

## Table of Contents

<b>Symbols</b> . . . . .	ix
<b>Abbreviations</b> . . . . .	xiii
<b>Introduction</b> . . . . .	xv
<b>Acknowledgements</b> . . . . .	xxi
<b>Chapter 1. Theoretical Framework of Quantum Transport in Semiconductors and Devices</b> . . . . .	1
1.1. The fundamentals: a brief introduction to phonons, quasi-electrons and envelope functions . . . . .	2
1.1.1. The basic concepts: band structure and phonon dispersion . . . . .	2
1.1.2. Quasi-electron/phonon scattering . . . . .	8
1.1.3. Quasi-electron/quasi-electron and quasi-electron/impurity scattering . . . . .	9
1.2. The semi-classical approach of transport . . . . .	11
1.2.1. The Boltzmann transport equation . . . . .	11
1.2.2. Quantum corrections to the Boltzmann equation . . . . .	13
1.3. The quantum treatment of envelope functions . . . . .	16
1.3.1. The density matrix formalism . . . . .	17
1.3.2. The Wigner function formalism . . . . .	20
1.3.3. The Green's functions formalism . . . . .	27
1.4. The two main problems of quantum transport . . . . .	29
1.4.1. The first problem: the modeling of contacts . . . . .	29
1.4.2. The second problem: the treatment of collisions/scattering in quantum transport . . . . .	37

<b>Chapter 2. Particle-based Monte Carlo Approach to Wigner-Boltzmann Device Simulation</b> . . . . .	57
2.1. The particle Monte Carlo technique to solve the BTE. . . . .	59
2.1.1. Principles and algorithm. . . . .	59
2.1.2. Multi-subband transport: mode-space approach . . . . .	62
2.2. Extension of the particle Monte Carlo technique to the WBTE: principles . . . . .	71
2.2.1. The Wigner paths method . . . . .	72
2.2.2. The “full Monte Carlo” method . . . . .	73
2.2.3. The “continuous affinity” method technique. . . . .	76
2.3. Simple validations via two typical cases. . . . .	83
2.3.1. First validation of the quantum mechanical treatment: interaction of a wave packet with a tunneling barrier. . . . .	83
2.3.2. Validation of the semi-classical treatment: $N^+/N/N^+$ diode . . . . .	84
2.4. Conclusion . . . . .	86
<b>Chapter 3. Application of the Wigner Monte Carlo Method to RTD, MOSFET and CNTFET</b> . . . . .	89
3.1. The resonant tunneling diode (RTD) . . . . .	90
3.1.1. Introduction to the RTD . . . . .	90
3.1.2. Model, simulated structure and current-voltage characteristics . . . . .	92
3.1.3. Microscopic quantities. . . . .	94
3.1.4. Comparison with experiment . . . . .	96
3.1.5. Comparison with the Green’s function formalism. . . . .	96
3.2. The double-gate metal-oxide-semiconductor field-effect transistor (DG-MOSFET) . . . . .	99
3.2.1. Introduction to the DG-MOSFET . . . . .	99
3.2.2. Simulated devices. . . . .	102
3.2.3. Model: transport and scattering. . . . .	103
3.2.4. Subband profiles and mode-space wave functions . . . . .	109
3.2.5. Quantum transport effects. . . . .	111
3.2.6. Impact of scattering . . . . .	117
3.2.7. Design of nano-MOSFET and factors of merit for CMOS applications . . . . .	121
3.2.8. Degeneracy effects in source and drain access. . . . .	125
3.2.9. Some comparisons with experiments . . . . .	132
3.3. The carbon nanotube field-effect transistor (CNTFET) . . . . .	134
3.3.1. Introduction to the CNTFET . . . . .	134
3.3.2. Simulated device . . . . .	136
3.3.3. Model: band structure, transport and scattering . . . . .	137
3.3.4. Quantum transport effect . . . . .	142
3.4. Conclusion . . . . .	148
3.4.1. Summary of main results . . . . .	148

3.4.2. Prospective conclusions regarding CMOS devices . . . . .	149
<b>Chapter 4. Decoherence and Transition from Quantum to Semi-classical Transport</b> . . . . .	151
4.1. Simple illustration of the decoherence mechanism. . . . .	152
4.2. Coherence and decoherence of Gaussian wave packets in GaAs . . . . .	157
4.2.1. Introduction . . . . .	157
4.2.2. Decoherence of free wave packets in GaAs . . . . .	160
4.2.3. Impact of decoherence on the interaction of a wave packet with single or double tunnel barrier . . . . .	166
4.3. Coherence and decoherence in RTD: transition between semi-classical and quantum regions . . . . .	171
4.3.1. Decoherence in RTD. . . . .	171
4.3.2. Transition between quantum and semi-classical regions. . . . .	174
4.4. Quantum coherence and decoherence in DG-MOSFET. . . . .	175
4.4.1. Electron decoherence . . . . .	177
4.4.2. Emergence of semi-classical behavior . . . . .	179
4.5. Conclusion . . . . .	180
<b>Conclusion</b> . . . . .	183
<b>Appendix A. Average Value of Operators in the Wigner Formalism</b> . . . . .	187
<b>Appendix B. Boundaries of the Wigner Potential</b> . . . . .	189
<b>Appendix C. Hartree Wave Function</b> . . . . .	191
<b>Appendix D. Asymmetry Between Phonon Absorption and Emission Rates</b> . . . . .	193
<b>Appendix E. Quantum Brownian Motion</b> . . . . .	195
<b>Appendix F. Purity in the Wigner formalism</b> . . . . .	201
<b>Appendix G. Propagation of a Free Wave Packet Subject to Quantum Brownian Motion</b> . . . . .	203
<b>Appendix H. Coherence Length at Thermal Equilibrium</b> . . . . .	205
<b>Bibliography</b> . . . . .	207
<b>Index</b> . . . . .	241