

Contents

Foreword	xvii
Peter Fulde	
1 Density Functional Theory: A Personal View	1
Robert O. Jones	
1.1 Introduction.....	1
1.2 The Early Years: The Density as a Basic Variable.....	3
1.3 Towards an “Approximate Practical Method”	6
1.4 Density Functional Formalism.....	8
1.4.1 Single-Particle Description of a Many-Particle System	8
1.4.2 Approximations to E_{xc}	9
1.4.3 Exchange-Correlation Energy, E_{xc}	11
1.4.4 DF Theory in Retrospect	13
1.5 The Beryllium Dimer	15
1.5.1 The Story to Late 1979	15
1.5.2 1980–1984	20
1.5.3 After 1984.....	21
1.6 Concluding Remarks	23
References.....	27
2 Projected Wavefunctions and High T_c Superconductivity in Doped Mott Insulators	29
Mohit Randeria, Rajdeep Sensarma, and Nandini Trivedi	
2.1 Introduction.....	29
2.2 Hubbard Model and Projected Wavefunctions	32
2.3 Particle-hole Asymmetry in Doped Mott Insulators	35
2.4 Gutzwiller Approximation	38
2.5 Superconducting Ground State	41
2.5.1 Energy Gap	42
2.5.2 Order Parameter	43

2.6	Momentum Distribution	45
2.7	Electronic Excitations and Spectral Properties	46
2.7.1	Nodal Fermi Velocity	47
2.7.2	Spectral Function	48
2.7.3	Sum Rules	49
2.7.4	Fermi Surface	50
2.8	Superfluid Density	51
2.8.1	Doping Dependence of D_s	52
2.8.2	Temperature Dependence of D_s	54
2.9	Disorder and Strong Correlations	56
2.10	Competing Orders: Antiferromagnetism	59
2.11	Conclusion	60
	References	62
3	The Pseudoparticle Approach to Strongly Correlated Electron Systems	65
	Raymond Frésard, Johann Kroha, and Peter Wölfle	
3.1	Introduction	66
3.2	Pseudoparticle Representations of Quantum Operators	67
3.2.1	Spin Operators	67
3.2.2	Electron Operators	70
3.3	Mean-Field Approximations	77
3.3.1	Saddle-Point Approximation to the Barnes Representation	77
3.3.2	Saddle-Point Approximation to the KR Representation	79
3.4	Fluctuation Corrections to the Saddle-Point Approximation: SRI Representation of the Hubbard Model	83
3.4.1	Magnetic and Stripe Phases	84
3.5	Conserving Self-Consistent Approximations	85
3.5.1	General Properties	85
3.5.2	Exact Infrared Properties of Pseudoparticle Propagators	87
3.5.3	Fock Space Projection in Saddle-Point Approximation	87
3.5.4	Noncrossing Approximation (NCA)	88
3.5.5	Conserving T -Matrix Approximation (CTMA)	90
3.6	Renormalization Group Approaches	93
3.6.1	“Poor Man’s Scaling” in the Equilibrium Kondo Model	94
3.6.2	Functional RG for the Kondo Model Out of Equilibrium	95
3.6.3	RG Approach to the Kondo Model at Strong Coupling	96

3.6.4	Functional RG Approach to Frustrated Heisenberg Models	97
3.7	Conclusion	98
	References	98
4	The Composite Operator Method (COM)	103
	Adolfo Avella and Ferdinando Mancini	
4.1	Strong Correlations and Composite Operators	103
4.2	The Composite Operator Method (COM)	106
4.2.1	Basis ψ	106
4.2.2	Equations of Motion of ψ	108
4.2.3	Dyson Equation for G	110
4.2.4	Propagator G_0	111
4.2.5	Residual Self-Energy Σ	114
4.2.6	Self-Consistency	115
4.2.7	Summary	116
4.3	Case Study: The Hubbard Model	116
4.3.1	The Hamiltonian	116
4.3.2	The Residual Self-Energy $\Sigma(\mathbf{k}, \omega)$	131
4.3.3	Four-Pole Solution	134
4.3.4	Superconducting Solution	136
4.4	Conclusions and Outlook	138
	References	139
5	LDA+GTB Method for Band Structure Calculations in the Strongly Correlated Materials	143
	Sergey G. Ovchinnikov, Vladimir A. Gavrichkov, Maxim M. Korshunov, and Elena I. Shneyder	
5.1	Introduction	144
5.2	Quasiparticle Definition of an Electron From the Lehmann Representation	145
5.3	The Main Steps of the LDA+GTB Method	146
5.3.1	Step I: LDA	148
5.3.2	Step II: Exact Diagonalization	148
5.4	Step III: Perturbation Theory	154
5.4.1	Perturbation Theory in the X -Operators Representation	154
5.4.2	Virtual and In-Gap States	157
5.4.3	Summary of Step III	158
5.5	LDA+GTB Band Structure of the Hole and Electron Doped Cuprates	159
5.5.1	LDA+GTB Band Structure of the Undoped La_2CuO_4	159
5.5.2	Low-Energy Effective $t - t' - t'' - J^*$ Model and the Fermi Surface of $\text{Sm}_{2-x}\text{Ce}_x\text{CuO}_4$	161

5.5.3	Doping-Dependent Evolution of the Fermi Surface and Lifshitz Quantum Phase Transitions in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$	163
5.6	LDA+GTB Band Structure of Manganite $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$	165
5.7	Finite-Temperature Effect on the Electronic Structure of LaCoO_3	166
5.8	Conclusions	169
	References	170
6	Projection Operator Method	173
	Nikolay M. Plakida	
6.1	Introduction	173
6.2	Equation of Motion Method for Green Functions	175
6.2.1	General Formulation	175
6.2.2	Projection Technique for Green Functions	177
6.3	Superconducting Pairing in the Hubbard Model	180
6.3.1	Hubbard Model	180
6.3.2	Dyson Equation	181
6.3.3	Mean-Field Approximation	183
6.3.4	Self-Energy Operator	184
6.3.5	Equation for Superconducting Gap and T_c	186
6.4	Spin-Excitation Spectrum	189
6.4.1	Dynamical Spin Susceptibility	189
6.4.2	Spin Susceptibility in the $t - J$ Model	192
6.4.3	Magnetic Resonance Mode	196
6.5	Conclusion	201
	References	201
7	Dynamical Mean-Field Theory	203
	Dieter Vollhardt, Krzysztof Byczuk, and Marcus Kollar	
7.1	Motivation	203
7.1.1	Electronic Correlations	203
7.1.2	The Hubbard Model	204
7.1.3	Construction of Comprehensive Mean-Field Theories for Many-Particle Models	205
7.2	Lattice Fermions in the Limit of High Dimensions	206
7.2.1	Scaling of the Hopping Amplitude	206
7.2.2	Simplifications of the Many-Body Perturbation Theory	207
7.2.3	Interactions Beyond the On-Site Interaction	209
7.2.4	Single-Particle Propagator	210
7.2.5	Consequences of the Momentum Independence of the Self-Energy	210

7.3	Dynamical Mean-Field Theory for Correlated Lattice Fermions.....	212
7.3.1	Construction of the DMFT as a Self-Consistent Single-Impurity Anderson Model	212
7.3.2	Solution of the Self-Consistency Equations of the DMFT	217
7.4	The Mott–Hubbard Metal–Insulator Transition.....	217
7.4.1	DMFT and the Three-Peak Structure of the Spectral Function	218
7.5	Theory of Electronic Correlations in Materials	221
7.5.1	The LDA+DMFT Approach	221
7.5.2	Single-Particle Spectrum of Correlated Electrons in Materials	224
7.6	Electronic Correlations and Disorder.....	227
7.7	DMFT for Correlated Bosons in Optical Lattices	228
7.8	DMFT for Nonequilibrium	229
7.9	Summary and Outlook	231
	References.....	232
8	Cluster Perturbation Theory	237
	David Sénéchal	
8.1	Introduction: CPT in a Nutshell	237
8.2	Cluster Kinematics	240
8.3	Lehmann Representation of the Green Function.....	244
8.3.1	The Lehmann Representation and the CPT Green Function	245
8.4	The Impurity Solver.....	246
8.4.1	Coding of the Basis States	247
8.4.2	The Lanczos Algorithm for the Ground State	249
8.4.3	The Lanczos Algorithm for the Green Function	250
8.4.4	The Band Lanczos Algorithm for the Green Function....	252
8.4.5	Cluster Symmetries	253
8.4.6	Green Functions Using Cluster Symmetries	255
8.4.7	Other Solvers	256
8.5	Periodization.....	257
8.6	Computing Physical Quantities.....	261
8.7	Results on the Hubbard Model	263
8.8	Applications to Other Models	266
8.8.1	Multi-Band Hubbard Models	266
8.8.2	t – J or Spin Models	267
8.8.3	Extended Hubbard Models	268
8.8.4	Phonons	269
	References.....	269

9	Dynamical Cluster Approximation	271
	H. Fotsos, S. Yang, K. Chen, S. Pathak, J. Moreno, M. Jarrell, K. Mielson, E. Khatami, and D. Galanakis	
9.1	Introduction	271
9.2	The Dynamical Mean Field and Cluster Approximations	273
9.2.1	The Dynamical Mean-Field Approximation	273
9.2.2	The Dynamical Cluster Approximation	276
9.2.3	Φ Derivability	277
9.2.4	Algorithm	280
9.3	Physical Quantities	281
9.3.1	Particle–Hole Channel	281
9.3.2	Particle–Particle Channel	283
9.4	DCA and Quantum Criticality in the Hubbard Model	285
9.4.1	Evidence of the Quantum Critical Point at Optimal Doping	285
9.4.2	Nature of the Quantum Critical Point in the Hubbard Model	291
9.4.3	Relationship Between Superconductivity and the Quantum Critical Point	294
9.5	Conclusion	300
	References	300
10	Self-Energy-Functional Theory	303
	Michael Potthoff	
10.1	Motivation	303
10.2	Self-Energy Functional	305
10.2.1	Hamiltonian, Grand Potential and Self-Energy	305
10.2.2	Luttinger–Ward Functional	306
10.2.3	Diagrammatic Derivation	308
10.2.4	Derivation Using the Path Integral	308
10.2.5	Variational Principle	311
10.2.6	Approximation Schemes	312
10.3	Variational Cluster Approach	313
10.3.1	Reference System	313
10.3.2	Domain of the Self-Energy-Functional	314
10.3.3	Construction of Cluster Approximations	315
10.4	Consistency of Approximations	320
10.4.1	Analytical Structure of the Green’s Function	320
10.4.2	Thermodynamical Consistency	321
10.4.3	Symmetry Breaking	322
10.4.4	Non-perturbative Conserving Approximations	325
10.5	Bath Degrees of Freedom	327
10.5.1	Motivation and Dynamical Impurity Approximation	327
10.5.2	Relation to Dynamical Mean-Field Theory	328
10.5.3	Cluster Mean-Field Approximations	330
10.5.4	Translation Symmetry	332

10.6	Systematics of Approximations	333
10.7	Summary	336
	References	337
11	Cluster Dynamical Mean Field Theory	341
	David Sénéchal	
11.1	The CDMFT Procedure	342
11.1.1	The Effective Hamiltonian	342
11.1.2	The Self-Consistency Condition	345
11.1.3	The SFA Point of View	346
11.2	The Exact Diagonalization Implementation	347
11.2.1	Working with a Small Bath System: The Distance Function	347
11.2.2	Bath Parametrization	348
11.2.3	The Distance Function	352
11.3	Quantum Monte Carlo Solvers	355
11.3.1	The Hirsch-Fye Method	356
11.3.2	The Continuous-Time Method	358
11.4	The Mott Transition	360
11.5	Application to the Cuprates	364
11.6	CDMFT and DCA	367
	References	370
12	Functional Renormalization Group for Interacting Many-Fermion Systems on Two-Dimensional Lattices	373
	Carsten Honerkamp	
12.1	Introduction	373
12.2	Functional RG Schemes for Fermions: Exact Flow Equations and Truncations	376
12.2.1	Basic Elements	376
12.2.2	Functional Renormalization Group Differential Equations	378
12.2.3	Choice of Flow Parameter	383
12.3	Implementation of the Fermionic fRG for Two Dimensional Lattices	386
12.4	Instabilities in Two-Dimensional Lattice Systems	388
12.4.1	Two-Dimensional Hubbard Model Near Half Filling	388
12.4.2	Iron Pnictides	395
12.5	Remarks on the fPI fRG Scheme	398
12.5.1	Differences to Standard Wilsonian RG	398
12.5.2	Higher Loops	399
12.5.3	Connection to Infinite-Order Single-Channel Summations	399
12.5.4	Symmetry-Breaking: Connection to Mean-Field and Eliashberg Theory	400

12.5.5	Normal-State Self-Energy	402
12.5.6	Refined Studies	404
12.6	Conclusions and Outlook	405
	References	405
13	Two-Particle-Self-Consistent Approach for the Hubbard Model	409
	André-Marie S. Tremblay	
13.1	Introduction	409
13.2	The Method	412
13.2.1	Physically Motivated Approach, Spin and Charge Fluctuations	413
13.2.2	Mermin–Wagner, Kanamori–Brueckner and Benchmarking Spin and Charge Fluctuations	416
13.2.3	Self-Energy	420
13.2.4	Internal Accuracy Checks	423
13.2.5	A More Formal Derivation	425
13.2.6	Pseudogap in the Renormalized Classical Regime	429
13.3	Case Studies	432
13.3.1	Pseudogap in Electron-Doped Cuprates	432
13.3.2	<i>d</i> -Wave Superconductivity	435
13.4	More Insights on the Repulsive Model	441
13.4.1	Critical Behavior and Phase Transitions	441
13.4.2	Longer Range Interactions	442
13.4.3	Frustration	443
13.4.4	Thermodynamics, Conserving Aspects	443
13.4.5	Vertex Corrections and Conservation Laws	446
13.5	Attractive Hubbard Model	446
13.5.1	Pseudogap from Superconductivity in Attractive Hubbard Model	447
13.6	Open Problems	448
	References	450
	Index	455