CONTENTS

Preface **xiii**

I Nonlinear Continuum Mechanics **1**

1 Kinematics of Deformable Bodies **3**
1.1 Motion 4
1.2 Strain and Deformation Tensors 7
1.3 Rates of Motion 10
1.4 Rates of Deformation 13
1.5 The Piola Transformation 15
1.6 The Polar Decomposition Theorem 19
1.7 Principal Directions and Invariants of Deformation and Strain 20
1.8 The Reynolds' Transport Theorem 23

2 Mass and Momentum **25**
2.1 Local Forms of the Principle of Conservation of Mass . . 26
2.2 Momentum 28

3 Force and Stress in Deformable Bodies **29**

4 The Principles of Balance of Linear and Angular Momentum **35**
4.1 Cauchy's Theorem: The Cauchy Stress Tensor 36

4.2 The Equations of Motion (Linear Momentum) 38
4.3 The Equations of Motion Referred to the Reference Configuration: The Piola–Kirchhoff Stress Tensors . . . 40
4.4 Power 42

5 The Principle of Conservation of Energy 45
5.1 Energy and the Conservation of Energy 45
5.2 Local Forms of the Principle of Conservation of Energy . 47

6 Thermodynamics of Continua and the Second Law 49

7 Constitutive Equations 53
7.1 Rules and Principles for Constitutive Equations 54
7.2 Principle of Material Frame Indifference 57
7.2.1 Solids 57
7.2.2 Fluids 59
7.3 The Coleman–Noll Method: Consistency with the Second Law of Thermodynamics 60

8 Examples and Applications 63
8.1 The Navier–Stokes Equations for Incompressible Flow . 63
8.2 Flow of Gases and Compressible Fluids: The Compressible Navier–Stokes Equations 66
8.3 Heat Conduction 67
8.4 Theory of Elasticity 69

II Electromagnetic Field Theory and Quantum Mechanics 73

9 Electromagnetic Waves 75
9.1 Introduction 75
9.2 Electric Fields 75
9.3 Gauss's Law 79
9.4 Electric Potential Energy 80
9.4.1 Atom Models 80
9.5 Magnetic Fields 81

9.6 Some Properties of Waves 84
9.7 Maxwell's Equations 87
9.8 Electromagnetic Waves 91

10 Introduction to Quantum Mechanics 93
10.1 Introductory Comments 93
10.2 Wave and Particle Mechanics 94
10.3 Heisenberg's Uncertainty Principle 97
10.4 Schrödinger's Equation 99
10.4.1 The Case of a Free Particle 99
10.4.2 Superposition in $\mathbb{R}^n$ 101
10.4.3 Hamiltonian Form 102
10.4.4 The Case of Potential Energy 102
10.4.5 Relativistic Quantum Mechanics 102
10.4.6 General Formulations of Schrödinger's Equation 103
10.4.7 The Time-Independent Schrödinger Equation . . 104
10.5 Elementary Properties of the Wave Equation 104
10.5.1 Review 104
10.5.2 Momentum 106
10.5.3 Wave Packets and Fourier Transforms 109
10.6 The Wave–Momentum Duality 110
10.7 Appendix: A Brief Review of Probability Densities . . . 111

11 Dynamical Variables and Observables in Quantum Mechanics: The Mathematical Formalism 115
11.1 Introductory Remarks 115
11.2 The Hilbert Spaces $L^2(\mathbb{R})$ (or $L^2(\mathbb{R}^d)$) and $H^1(\mathbb{R})$ (or $H^1(\mathbb{R}^d)$) 116
11.3 Dynamical Variables and Hermitian Operators 118
11.4 Spectral Theory of Hermitian Operators: The Discrete Spectrum 121
11.5 Observables and Statistical Distributions 125
11.6 The Continuous Spectrum 127
11.7 The Generalized Uncertainty Principle for Dynamical Variables 128
11.7.1 Simultaneous Eigenfunctions 130

12 Applications: The Harmonic Oscillator and the Hydrogen Atom **131**
12.1 Introductory Remarks 131
12.2 Ground States and Energy Quanta: The Harmonic Oscillator 131
12.3 The Hydrogen Atom 133
12.3.1 Schrödinger Equation in Spherical Coordinates . 135
12.3.2 The Radial Equation 136
12.3.3 The Angular Equation 138
12.3.4 The Orbitals of the Hydrogen Atom 140
12.3.5 Spectroscopic States 140

13 Spin and Pauli's Principle **145**
13.1 Angular Momentum and Spin 145
13.2 Extrinsic Angular Momentum 147
13.2.1 The Ladder Property: Raising and Lowering States 149
13.3 Spin 151
13.4 Identical Particles and Pauli's Principle 155
13.5 The Helium Atom 158
13.6 Variational Principle 161

14 Atomic and Molecular Structure **165**
14.1 Introduction 165
14.2 Electronic Structure of Atomic Elements 165
14.3 The Periodic Table 169
14.4 Atomic Bonds and Molecules 173
14.5 Examples of Molecular Structures 180

15 Ab Initio Methods: Approximate Methods and Density Functional Theory **189**
15.1 Introduction 189
15.2 The Born–Oppenheimer Approximation 190
15.3 The Hartree and the Hartree–Fock Methods 194
15.3.1 The Hartree Method 196
15.3.2 The Hartree–Fock Method 196
15.3.3 The Roothaan Equations 199

15.4 Density Functional Theory 200
15.4.1 Electron Density 200
15.4.2 The Hohenberg–Kohn Theorem 205
15.4.3 The Kohn–Sham Theory 208

III Statistical Mechanics 213

16 Basic Concepts: Ensembles, Distribution Functions, and Averages 215
16.1 Introductory Remarks 215
16.2 Hamiltonian Mechanics 216
16.2.1 The Hamiltonian and the Equations of Motion . . 218
16.3 Phase Functions and Time Averages 219
16.4 Ensembles, Ensemble Averages, and Ergodic Systems . . 220
16.5 Statistical Mechanics of Isolated Systems 224
16.6 The Microcanonical Ensemble 228
16.6.1 Composite Systems 230
16.7 The Canonical Ensemble 234
16.8 The Grand Canonical Ensemble 239
16.9 Appendix: A Brief Account of Molecular Dynamics . . 240
16.9.1 Newtonian's Equations of Motion 241
16.9.2 Potential Functions 242
16.9.3 Numerical Solution of the Dynamical System . . 245

17 Statistical Mechanics Basis of Classical Thermodynamics 249
17.1 Introductory Remarks 249
17.2 Energy and the First Law of Thermodynamics 250
17.3 Statistical Mechanics Interpretation of the Rate of Work in Quasi-Static Processes 251
17.4 Statistical Mechanics Interpretation of the First Law of Thermodynamics 254
17.4.1 Statistical Interpretation of $\dot{Q}$ 256
17.5 Entropy and the Partition Function 257
17.6 Conjugate Hamiltonians 259
17.7 The Gibbs Relations 261

17.8 Monte Carlo and Metropolis Methods 262
17.8.1 The Partition Function for a Canonical Ensemble 263
17.8.2 The Metropolis Method 264
17.9 Kinetic Theory: Boltzmann's Equation of Nonequilibrium Statistical Mechanics 265
17.9.1 Boltzmann's Equation 265
17.9.2 Collision Invariants 268
17.9.3 The Continuum Mechanics of Compressible Fluids and Gases: The Macroscopic Balance Laws 269

Exercises **273**

Bibliography **317**

Index **325**