Contents

	Preface Acknowledgements	
	List of symbols	xii xiii
'1	Prologue: an atomistic view of electrical resistance	1
	1.1 Energy level diagram	3
	1.2 What makes electrons flow?	7
	1.3 The quantum of conductance	11
	1.4 Potential profile	14
	1.5 Coulomb blockade	18
	1.6 Towards Ohm's law	21
	Exercises	30
	-	
2	Schrödinger equation	33
	2.1 Hydrogen atom	33
	2.2 Method of finite differences	38
	2.3 Examples	41
	Exercises	49
· · ·	Self-consistent field	
3	Sen-consistent neid —	51
	3.1 The self-consistent field (SCF) procedure	51
	3.2 Relation to the multi-electron picture	57
	3.3 Bonding	63
	3.4 Supplementary notes: multi-electron picture	71
	Exercises	78

LO	nte	nts

4	Basi	is functions	81
	*4.1	Basis functions as a computational tool	81
	*4.2	Basis functions as a conceptual tool	87
	4.3	Equilibrium density matrix	93
	4.4	Supplementary notes	97
		Exercises	103
5	Ban	dstructure	104
	*5.1	Toy examples	104
	*5.2	General result	109
	*5.3	Common semiconductors	116
	5.4	Effect of spin-orbit coupling	120
	5.5	Supplementary notes: the Dirac equation	126
		Exercises	128
6	Subbands		129
	*6.1	Quantum wells, wires, dots, and "nanotubes"	129
	*6.2	Density of states	138
	*6.3	Minimum resistance of a wire	145
	6.4	Velocity of a (sub)band electron	150
		Exercises	154
7	 Capa	acitance	155
	*7.1	Model Hamiltonian	156
	7.2	Electron density/density matrix	162
	*7.3	Quantum vs. electrostatic capacitance	170
	7.4	Supplementary notes: multi-band effective mass Hamiltonian	176
		Exercises	180
			100

*8	Level broadening	183
	8.1 Open systems	185
	8.2 Local density of states	191
	8.3 Lifetime	200
	8.4 What constitutes a contact (reservoir)?	207
	Exercises	213
9	Coherent transport	217
	*9.1 Overview	217
	9.2 Density matrix	223
	9.3 Inflow/outflow	230
	*9.4 Transmission	232
	*9.5 Examples	240
	Exercises	249
10	Non-coherent transport	
	10.1 Why does an atom emit light?	254
	10.2 Examples	263
	10.3 Inflow and outflow	271
	10.4 Supplementary notes: phonons	275
	Exercises	282
11	Atom to transistor	285
	11.1 Quantum transport equations	285
	*11.2 Physics of Ohm's law	290
	*11.3 Where is the heat dissipated?	298
	*11.4 Where is the voltage drop?	301
	Exercises	308
12	 Epilogue	312

Appendix:	319	
A.1	Correlation functions	320
A.2	Non-equilibrium density matrix	324
A.3	Inflow and outflow	329
A.4	Inelastic flow	332
A.5	Coulomb blockade/Kondo resonance	337
MATLAB COO	des used to generate text figures	343
Furt	ther reading	394
Refe	rences	399
Inde	x	402

^{*} Asterisked sections indicate those that I use for undergraduate teaching.