
Contents

Preface	xiii
List of Symbols	xv
List of Abbreviations	xvii
Chapter 1. Introduction: Nanoelectronics, Quantum Mechanics, and Solid State Physics	1
Philippe DOLLFUS and François TRIOZON	
1.1. Nanoelectronics	1
1.1.1. Evolution of complementary metal–oxide–semiconductor microelectronics toward the nanometer scale	1
1.1.2. Post-CMOS nanoelectronics	3
1.1.3. Theory and simulation	3
1.2. Basic notions of solid-state physics.	4
1.2.1. Simplifications of the many-body problem.	4
1.2.2. Basic notions of quantum mechanics	6
1.2.3. Bloch waves in crystals	17
1.2.4. Effective mass approximation	19
1.3. Quantum mechanics and electronic transport	20
1.3.1. Wavepacket in a slowly varying potential: the semiclassical equations of motion.	20
1.3.2. Square potential barrier: tunneling and quantum reflection	22
1.3.3. Quantum confinement	25
1.3.4. Scattering.	28
1.4. Conclusion	29
1.5. Bibliography	30

Chapter 2. Electronic Transport: Electrons, Phonons and Their Coupling within the Density Functional Theory	31
Nathalie VAST, Jelena SJAKSTE, Gaston KANÉ and Virginie TRINITÉ	
2.1. Introduction	31
2.2. Electronic structure	34
2.2.1. The time-independent Schrödinger equation	35
2.2.2. Born–Oppenheimer separation	35
2.2.3. The many-electron problem	36
2.2.4. The DFT	38
2.2.5. Conclusions and remarks about and beyond DFT	44
2.3. Phonons	46
2.3.1. Schrödinger equation for the ions	46
2.3.2. The harmonic approximation	47
2.3.3. The Hellmann–Feynman theorem	47
2.3.4. The linear response	48
2.3.5. The frozen-phonon method	48
2.3.6. Density functional perturbation theory	49
2.3.7. Beyond the harmonic approximation: computing the phonon–phonon interaction	52
2.4. Electron–phonon coupling	52
2.4.1. Electron–phonon matrix element	53
2.4.2. Wavefunctions of the initial and final electronic states	54
2.4.3. Selection rules and strong dispersion of electron–phonon matrix elements	55
2.4.4. Electron–phonon transition probability: use of the Fermi golden rule	58
2.4.5. Measurable quantities and comparison with DFPT calculations	59
2.4.6. Different electron–phonon scattering mechanisms and their role in the transport properties of semiconductors	60
2.4.7. Electron–phonon coupling beyond standard approximations	62
2.5. Semiclassical transport properties	62
2.5.1. Semiclassical transport: BTE	63
2.5.2. Scattering mechanisms	64
2.5.3. Linear and nonlinear transport	67
2.5.4. Coupling BTE with DFT	68
2.5.5. Limits of the semiclassical approach	69

2.6. Quantum transport	70
2.6.1. Quantum ballistic transport: the Landauer-Büttiker approach.	70
2.6.2. The master equation	77
2.6.3. Dynamics of the density matrix operator: closed and open system.	78
2.6.4. Non-equilibrium Green's functions	84
2.7. Conclusion	84
2.8. Appendix A	85
2.8.1. Derivation of the single-particle master equation	85
2.9. Bibliography	86
Chapter 3. Electronic Band Structure: Empirical Pseudopotentials, $k \cdot p$ and Tight-Binding Methods	97
Denis RIDEAU, François TRIOZON and Philippe DOLLFUS	
3.1. Band structure problem	97
3.1.1. Introduction	97
3.1.2. Bulk semiconductors	99
3.1.3. Confined systems	101
3.2. Empirical pseudopotentials method	102
3.2.1. Principles of the model – basic equations	104
3.2.2. The EPM equation in matrix form	106
3.2.3. Effects of strain within EPM	108
3.3. The $k \cdot p$ method	109
3.3.1. Principles of the model – basic equations	110
3.3.2. Solution of the eigenvalue problem	112
3.3.3. Effect of strain within the $k \cdot p$ model	114
3.4. The TB method	115
3.4.1. Principles of the model	116
3.4.2. The sp ³ d ⁵ s* TB model for Si and Ge	116
3.4.3. The simple case of graphene	118
3.4.4. Strain effects in the TB model	121
3.5. Optimization of empirical models	122
3.5.1. Reference data and methodology	122
3.5.2. Model parameters for Si and Ge	123
3.5.3. Comparison of the models for bulk Si and Ge	125
3.6. Bibliography	126

Chapter 4. Relevant Semiempirical Potentials for Phonon Properties	131
Sebastian VOLZ	
4.1. Introduction	131
4.1.1. Criteria for choosing the adequate potential in phonon computations	132
4.1.2. Derivation of the phonon properties	133
4.2. Generic pair potentials: the Lennard-Jones potential	134
4.3. Semiconductors: Stillinger–Weber and Tersoff potentials	136
4.3.1. Stillinger–Weber potential	136
4.3.2. Silicon crystal modeled with Stillinger– Weber potential	137
4.3.3. Germanium crystal modeled with Stillinger– Weber	138
4.3.4. Tersoff potential	140
4.4. Oxydes: Van Beest, Kramer and van Santen potential	143
4.4.1. Application of BKS potential to ZnO crystal	145
4.4.2. Application of BKS potential to MgO crystal	147
4.5. Metals – isotropic many-body pair-functional potentials for metals: the modified embedded-atom method	148
4.5.1. Example: phonon dispersion relation of gold	149
4.6. Polymers and carbon-based compounds: adaptive intermolecular reactive bond order, adaptive intermolecular REBO and Dreiding potentials	149
4.6.1. Adaptive intermolecular REBO potential	149
4.6.2. Dreiding potential	152
4.6.3. Example: DOS of the Jeffamine	155
4.7. Water: TIP3P potential	156
4.7.1. Example: radial density function and DOS	157
4.8. Conclusion	158
4.9. Bibliography	158
Chapter 5. Introduction to Quantum Transport	163
François TRIOZON, Stephan ROCHE and Yann-Michel NIQUET	
5.1. Quantum transport from the point of view of wavepacket propagation	164
5.1.1. Calculation of wavepacket evolution	164
5.1.2. The semi-classical limit	169
5.1.3. Tunneling and quantum reflection	171
5.1.4. Beyond 1D models	174
5.1.5. Simulation methods for quantum transport	177

5.2. The transmission formalism for the conductance.	177
5.2.1. The scattering matrix.	177
5.2.2. Landauer–Büttiker conductance	180
5.2.3. Conductance of an ideal wire and energy dissipation	184
5.2.4. Application to planar and bulk systems	184
5.3. The Green’s function method for quantum transmission	185
5.3.1. One-electron Green’s functions: definitions and basic properties	185
5.3.2. Calculation of the transmission through a conductor connected to two electrodes	199
5.3.3. Application to a 1D system	208
5.3.4. Application to a multichannel system	212
5.4. Conclusion	219
5.5. Matlab/Octave codes	219
5.6. Bibliography	220
Chapter 6. Non-Equilibrium Green’s Function Formalism	223
Michel LANNOO and Marc BESCOND	
6.1. Second quantization and time evolution pictures.	223
6.2. General definition of the Green’s functions, their physical meaning and their perturbation expansion.	225
6.2.1. Equilibrium perturbation expansion at $T = 0$ K	226
6.2.2. Non-equilibrium perturbation expansion	227
6.3. Stationary Green’s functions and fluctuation-dissipation theorem	229
6.3.1. General relations	229
6.3.2. Equilibrium: the fluctuation-dissipation theorem	231
6.4. Dyson’s equation and self-energy: general formulation.	232
6.4.1. Equation of motion for non-interacting electrons	232
6.4.2. Dyson’s equation and its justification for interacting electrons	233
6.4.3. Detailed form of Dyson’s equation for non-equilibrium	236
6.5. Some examples.	237
6.5.1. 1D free electron retarded Green’s function.	237
6.5.2. 1D tight-binding chain	238
6.5.3. Contact self-energy	239
6.6. The ballistic regime	240
6.6.1. The Landauer formula	240

6.6.2. The NEGF derivation of the Landauer formula	241
6.6.3. Relation with scattering theory	244
6.7. The electron–phonon interaction	245
6.7.1. The phonon Hamiltonian	245
6.7.2. Electron–phonon interaction	246
6.7.3. Electron–phonon self-energy	246
6.7.4. Explicit expressions for $\Sigma\omega_{e-ph}$ in the effective mass approximation	248
6.7.5. Conserving properties: continuity equations	251
6.7.6. Summary of the important formulae.	255
6.8. Bibliography	257
Chapter 7. Electron Devices Simulation with Bohmian Trajectories	261
Guillermo ALBAREDA, Damiano MARIAN, Abdelilah BENALI, Alfonso ALARCÓN, Simeon MOISES and Xavier ORIOLS	
7.1. Introduction: why Bohmian mechanics?	261
7.1.1. Quantum continuous measurement of the electrical current	263
7.1.2. Coulomb correlations and displacement current.	266
7.2. Theoretical framework: Bohmian mechanics	267
7.2.1. Postulates and basic equations	268
7.2.2. Bohmian explanation of the measurement process	269
7.2.3. Bohmian mechanics for many-particle systems	273
7.3. The BITLLES simulator: time-resolved electron transport	276
7.3.1. On the role of the measuring apparatus	278
7.3.2. Coulomb correlations beyond mean field.	285
7.3.3. Stochastic injection of electrons	288
7.4. Computation of the electrical current and its moments with BITLLES	291
7.4.1. Preliminary considerations	291
7.4.2. Practical method to compute DC, AC, transients and higher moments	294
7.5. Conclusion	299
7.6. Acknowledgments.	301
7.7. Appendix A: Practical algorithm to compute Bohmian trajectories	301
7.8. Appendix B: Ramo–Shockley–Pellegrini theorems	306
7.9. Appendix C: Bohmian mechanics with operators	307

7.10. Appendix D: Relation between the Wigner distribution function and the Bohmian trajectories	310
7.11. Bibliography	314
Chapter 8. The Monte Carlo Method for Wigner and Boltzmann Transport Equations	319
Philippe DOLLFUS, Damien QUERLIOZ and Jérôme SAINT MARTIN	
8.1. The WTE	320
8.1.1. Density matrix and Liouville equation	320
8.1.2. The Wigner function	322
8.1.3. Dynamic equation: The Wigner equation.	323
8.2. The semiclassical limit: BTE	325
8.2.1. Distribution function and Boltzmann equation: the standard point of view	326
8.2.2. The connection between WTE and BTE	328
8.3. Scattering in Boltzmann and Wigner equations	329
8.3.1. The Boltzmann collision operator: phonon and impurity scattering	330
8.3.2. Phonon and impurity scattering in the Wigner formalism	339
8.3.3. Wigner–Boltzmann equation	340
8.4. The MC method for solving the BTE	341
8.4.1. Main features of the MC algorithm	341
8.4.2. Interaction with single impurities	347
8.4.3. Quantization effects: the multi-subband approach	348
8.4.4. Quantization effects: the effective potential approach	351
8.4.5. Full-band MC simulation	352
8.5. Extension of the MC method for solving the WBTE	352
8.5.1. Overview of the different methods.	353
8.5.2. The “continuous affinity” method	355
8.5.3. About the validity of the method.	359
8.6. Bibliography	360
List of Authors	371
Index	373
