

CONTENTS

<i>Contributors</i>	<i>ix</i>
<i>Preface</i>	<i>xiii</i>
1. Paradox of Self-Interaction Correction: How Can Anything So Right Be So Wrong?	1
John P. Perdew, Adrienn Ruzsinszky, Jianwei Sun, and Mark R. Pederson	
1. Introduction	2
2. What Is Right About PZ SIC?	6
3. What Is Wrong About PZ SIC?	7
4. SIC: How Can Anything So Right Be So Wrong? (Conclusions)	8
Acknowledgments	10
Appendix. Do Complex Orbitals Resolve the Paradox of SIC?	11
References	12
2. Local Spin Density Treatment of Substitutional Defects in Ionic Crystals with Self-Interaction Corrections	15
Koblar Alan Jackson	
1. Introduction	15
2. Free-Ion Calculations	18
3. Pure Crystal Calculation	20
4. Embedded-Cluster Approach to Isolated Impurities	21
5. Discussion	26
Acknowledgment	27
References	27
3. Electronic Transport as a Driver for Self-Interaction-Corrected Methods	29
Anna Pertsova, Carlo Maria Canali, Mark R. Pederson, Ivan Rungger, and Stefano Sanvito	
1. Electron Transport Formalism	32
2. Atomic Self-Interaction Correction	35
3. Linear Response: Energy Level Alignment	39
4. Derivative Discontinuity of Exchange–Correlation Functional	47
5. Recent Developments: DFT-NEGF with Improved Exchange–Correlation Functionals	62

6. Tunneling Transport Through Magnetic Molecules	64
Acknowledgments	80
References	80
4. The Two-Set and Average-Density Self-Interaction Corrections Applied to Small Electronic Systems	87
Phuong Mai Dinh, Paul-Gerhard Reinhard, Eric Suraud, and Marc Vincendon	
1. The Two-Set SIC Scheme	88
2. Average-Density SIC—A Very Simple Approach	92
3. Results	92
4. Test of Molecular Binding for the N_2 Dimer	93
5. Dynamical Simulation of Ionization and IP	94
6. On Koopmans' Theorem	96
7. A Critical Example: $Na(H_2O)_n$	98
8. PES and the Impact of s.p. Energies	101
References	102
5. Koopmans-Compliant Self-Interaction Corrections	105
Nicolas Poilvert, Giovanni Borghi, Ngoc Linh Nguyen, Nathan Daniel Keilbart, Kevin Wang, and Ismaila Dabo	
1. Introduction: Toward Many-Electron Self-Interaction Corrections	105
2. Defining Self-Interaction Errors	106
3. Classifying Self-Interaction Corrections	111
4. Koopmans-Compliant PZ Correction	114
5. Conclusion	123
Acknowledgments	123
References	123
6. Constrained Local Potentials for Self-Interaction Correction	129
Nikitas Gidopoulos and Nektarios N.N. Lathiotakis	
1. Constraining the Optimal Local Potential to Heal Self-Interaction	129
2. Applications of the Approach of Constrained Local Potential	133
3. Perspectives	139
Acknowledgment	141
References	141
7. Self-Interaction Correction as a Kohn–Sham Scheme in Ground-State and Time-Dependent Density Functional Theory	143
Stephan Kümmel	
References	149

8. Self-Interaction Corrections Within the Fermi-Orbital-Based Formalism	153
Mark R. Pederson and Tunna Baruah	
1. Introduction	154
2. Fermi-Orbital SIC	157
3. Energies and Derivatives Within Fermi-Orbital SIC	161
4. Applications	168
5. Outlook	177
Acknowledgments	178
References	178
9. Laser Spectroscopy and Quantum Optics in GaAs and InAs Semiconductor Quantum Dots	181
Duncan G. Steel	
1. Introduction	182
2. Early Experiments on Fluctuation and Self-Assembled Quantum Dots: Suppression of the Usual Many-Body Physics Seen in Higher Dimensional Structures	185
3. Quantum Coherence, Coherent Optical Control, and Application to Quantum Information	192
4. Summary	218
Acknowledgments	218
References	219
10. Ultracold Neutral Plasmas Well into the Strongly Coupled Regime	223
Michael S. Murillo and Scott D. Bergeson	
1. Introduction	224
2. Transport in Dense Plasmas	227
3. UNP Experiment	231
4. Electron Shielding, $1 \leq \Gamma \leq 4$	235
5. Strong Coupling in Screened Plasmas	238
6. Structure of Ultracold Plasmas	240
7. Using Rydberg States to Preorder the Neutral Gas	242
8. Multiple Ionization	249
9. Laser-Cooling the Ions	257
10. Dual-Species Plasmas	264
11. Conclusion	264
Acknowledgments	265
References	265

11. Coherent Population Trapping, Nuclear Spin Cooling, and Lévy Flights in Solid-State Atom-Like Systems	273
Swati Singh, Yiwen Chu, Mikhail Lukin, and Susanne Yelin	
1. Introduction	274
2. Physical System and Experiments: Overview	277
3. Simulating Spin Bath Cooling	290
4. Photon Statistics	297
5. Conclusion	306
Acknowledgments	307
Appendix A. NV–Laser Interaction Details	307
Appendix B. Details of Hyperfine Interaction	309
Appendix C. Simulating a Realistic ^{13}C Spin Bath	314
References	324
12. Thermodynamics of Quantum Systems Under Dynamical Control	329
David Gelbwaser-Klimovsky, Wolfgang Niedenzu, and Gershon Kurizki	
1. Introduction	331
2. Steady-State Cycles Under Periodic Modulation	343
3. Periodically Modulated Qubit-Based Heat Machine	350
4. QHMs Based on Periodically Modulated Multilevel Systems	356
5. Quantum Heat Engines Driven by a Quantum Piston	362
6. Self-contained QR with a Quantum Piston	368
7. Continuously Driven Qubit as Quantum Cooler	370
8. Cooling Speed of Quantum Baths	374
9. Control of Non-Markovian Thermodynamic Processes	377
10. Work-Information Relation Under Non-Markovian Evolution: Violation of the SL Bound	383
11. Discussion and Outlook	389
Acknowledgments	396
References	397
Index	409
Contents of Volumes in This Serial	421