

Contents

Acknowledgment	iii
Abstract	v
Zusammenfassung	vii
1 Introduction	1
2 Theory of Quantum Transport	5
2.1 Landauer Transport Theory	5
2.2 Landauer-Büttiker Transport Theory	9
2.3 Scaling, Ohm's Law, Coherence	12
2.4 Scattering States	14
2.5 Quantum Transport Simulations	15
2.5.1 Characterization of the Transport Model . . .	15
2.5.2 Decoupling of the Schrödinger Equation . . .	18
2.5.3 Devices	21
3 Ballistic Transport	25
3.1 Physical Motivation	25
3.2 Scattering Matrix Approach (SMA)	26
3.2.1 The Quasi 1D Transport Problem	26
3.2.2 Physical Constraints	27
3.2.3 Recursive Construction Algorithm	28

3.2.4	Scaling of the SMA Algorithm	30
3.2.5	Boundary Conditions for Ballistic Transport	31
3.2.6	Calculation of Observables	33
3.3	Limits of Ballistic Transport	36
3.4	Simulation Results	38
4	Büttiker Scattering	45
4.1	Physical Motivation	45
4.2	Scattering Matrix Approach (SMA)	46
4.2.1	Generalization of the SMA Algorithm	46
4.2.2	Interpretation of the Generalized SMA Algorithm	50
4.2.3	Scaling of the Generalized SMA Algorithm	52
4.2.4	Calculation of Observables	53
4.3	Self-Consistency: Current Conservation	54
4.3.1	Energy Relaxation	54
4.3.2	Momentum Relaxation	55
4.4	Simulation Results	57
4.5	Shortcomings and Advantages	61
5	Non-Equilibrium Green's Functions	63
5.1	Physical Motivation	63
5.2	Quantum Transport Equations	64
5.2.1	Steady-state Formulation	64
5.2.2	Choice of Basis	65
5.3	Local Phonon Scattering	68
5.3.1	The Lesser Scattering Self-Energy	68
5.3.2	The Retarded Scattering Self-Energy	69
5.3.3	Intravalley Acoustic Phonon Scattering	70
5.3.4	Intervalley Phonon Scattering	71
5.4	Calculation of Observables	71
5.5	Computational Aspects	74
5.5.1	Ballistic Transport	74
5.5.2	Büttiker Scattering	74
5.5.3	Local Scattering	75

5.5.4	Non-local Scattering	76
5.5.5	Self-Consistency: Current Conservation	76
5.6	Boundary Conditions	79
5.6.1	Decomposition of the System	79
5.6.2	Coherent Boundary Conditions	80
5.6.3	Incoherent Boundary Conditions	81
5.7	Simulation Results	84
5.7.1	Approximations of the Retarded Electron-Phonon Self-Energy	84
5.7.2	General Aspects of Scattering	87
5.7.3	Analysis of the Boundary Conditions	91
5.7.4	Conductivity and Mobility	97
5.8	Comments on NEGF and Scattering	102
6	Electrostatic Solution	103
6.1	Poisson Equation	103
6.2	The Predictor Corrector Approach	104
6.3	Boundary Conditions	106
7	Conclusion and Outlook	109
A	NEGF Theory	113
B	Detailed Balance	115
C	Principal Part Integral	119
D	Current Conservation	121
E	Scattering States	125
	Bibliography	129
	Curriculum Vitae	139