methods | 7 | | | |
| 2 | Electronic Structure Calculations in One-Electron | | | | | |
| | Ap | proximation | 9 | | | |
| | 2.1 | Density Functional Theory and Electronic | | | | |
| | | Structure Calculations Methods | | | | |
| | | 2.1.1 Density Functional Theory | 9 | | | |
| | | 2.1.2 Electronic Structure Calculations Methods Based | | | | |
| | | on DFT | 11 | | | |
| | | 2.1.3 Breakdown of Local Density Approximation | | | | |
| | | for Strongly Correlated Systems | 14 | | | |
| | | 2.1.4 Corrections for Electron–Electron Correlations | 15 | | | |
| | 2.2 | Determining Problem Hamiltonian from Density | | | | |
| | | Functional Theory | 18 | | | |
| | | 2.2.1 Problem Definition | 18 | | | |
| | | 2.2.2 Coulomb Interaction Hamiltonian | 19 | | | |
| | | 2.2.3 Double-Counting Problem for Coulomb Interaction | 20 | | | |
| | | 2.2.4 Wannier Functions as Coulomb Interaction | | | | |
| | | Hamiltonian Basis | 21 | | | |
| | | 2.2.5 Coulomb Parameter U Value from Constrain | | | | |
| | | DFT Calculation | 26 | | | |
| | 2.3 | Static Mean-Field Approximation: $LDA + U$ Method | 30 | | | |
| | 2.4 | LDA + U Method Applications | 33 | | | |
| | | 2.4.1 Mott Insulators: NiO, CoO, and CaCuO ₂ | 33 | | | |
| | | 2.4.2 Charge Ordering: Fe_3O_4 | 35 | | | |
| | | 2.4.3 Orbital Ordering: KCuF ₃ | 38 | | | |
| | | 2.4.4 Orbital and Charge Ordering: Pr _{0.5} Ca _{0.5} MnO ₃ | 41 | | | |
| | | 2.4.5 Spin Ordering: CaV_nO_{2n+1} | 43 | | | |



| 3 | Hubbard Model in Dynamical Mean-Field Theory | | | | |
|---|--|--------|--|-----|--|
| | 3.1 | Reduc | ring Lattice Model to Effective Single | | |
| | | Impu | rity Anderson Model | 47 | |
| | | 3.1.1 | Electronic Green Function | 47 | |
| | | 3.1.2 | Single Impurity Anderson Model | 49 | |
| | | 3.1.3 | Basic DMFT Equations | 53 | |
| | | 3.1.4 | DMFT Equations for Bethe Lattice | 55 | |
| | | 3.1.5 | Methods for Solution of Single Impurity | | |
| | | 0.110 | Anderson Model | 55 | |
| | 3.2 | Quant | tum Monte Carlo Method as Single | | |
| | | Impui | rity Anderson Model Solver | 59 | |
| | | 3.2.1 | Hirsch–Fve Algorithm | 59 | |
| | | 3.2.2 | Maximum Entropy Method for Spectral | | |
| | | | Function Calculation | 66 | |
| | | 3.2.3 | QMC for Single Impurity Anderson Model | | |
| | | | with Orbital Degrees of Freedom | 72 | |
| | | 3.2.4 | Projective Quantum Monte Carlo Method | 73 | |
| | | 3.2.5 | Continuous-Time <i>QMC</i> | 76 | |
| | 3.3 | Hubb | ard Model Spectral Function in DMFT | | |
| | 0.0 | Appro | ximation | 82 | |
| | | 3.3.1 | Three Peak Spectral Structure for Half-Filling | 82 | |
| | | 3.3.2 | Metal–Insulator Phase Transition | 87 | |
| | 3.4 | Hubba | ard Model with Deviation from Half-Filling | 90 | |
| | | 3.4.1 | Quasiparticle Peak Evolution | 90 | |
| | | 3.4.2 | Phase Diagram for $T = 0$ | 90 | |
| | | 3.4.3 | Spin-Polarized Case | 94 | |
| | 3.5 | Antife | erromagnetism | 98 | |
| | 0.0 | 3.5.1 | DMFT Equations with Antiferromagnetic | | |
| | | | Order Parameter | 98 | |
| | | 3.5.2 | NRG Method Results for AFM Phase | 101 | |
| | 3.6 | Super | conductivity in Two-Dimensional Hubbard Model | 106 | |
| | | 3.6.1 | DMFT Equations for Superconducting State | 106 | |
| | | 3.6.2 | Coexistence Problem for Superconducting | | |
| | | 0.0.2 | and Antiferromagnetic Order Parameters | 109 | |
| | 3.7 | Trans | port Properties and Susceptibility | 111 | |
| | 0.1 | 3.7.1 | Optical Conductivity | 111 | |
| | | 3.7.2 | Magnetic Susceptibility | 114 | |
| | | | | | |
| 4 | DM | FT E | xtensions | 121 | |
| | 4.1 | t - J | Model as a Hubbard Model Limit | 121 | |
| | | 4.1.1 | Hamiltonian and Green Function | 121 | |
| | | 4.1.2 | DMFT Equations Derivation | 123 | |
| | | 4.1.3 | Reformulation of <i>DMFT</i> Equations | 125 | |
| | | 4.1.4 | Numerical Calculation Results | 128 | |

| | 4.2 DMFT Extensions for Nonlocal Coulomb | | | |
|---|--|---------------|--|--------------|
| | | and E | Exchange Interaction Case | . 130 |
| | | 4.2.1 | Hamiltonian and Green Function for Extended | |
| | | | Model | . 130 |
| | | 4.2.2 | EDMFT for Homogeneous System | . 132 |
| | | 4.2.3 | EDMFT for the System with Two Sublattices | . 134 |
| | | 4.2.4 | DMFT with Orbital Degeneracy | . 137 |
| | | 4.2.5 | QMC Impurity Solver for the Problem with Orbital | |
| | | | Degeneracy | . 139 |
| | | 4.2.6 | Exchange Interactions in QMC | . 140 |
| | | 4.2.7 | Continuous-Time QMC for Two-Orbital Model | . 141 |
| | 4.3 | Takin | g into Account Spatial Fluctuations | . 144 |
| | | 4.3.1 | Heuristic Approach to DMFT Extension | |
| | | | for Spatial Fluctuations | . 144 |
| | | 4.3.2 | Dynamical Vertex Approximation | . 148 |
| | | 4.3.3 | Pseudogap | .151 |
| | | 4.3.4 | Dynamical Cluster Method | . 157 |
| | 4.4 | Gener | ating Functional for Green Functions | . 161 |
| | | 4.4.1 | Baym-Kadanoff Functional | . 161 |
| | | 4.4.2 | Total Energy | . 162 |
| | 4.5 | DMF | T for Systems with Disorder | . 164 |
| | | 4.5.1 | Anderson-Hubbard Model | .164 |
| | | 4.5.2 | Phase Diagram for Nonmagnetic State | . 165 |
| | | 4.5.3 | Optical Conductivity | . 169 |
| F | Dom | india. | Anderson Model (DAM) | 179 |
| Э | Fer | TOULC . | Studios for DAM | 179 |
| • | 9.1 | | DAM og a Dagia Madel for Hasser Fermion Systems | 179 |
| | | 5.1.1 | PAM as a Basic Model for Heavy Fermion Systems | 175 |
| | | 0.1.2 | DMET for DAM | . 170 |
| | 50 | 0.1.0 | Studies by DMET Method | 190 |
| | 0.2 | PAM E 0 1 | Studies by $DMFT$ Method | . 100 |
| | ۳۹ | 0.2.1 Vand | DMFI(NRG) Results at $I = 0$ | . 100 |
| | ე.ა | Kond 5 2 1 | O Lattice | . 100 |
| | | 0.3.1 | Numerical Density Croup Mathed for Single Impurity | . 100 |
| | | 5.3.2 | Numerical Renorm-Group Method for Single Impurity | 107 |
| | | F 0 0 | Kondo Problem Solution | . 187 |
| | | 5.3.3 | I wo Energy Scales | . 189 |
| | | 5.3.4 | Method | 101 |
| | | EDE | Method | . 191 |
| | | ə.ə.ə | hughetic Ordering in Kondo Lattice Study | 109 |
| | F / | Dames | by Continuous-Time QMC Method | - 193 100 |
| | ə. 4 | | DMET Equations for ad Madel with Classical Sair | 100 |
| | | 5.4.1 | DMF1 Equations for sa-Model with Classical Spin | . 190 |
| | | 5.4.2 | Analysis of DMFT Equations Solution | . 198 |

.

| 6 | Electronic Structure Calculations for Real Materials | | | | | |
|-----|--|-------------------|---|--|--|--|
| | by | $LDA \rightarrow$ | $\vdash DMFT$ Method | | | |
| | 6.1 | Comb | aning Density Functional Theory and Dynamical | | | |
| | | Mean | -Field Theory: $LDA + DMFT$ method | | | |
| | | 6.1.1 | Coulomb Interaction | | | |
| | | 6.1.2 | Computation of Lattice and Local Green Functions | | | |
| | | | in General Case | | | |
| | | 6.1.3 | Total Energy Calculation in $LDA + DMFT \dots 206$ | | | |
| | 6.2 | Early | Transition Metal Oxides: Mott Insulators and Strongly | | | |
| | | Correlated Metals | | | | |
| | | 6.2.1 | SrVO ₃ : One Electron in Degenerate <i>d</i> -Band, Strongly | | | |
| | | | Correlated Metal | | | |
| | | 6.2.2 | V_2O_3 : Two Electrons in <i>d</i> -Band with Trigonal | | | |
| | | | Crystal-Field Splitting | | | |
| | | 6.2.3 | LiV_2O_4 : Heavy Fermion in <i>d</i> -Electron System | | | |
| | 6.3 | Late ' | Iransition Metal Oxides: Charge Transfer Insulators 220 | | | |
| | | 6.3.1 | NiO: Band Structure for Charge Transfer Insulator 220 | | | |
| | | 6.3.2 | MnO: Metal–Insulator Transition with Pressure | | | |
| | | | and <i>d</i> -ion Magnetic Moment Collapse | | | |
| | 6.4 | f-Elec | ectron Systems: $\alpha - \gamma$ Transition in Ce | | | |
| | 6.5 | Mang | anites | | | |
| | | 6.5.1 | Manganites Physical Properties | | | |
| | | 6.5.2 | Electronic Model for Manganites | | | |
| | | 6.5.3 | QMC for Systems with Electron–Lattice Coupling 235 | | | |
| | | 6.5.4 | $LDA + DMFT(QMC)$ Results for $La_{1-x}Sr_{x}MnO_{3}239$ | | | |
| | 6.6 | High- | $T_{\rm c}$ Superconductors Based on Pnictides Compounds 244 | | | |
| | 6.7 | The I | ist of Strongly Correlated Materials Investigated | | | |
| | | by DI | <i>MFT</i> Method | | | |
| 7 | Cor | nclusio | n | | | |
| ۸ | Fur | etions | Integral and Partition Function 257 | | | |
| A | run | | | | | |
| В | Gre | en Fu | nctions Formalism | | | |
| Re | feren | ices | | | | |
| Ind | lex | | | | | |