

# Contents

## Part I Overview and physical equations

<b>1</b>	<b>Overview of device modelling</b> . . . . .	3
1.1	Devices . . . . .	5
1.2	Physical theory and modelling equations . . . . .	8
1.2.1	Physical theory . . . . .	9
1.2.2	Modelling equations . . . . .	11
1.3	Mathematical and numerical techniques . . . . .	14
1.4	What is in this book, and its limitations . . . . .	19
<b>2</b>	<b>Quantum mechanics</b> . . . . .	21
2.1	The physical basis of quantum mechanics . . . . .	21
2.2	The Schrödinger equation . . . . .	23
2.2.1	Derivation of the time-dependent Schrödinger equation . . . . .	24
2.2.2	The time-independent Schrödinger equation . . . . .	25
2.3	Boundary and continuity conditions, and parity . . . . .	26
2.3.1	Boundary and continuity conditions . . . . .	26
2.3.2	Parity . . . . .	27
2.4	The probability current density . . . . .	27
2.5	One dimensional motion . . . . .	28
2.5.1	General considerations . . . . .	28
2.5.2	Reflection and Transmission coefficients . . . . .	31
2.5.3	Single finite step for $E < V_0$ . . . . .	33
2.5.4	Infinite barrier . . . . .	34
2.5.5	Infinite square well . . . . .	34
2.5.6	Finite square well . . . . .	35
2.5.7	$\delta$ -function potential . . . . .	37
2.5.8	Square potential barrier . . . . .	38
2.5.9	The $\text{sech}^2$ potential . . . . .	40

2.6	Operators and observables	43
2.7	The Uncertainty Principle	49
2.8	The postulates of quantum mechanics	51
2.9	The harmonic oscillator	54
2.9.1	Solution of the differential equation	54
2.9.2	The ladder operator method	59
2.9.3	Oscillations in more than one dimension	61
2.9.4	The displaced harmonic oscillator	63
2.10	Spherically symmetric potentials	63
2.10.1	The Schrödinger equation in spherical polar coordinates	64
2.10.2	Solution of the angular components	65
2.10.3	Angular momentum	68
2.10.4	The hydrogen atom	70
2.11	Angular momentum and spin	75
2.11.1	The necessity for extra energy levels	75
2.11.2	Generalised angular momentum	76
2.11.3	Particles with spin $\frac{1}{2}$	78
2.11.4	Energy splitting using spin	80
2.12	Systems of identical particles: BE and FD statistics	82
2.12.1	Symmetric and antisymmetric wave functions	82
2.12.2	The Pauli exclusion principle	83
2.12.3	Non-interacting identical particles	84
2.13	The Schrödinger equation in device modelling	85
	Problems	86
<b>3</b>	<b>Equilibrium thermodynamics and statistical mechanics</b>	<b>89</b>
3.1	The scope and laws of thermodynamics	89
3.1.1	The Zeroth Law of thermodynamics	90
3.1.2	The First Law of thermodynamics	92
3.1.3	The Second Law of thermodynamics	96
3.1.4	Properties of the thermodynamic entropy	99
3.2	The statistical entropy	100
3.3	Maximisation of entropy subject to constraints	102
3.4	The distributions	104
3.4.1	The Canonical distribution	105
3.4.2	The Grand Canonical distribution	106
3.4.3	The Microcanonical distribution	107
3.5	Fermi-Dirac and Bose-Einstein statistics	108
3.6	The continuous approximation and the Ideal Quantum Gas	109
	Problems	112
<b>4</b>	<b>Density of states and applications—1</b>	<b>115</b>
4.1	Electron number and energy densities	115
4.1.1	Density of states—general	116
4.1.2	Density of states—particles free in three dimensions	117

- 4.1.3 Density of states—particles free in two dimensions . . . . . 119
- 4.1.4 Density of states—particles free in one dimension . . . . . 120
- 4.2 Blackbody radiation . . . . . 122
- 4.3 Classical aspects of specific heat . . . . . 124
  - 4.3.1 The Equipartition of Energy theorem . . . . . 124
  - 4.3.2 Examples on the Equipartition of Energy theorem . . . . . 125
- 4.4 Quantum aspects of specific heat . . . . . 127
  - 4.4.1 Quantum vibrational aspects: the Einstein solid . . . . . 127
  - 4.4.2 Quantum rotational aspects . . . . . 128
  - 4.4.3 Schottky peaks . . . . . 131
- 4.5 Bose-Einstein condensation . . . . . 132
- 4.6 Thermionic emission . . . . . 133
- 4.7 Semiconductor statistics . . . . . 136
  - 4.7.1 Allowed and forbidden bands . . . . . 136
  - 4.7.2 The effective mass . . . . . 138
  - 4.7.3 Electron and hole densities . . . . . 138
  - 4.7.4 The non-degenerate approximation . . . . . 140
- Problems . . . . . 141
  
- 5 Density of states and applications—2 . . . . . 143**
  - 5.1 Periodic potential: the Bloch theorem . . . . . 143
  - 5.2 Heterostructures: position-dependent mass . . . . . 147
  - 5.3 Heterostructures: the effective mass approximation . . . . . 149
  - 5.4 Quantum wells . . . . . 152
    - 5.4.1 The general structure of a quantum well . . . . . 152
    - 5.4.2 Density of states in quantum wells . . . . . 153
    - 5.4.3 Quantum wells—particles free in two dimensions . . . . . 156
    - 5.4.4 Quantum wells—particles free in one dimension . . . . . 157
  - Problems . . . . . 158
  
- 6 The transport equations and the device equations . . . . . 161**
  - 6.1 The Boltzmann transport equation . . . . . 162
    - 6.1.1 Derivation of the BTE . . . . . 162
    - 6.1.2 The relaxation-time approximation . . . . . 163
  - 6.2 The moments of the BTE . . . . . 164
    - 6.2.1 The general moment . . . . . 165
    - 6.2.2 First moment: carrier concentration equation . . . . . 166
    - 6.2.3 Second moment: momentum conservation equation . . . . . 167
    - 6.2.4 Third moment: energy transport equation . . . . . 168
  - 6.3 Models based on the BTE moments . . . . . 169
    - 6.3.1 The Poisson equation . . . . . 170
    - 6.3.2 The simplified energy transport model . . . . . 171
    - 6.3.3 The drift-diffusion model . . . . . 172
  - 6.4 The Wigner distribution function . . . . . 172
    - 6.4.1 Definition of the Wigner function . . . . . 173

6.4.2	Properties of the Wigner function . . . . .	173
6.5	The Wigner transport equation . . . . .	174
6.5.1	Derivation of the Wigner equation . . . . .	175
6.5.2	Special cases of the Wigner equation . . . . .	177
6.5.3	Moments of the Wigner equation . . . . .	178
6.6	Description of a typical device . . . . .	178
6.7	Material properties . . . . .	180
6.7.1	GaAs . . . . .	180
6.7.2	AlGaAs . . . . .	181
6.7.3	InGaAs . . . . .	182
6.7.4	The electron mobility . . . . .	182
6.8	The Schrödinger equation applied to the HEMT . . . . .	183
6.9	The overall nature of the modelling equations . . . . .	184
	Problems . . . . .	185

## Part II Mathematical and numerical methods

<b>7</b>	<b>Basic approximation and numerical methods . . . . .</b>	<b>189</b>
7.1	Reading the C programmes . . . . .	189
7.2	Finite differences . . . . .	193
7.2.1	Description of the mesh . . . . .	193
7.2.2	Numerical differentiation . . . . .	193
7.2.3	Numerical integration . . . . .	196
7.2.4	Discretisation of the Poisson and Schrödinger equations . . . . .	198
7.3	Solution of simultaneous equations . . . . .	199
7.3.1	Linear equations: direct method . . . . .	200
7.3.2	Linear equations: relaxation method . . . . .	202
7.3.3	The Newton method: a brief introduction . . . . .	206
7.4	Time discretisation . . . . .	207
7.4.1	Explicit and implicit schemes . . . . .	208
7.4.2	The ADI method . . . . .	211
7.5	Function updating and fitting . . . . .	213
7.5.1	Updating due to altered boundary conditions . . . . .	213
7.5.2	Discretising mixed boundary conditions . . . . .	216
7.5.3	Modelling abrupt junctions . . . . .	217
	Problems . . . . .	218
<b>8</b>	<b>Fermi and associated integrals . . . . .</b>	<b>221</b>
8.1	Definition of the Fermi integrals . . . . .	221
8.1.1	The standard Fermi integrals . . . . .	222
8.1.2	The associated Fermi integrals . . . . .	222
8.2	Approximation of the associated integrals . . . . .	223
8.3	Implementation of the approximation scheme . . . . .	225
8.3.1	Method of implementation . . . . .	225
8.3.2	Results of the implementation . . . . .	226

8.3.3	Improvements to the scheme	227
8.4	Calculation of the standard Fermi integrals	227
	Problems	228
<b>9</b>	<b>The upwinding method</b>	229
9.1	Description of the upwinding approach	229
9.2	Upwinding applied to device equations	230
9.3	Upwinding in terms of the C-function	233
9.3.1	Definition of the C-function	233
9.3.2	Properties of the C-function and related functions	234
9.4	Upwinding using the C-function	237
9.5	Numerical diffusion	239
9.6	The limit of uniform temperature	243
	Problems	244
<b>10</b>	<b>Solution of equations: the Newton and reduced method</b>	247
10.1	The Newton method for one variable	247
10.2	Error analysis of the Newton method	249
10.3	The multi-variable Newton method	251
10.4	The reduced Newton method	253
10.5	The Newton method applied to device modelling	254
10.5.1	The reduced method applied to device modelling	254
10.5.2	Example	257
<b>11</b>	<b>Solution of equations: the phaseplane method</b>	259
11.1	The basis of the phaseplane method	259
11.2	The phaseplane method for one variable	260
11.3	Discretisation of the equation	261
11.4	The condition for a stable solution	262
11.5	Exact correspondence between the differential and discretised equations	265
11.6	A one-variable example	266
11.7	The phaseplane equations for several variables	267
11.8	Connection with the Newton and SOR/SUR schemes	270
11.9	Error analysis of the phase plane method	271
11.9.1	One-variable case using exact derivatives	271
11.9.2	One-variable case using central difference derivatives	272
11.9.3	Multi-variable case using exact derivatives	272
11.9.4	Multi-variable case using central difference derivatives	275
11.9.5	Multi-variable case using forward difference derivatives	276
11.10	The phaseplane method applied to device modelling	277
11.11	Case study: a four-layer four-contact HEMT	281

<b>12</b>	<b>Solution of equations: the multigrid method</b>	283
12.1	Description of the multigrid method	283
12.2	Moving between grids: restriction and prolongation	286
12.3	Implementation of the multigrid method	287
12.4	Efficiency of the multigrid scheme	290
12.5	Multigrids applied to device modelling	292
12.5.1	Case study 1: application to a one-dimensional device	293
12.5.2	Case study 2: application to a two-dimensional device	299
<b>13</b>	<b>Approximate and numerical solutions of the Schrödinger equation</b>	303
13.1	The WKB approximation	303
13.1.1	The basis of the WKB method	303
13.1.2	The limit of the approximation	305
13.1.3	The connection formulae	306
13.1.4	Examples	309
13.2	Time independent perturbation theory	313
13.2.1	The first order non-degenerate case	314
13.2.2	The second order non-degenerate case	315
13.2.3	The degenerate case	316
13.2.4	Example: linear perturbation to the harmonic oscillator	316
13.3	Time dependent perturbation theory	318
13.4	The Variational Principle	320
13.5	Discretisation of the Schrödinger equation	322
13.5.1	Discretisation in two dimensions	323
13.5.2	Discretisation in one dimension	324
13.6	Numerical solution: the iteration method	325
13.6.1	The basis of the iteration method	325
13.6.2	Numerical implementation of the iteration method	326
13.7	Numerical solution: the trial function method	328
13.7.1	The basis of the trial function method	329
13.7.2	Choice of trial functions	333
13.7.3	Numerical implementation of the trial function method	333
13.8	Numerical solution: the matrix method	336
<b>14</b>	<b>Genetic algorithms and simulated annealing</b>	339
14.1	How genetic algorithms work	340
14.2	Chromosome representation	343
14.3	The genetic operators	345
14.3.1	Stage 1: Roulette wheel selection	346
14.3.2	Stage 2: Crossover	348
14.3.3	Stage 3: Mutation	350
14.4	The multivariable and multifunction cases	351
14.4.1	The multivariable case	352
14.4.2	The multifunction case	353
14.4.3	Example: maximising a function of two variables	354

- 14.5 Refinements to the GA approach ..... 355
  - 14.5.1 Differential mutation ..... 355
  - 14.5.2 Contractive mapping ..... 356
  - 14.5.3 Range refinement ..... 358
- 14.6 Simulated annealing ..... 358
  - 14.6.1 How simulated annealing works ..... 359
  - 14.6.2 Acceptance function based on MB statistics ..... 362
  - 14.6.3 Acceptance function based on Tsallis statistics ..... 363
  - 14.6.4 Acceptance function based on BE statistics ..... 365
  - 14.6.5 The cooling schedule ..... 368
- 14.7 Application: approximation to the Associated Fermi integrals ..... 372
  - 14.7.1 Approximation method ..... 372
  - 14.7.2 Results ..... 374
- 15 Grid generation ..... 377**
  - 15.1 Overview of grid generation ..... 378
  - 15.2 Functions of a grid generation programme ..... 379
  - 15.3 Results from the programme ..... 385
- A The theory of contractive mapping ..... 389**
- References ..... 393**
- Index ..... 401**



<http://www.springer.com/978-1-84882-936-7>

Mathematical and Numerical Modelling of  
Heterostructure Semiconductor Devices: From Theory  
to Programming

Cole, E.A.B.

2009, XV, 406 p. 40 illus., Softcover

ISBN: 978-1-84882-936-7