Contents

Acknowledgments xv

Series Preface xvii

Preface xix

About the Authors xxi

Web Materials xxiii

1 Computational Basics for Physics 1
. 1
1.1 Chapter Overview 1
1.2 The Python Ecosystem 1
1.2.1 Visualization Tools 2
1.2.2 Matrix Tools 8
1.2.3 Algebraic Tools 11
1.3 Dealing with Floating Point Numbers 12
1.3.1 Uncertainties in Computed Numbers 13
1.4 Numerical Derivatives 14
1.5 Numerical Integration 15
1.5.1 Gaussian Quadrature 17
1.5.2 Monte Carlo (Mean Value) Integration 17
1.6 Random Number Generation 19
1.6.1 Tests of Random Generators 21
1.6.2 Central Limit Theorem 22
1.7 Ordinary Differential Equations Algorithms 24
1.7.1 Euler & Runge-Kutta Rules 25
1.8 Partial Differential Equations Algorithms 27
1.9 Code Listings 27

2 Data Analytics for Physics 39
. 39
2.1 Chapter Overview 39
2.2 Root Finding 39
2.3 Least-Squares Fitting 42
2.3.1 Linear Least Square Fitting 43
2.4 Discrete Fourier Transforms (DFT) 47
2.5 Fast Fourier Transforms (FFT)⊙ 51
2.6 Noise Reduction 54
2.6.1 via Autocorrelation Function 54
2.6.2 via Digital Filters 56
2.7 Spectral Analysis of Nonstationary Signals 58
2.7.1 Short-Time Fourier Transforms 59
2.7.2 Wavelet Analysis 60
2.7.3 Discrete Wavelet Transforms, Multi Resolution Analysis⊙ . . 65
2.8 Principal Components Analysis (PCA) 65
2.9 Fractal Dimension Determination 68
2.10 Code Listings 70

3 Classical & Nonlinear Dynamics 81
. 81
3.1 Chapter Overview 81
3.2 Oscillators 81
3.2.1 First a Linear Oscillator 81
3.2.2 Nonlinear Oscillators 83
3.2.3 Assessing Precision via Energy Conservation 85
3.2.4 Models of Friction 85
3.2.5 Linear & Nonlinear Resonances 86
3.2.6 Famous Nonlinear Oscillators 88
3.2.7 Solution via Symbolic Computing 90
3.3 Realistic Pendula 91
3.3.1 Elliptic Integrals 93
3.3.2 Period Algorithm 94
3.3.3 Phase Space Orbits 94
3.3.4 Vibrating Pivot Pendulum 96
3.4 Fourier Analysis of Oscillations 96
3.4.1 Pendulum Bifurcations 97
3.4.2 Sonification 98
3.5 The Double Pendulum 99
3.6 Realistic Projectile Motion 101
3.6.1 Trajectory of Thrown Baton 102
3.7 Bound States 103
3.8 Three-Body Problems: Neptune, Two Suns, Hénon-Heiles 106

3.8.1 Two Fixed Suns with a Single Planet . . . 107
3.8.2 Hénon-Heiles Bound States . . . 108
3.9 Scattering . . . 109
3.9.1 Rutherford Scattering . . . 109
3.9.2 Mott Scattering . . . 110
3.9.3 Chaotic Scattering . . . 112
3.10 Billiards . . . 114
3.11 Lagrangian and Hamiltonian Dynamics . . . 115
3.11.1 Hamilton's Principle . . . 115
3.11.2 Problems . . . 117
3.12 Weights Connected by Strings (Hard) . . . 118
3.13 Code Listings . . . 119

4 Wave Equations & Fluid Dynamics 125
. . . 125
4.1 Chapter Overview . . . 125
4.2 String Waves . . . 125
4.2.1 Extended Wave Equations . . . 128
4.2.2 Computational Normal Modes . . . 130
4.2.3 Masses on Vibrating String . . . 131
4.2.4 Wave Equation for Large Amplitudes . . . 133
4.3 Membrane Waves . . . 134
4.4 Shock Waves . . . 136
4.4.1 Advective Transport . . . 136
4.4.2 Burgers' Equation . . . 137
4.5 Solitary Waves (Solitons) . . . 138
4.5.1 Including Dispersion, KdeV Solitons . . . 138
4.5.2 Pendulum Chain Solitons, Sine Gordon Solitons . . . 141
4.6 Hydrodynamics . . . 143
4.6.1 Navier-Stokes Equation . . . 144
4.6.2 Flow Over Submerged Beam . . . 146
4.6.3 Vorticity Form of Navier-Stokes Equation . . . 147
4.6.4 Torricelli's Law, Orifice Flow . . . 150
4.6.5 Inflow and Outflow from Square Box . . . 153
4.6.6 Chaotic Convective Flow . . . 154
4.7 Code Listings . . . 155

5 Electricity & Magnetism 169
with Contributions from Viktor Podolski . . . 169
5.1 Chapter Overview . . . 169
5.2 Electric Potentials via Laplace's & Poisson's Equations . . . 170
5.2.1 Solutions via Finite Differences . . . 170
5.2.2 Problems . . . 173

5.2.3 Fourier Series *vs* Finite Differences . . . 176
5.2.4 Disk in Space, Polar Plots . . . 180
5.2.5 Potential Within Grounded Wedge . . . 180
5.2.6 Charge Between Parallel Planes . . . 181
5.3 E&M Waves via FDTD . . . 183
5.3.1 In Free Space . . . 183
5.3.2 In Dielectrics . . . 186
5.3.3 Circularly Polarized Waves . . . 187
5.3.4 Wave Plates . . . 188
5.3.5 On Telegraph Lines . . . 189
5.4 Thin Film Interference of Light . . . 192
5.5 Electric Fields . . . 194
5.5.1 Calculation & Visualization . . . 194
5.5.2 Fields in Dielectrics . . . 194
5.5.3 Via Direct Integration . . . 196
5.5.4 Via Image Method . . . 198
5.6 Magnetic Fields via Direct Integration . . . 200
5.6.1 Magnetic Field of Current Loop . . . 200
5.7 Motion of Charges in Magnetic Fields . . . 202
5.7.1 Mass Spectrometer . . . 202
5.7.2 Quadruple Focusing . . . 203
5.7.3 Magnetic Confinement . . . 205
5.8 Relativity in E&M . . . 206
5.8.1 Lorentz Transformations of Fields and Motion . . . 206
5.8.2 Two Interacting Charges, the Breit Interaction . . . 208
5.8.3 Field Propagation Effects . . . 209
5.9 Code Listings . . . 211

6 Quantum Mechanics 231
. . . 231
6.1 Chapter Overview . . . 231
6.2 Bound States . . . 232
6.2.1 In 1-D Box (Semi Analytic) . . . 232
6.2.2 Arbitrary Potential (ODE Solver + Search) . . . 233
6.2.3 Arbitrary Potential (Sloppy Shortcut) . . . 235
6.2.4 Relativistic Bound States of Klein-Gordon Equation . . . 236
6.3 Spontaneous Decay Simulation . . . 238
6.3.1 Fitting a Black Body Spectrum . . . 240
6.4 Wave Functions . . . 240
6.4.1 Harmonic Oscillator Wave Functions . . . 240
6.5 Partial Wave Expansions . . . 242
6.5.1 Associated Legendre Polynomials . . . 243
6.6 Hydrogen Wave Functions . . . 244

6.6.1 Radial . . . 244
6.6.2 3-D . . . 246
6.7 Wave Packets . . . 246
6.7.1 In Harmonic Oscillator . . . 246
6.7.2 In Momentum Space . . . 247
6.7.3 Solving Time Dependent Schrödinger Equation . . . 248
6.7.4 Time Dependent Schrödinger with E Field . . . 250
6.8 Scattering . . . 251
6.8.1 Square Well . . . 251
6.8.2 Coulomb . . . 254
6.8.3 Three Disks; Quantum Chaos . . . 256
6.8.4 Chaotic Quantum Billiards . . . 258
6.9 Matrix Quantum Mechanics . . . 259
6.9.1 In Momentum Space (Integral Equations) . . . 259
6.9.2 Delta Shell Potential . . . 261
6.9.3 Other Potentials . . . 262
6.9.4 Hydrogen Hyperfine Structure . . . 263
6.9.5 SU(3) Symmetry of Quarks . . . 265
6.10 Coherent States and Entanglement . . . 268
6.10.1 Glauber Coherent States . . . 268
6.10.2 Neutral Kaons as Superpositions of States . . . 269
6.10.3 Double Well Transitions . . . 272
6.10.4 Qubits . . . 273
6.11 Feynman Path Integral Quantum Mechanics ⊙ . . . 276
6.12 Code Listings . . . 279

7 Thermodynamics & Statistical Physics 303
. . . 303
7.1 Chapter Overview . . . 303
7.2 The Heat Equation . . . 303
7.2.1 Algorithm . . . 304
7.2.2 Solutions for Various Geometries . . . 305
7.3 Random Processes . . . 308
7.3.1 Random Walks . . . 308
7.3.2 Diffusion-Limited Aggregation, a Fractal Walk . . . 310
7.3.3 Surface Deposition . . . 311
7.4 Thermal Behavior of Magnetic Materials . . . 312
7.4.1 Roots of a Magnetization *vs* Temperature Equation . . . 313
7.4.2 Counting Spin States . . . 313
7.5 Ising Model . . . 315
7.5.1 Metropolis Algorithm . . . 316
7.5.2 Domain Formation . . . 319
7.5.3 Thermodynamic Properties . . . 320

7.5.4 Extensions 320
7.6 Molecular Dynamics 320
7.6.1 16 Particles in a Box 323
7.7 Code Listings 326

8 Biological Models: Population Dynamics & Plant Growth 339
. 339
8.1 Chapter Overview 339
8.2 The Logistic Map 339
8.2.1 Other Discrete and Chaotic Maps 342
8.3 Predator-Prey Dynamics 343
8.3.1 Predator-Prey Chaos 345
8.3.2 Including Prey Limits 346
8.3.3 Including Predation Efficiency 347
8.3.4 Two Predators, One Prey 349
8.4 Growth Models 350
8.4.1 Protein Folding as a Self-Avoiding Walks 350
8.4.2 Plant Growth Simulations 351
8.4.3 Barnsley's Fern 352
8.4.4 Self-Affine Trees 353
8.5 Code Listings 353

9 Additional Entry-Level Problems 361
. 361
9.1 Chapter Overview 361
9.2 Specular Reflection and Numerical Precision 361
9.3 Relativistic Rocket Golf 362
9.4 Stable Points in Electric Fields 364
9.5 Viewing Motion in Phase Space (Parametric Plots) 365
9.6 Other Useful Visualizations 366
9.7 Integrating Power into Energy 369
9.8 Rigid-Body Rotations with Matrices 371
9.9 Searching for Calibration of a Spherical Tank 373
9.10 AC Circuits via Complex Numbers 374
9.10.1 Using Complex Numbers 374
9.10.2 RLC Circuit 375
9.11 Beats and Satellites 377

10 Appendix: Python Codes 379
. 379
Bibliography 381