

Contents

<i>Preface</i>	vii
<i>Acknowledgments</i>	ix
1. Introduction to Multilayered Nanostructures	1
1.1 Thin Film Growth and Multilayered Nanostructures	2
1.2 Strongly Correlated Materials	14
1.3 The Proximity Effect	17
1.4 Electronic Charge Reconstruction at an Interface	20
1.5 Roadmap to Real-Materials Calculations	27
2. Dynamical Mean-Field Theory in the Bulk	31
2.1 Models of Strongly Correlated Electrons	31
2.2 Second Quantization	39
2.3 Imaginary Time Green's Functions	46
2.4 Real Time Green's Functions	53
2.5 The Limit $d \rightarrow \infty$ and the Mapping onto a Time-Dependent Impurity Problem	61
2.6 Impurity Problem Solvers	67
2.7 Computational Algorithms	77
2.8 Linear-Response dc -Transport in the Bulk	80
2.9 Metal-Insulator Transitions within DMFT	92
2.10 Bulk Charge and Thermal Transport	99
3. Dynamical Mean-Field Theory of a Multilayered Nanostructure	113
3.1 Potthoff-Nolting Approach to Multilayered Nanostructures	113

3.2	Quantum Zipper Algorithm (Renormalized Perturbation Expansion)	116
3.3	Computational Methods	119
3.4	Density of States for a Nanostructure	122
3.5	Longitudinal Charge Transport Through a Nanostructure	129
3.6	Charge Reconstruction (Schottky Barriers)	140
3.7	Longitudinal Heat Transport Through a Nanostructure .	152
3.8	Superconducting Leads and Josephson Junctions	172
3.9	Finite Dimensions and Vertex Corrections	193
4.	Thouless Energy and Normal-State Transport	197
4.1	Heuristic Derivation of the Generalized Thouless Energy	197
4.2	Thouless Energy in Metals	199
4.3	Thouless Energy in Insulators	206
4.4	Crossover from Tunneling to Incoherent Transport in Devices	209
5.	Josephson Junctions and Superconducting Transport	215
5.1	Introduction to Superconducting Electronics Devices . . .	215
5.2	Superconducting Proximity Effect	219
5.3	Josephson Current	224
5.4	Figure-of-Merit for a Josephson Junction	230
5.5	Effects of Temperature	234
5.6	Density of States and Andreev Bound States	238
6.	Thermal Transport	249
6.1	Electronic Charge Reconstruction Near a Metal-Insulator Transition	249
6.2	Thermal Transport Through a Barrier Near the Metal-Insulator Transition	253
7.	Future Directions	261
7.1	Spintronics Devices	261
7.2	Multiband Models for Real Materials	265
7.3	Nonequilibrium Properties	268
7.4	Summary	270

Appendix A	Problems	271
A.1	Jellium model	271
A.2	Density of states for the hypercubic lattice in 1, 2, 3, and ∞ dimensions	272
A.3	Noninteracting electron in a time-dependent potential . .	273
A.4	Relation between imaginary-time summations and real-axis integrals	274
A.5	The Green's functions of a local Fermi liquid	276
A.6	Rigid-band approximation to the Falicov-Kimball model .	276
A.7	Comparing the spectral formula to the Hilbert transform	278
A.8	Imaginary-time Green's functions	278
A.9	Partition function for a spinless electron in a general time-dependent field	279
A.10	Mapping the impurity in a field to an impurity coupled to a chain in the NRG approach	279
A.11	Impurity Green's function for the chain Hamiltonian in the NRG approach	281
A.12	Solving the NRG many-body Hamiltonian for the chain .	282
A.13	Metal-insulator transition in the half-filled Falicov-Kimball model	283
A.14	Kramers-Kronig analysis for the Green's function, and the effect of the pole in the Mott insulator	283
A.15	Metal-insulator transition on a simple cubic lattice	284
A.16	DC conductivity for the simple cubic lattice	287
A.17	Jonson-Mahan theorem	288
A.18	Charge and thermal conductivity for the Falicov- Kimball model	290
A.19	The particle-hole asymmetric metal-insulator transition .	291
A.20	Non Fermi-liquid behavior of the Falicov-Kimball model .	291
A.21	Thermopower of the Falicov-Kimball model and the figure-of-merit	292
A.22	$U \rightarrow \infty$ Green's functions	292
A.23	Determining $G_{\alpha\beta}$ from the quantum zipper algorithm . .	293
A.24	The stability of the left and right recursion relations of the quantum zipper algorithm	294
A.25	Efficient numerical evaluation of integrals via changes of variables	294
A.26	Equilibrium solutions with charge reconstruction	296

A.27	Local charge and heat current operators for a nanostructure	297
A.28	Operator identity for the Jonson-Mahan theorem	299
A.29	BCS gap equation	299
A.30	Equations of motion needed for the Nambu-Gor'kov formalism	300
A.31	Spin one-half atom in a time-dependent normal and anomalous dynamical mean field	300
A.32	Hilbert transformation in the Nambu-Gor'kov formalism .	301
A.33	Evaluating Hilbert transformation-like integrals needed for determining the bulk critical current on a simple-cubic lattice	302
A.34	The single-plane Mott-insulating barrier	304
A.35	Green's functions of the particle-hole symmetric Falicov-Kimball model nanostructure	305
A.36	Parallel implementation for the resistance calculation of a nanostructure	306
A.37	Resistance and Thouless energy of a nanostructure	306
	<i>Bibliography</i>	309
	<i>Index</i>	323