

Contents

Preface, *v*

How to use this book, *ix*

Chapter 1: Basic Mathematical Operations, *1*

- 1.1 Numerical differentiation, *2*
- 1.2 Numerical quadrature, *5*
- 1.3 Finding roots, *10*
- 1.4 Semiclassical quantization of molecular vibrations, *13*
- Project I: Scattering by a central potential, *18*

Chapter 2: Ordinary Differential Equations, *23*

- 2.1 Simple methods, *24*
- 2.2 Multistep and implicit methods, *27*
- 2.3 Runge-Kutta methods, *29*
- 2.4 Stability, *31*
- 2.5 Order and chaos in two-dimensional motion, *33*
- Project II: The structure of white dwarf stars, *42*
 - II.1 The equations of equilibrium, *42*
 - II.2 The equation of state, *43*
 - II.3 Scaling the equations, *45*
 - II.4 Solving the equations, *46*

Chapter 3: Boundary Value and Eigenvalue Problems, *49*

- 3.1 The Numerov algorithm, *50*
- 3.2 Direct integration of boundary value problems, *51*
- 3.3 Green's function solution of boundary value problems, *54*
- 3.4 Eigenvalues of the wave equation, *57*
- 3.5 Stationary solutions of the one-dimensional Schroedinger equation, *60*
- Project III: Atomic structure in the Hartree-Fock approximation, *64*

Contents

- III.1 Basis of the Hartree-Fock approximation, 65
- III.2 The two-electron problem, 67
- III.3 Many-electron systems, 69
- III.4 Solving the equations, 72

Chapter 4: Special Functions and Gaussian Quadrature, 77

- 4.1 Special functions, 77
- 4.2 Gaussian quadrature, 83
- 4.3 Born and eikonal approximations to quantum scattering, 87
- Project IV: Partial wave solution of quantum scattering, 94
 - IV.1 Partial wave decomposition of the wavefunction, 94
 - IV.2 Finding the phase shifts, 95
 - IV.3 Solving the equations, 97

Chapter 5: Matrix Operations, 101

- 5.1 Matrix inversion, 101
- 5.2 Eigenvalues of a tri-diagonal matrix, 104
- 5.3 Reduction to tri-diagonal form, 107
- 5.4 Determining nuclear charge densities, 112
- Project V: A schematic shell model, 125
 - V.1 Definition of the model, 125
 - V.2 The exact eigenstates, 127
 - V.3 Approximate eigenstates, 129
 - V.4 Solving the model, 134

Chapter 6: Elliptic Partial Differential Equations, 137

- 6.1 Discretization and the variational principle, 139
- 6.2 An iterative method for boundary value problems, 142
- 6.3 More on discretization, 146
- 6.4 Elliptic equations in two dimensions, 148
- Project VI: Steady-state hydrodynamics in two dimensions, 150
 - VI.1 The equations and their discretization, 150
 - VI.2 Boundary conditions, 154
 - VI.3 Solving the equations, 157

Chapter 7: Parabolic Partial Differential Equations, 161

- 7.1 Naive discretization and instabilities, 161
- 7.2 Implicit schemes and the inversion of tri-diagonal matrices, 165
- 7.3 Diffusion and boundary value problems in two dimensions, 169
- 7.4 Iterative methods for eigenvalue problems, 171
- 7.5 The time-dependent Schroedinger equation, 176
- Project VII: Self-organization in chemical reactions, 179
 - VII.1 Description of the model, 179
 - VII.2 Linear stability analysis, 180
 - VII.3 Numerical solution of the model, 183

Chapter 8: Monte Carlo Methods, 185

- 8.1 The basic Monte Carlo strategy, 186
- 8.2 Generating random variables with a specified distribution, 191
- 8.3 The algorithm of Metropolis *et al.*, 196
- 8.4 The Ising model in two dimensions, 200
- Project VIII: Quantum Monte Carlo for the H_2 molecule, 205
 - VIII.1 Statement of the problem, 206
 - VIII.2 Variational Monte Carlo and the trial wavefunction, 207
 - VIII.3 Monte Carlo evaluation of the exact energy, 210
 - VIII.4 Solving the problem, 214

Appendix A: Synopsis of the BASIC language, 217

Appendix B: Programs for the Examples, 227

- B.1 Example 1, 229
- B.2 Example 2, 235
- B.3 Example 3, 247
- B.4 Example 4, 261
- B.5 Example 5, 274

Contents

B.6 Example 6, *290*

B.7 Example 7, *304*

B.8 Example 8, *322*

Appendix C: Programs for the Projects, *331*

C.1 Project I, *331*

C.2 Project II, *337*

C.3 Project III, *344*

C.4 Project IV, *355*

C.5 Project V, *369*

C.6 Project VI, *376*

C.7 Project VII, *387*

C.8 Project VIII, *394*

References, *405*

The problem with computers is that they only give answers
-attributed to P. Picasso

