

# Contents

---

## Part I I-Introductory Many-Body Physics

---

|          |   |    |
|----------|---|----|
| <b>1</b> | <b>Basic Many-Body Quantum Mechanics</b> .....                        | 1  |
| 1.1      | Slater Determinants and Matrix Elements .....                         | 1  |
| 1.1.1    | Many-electron Matrix Elements .....                                   | 2  |
| 1.1.2    | Derivation of the Rules .....   | 4  |
| 1.2      | Second Quantization .....   | 5  |
| 1.2.1    | Bosons .....  | 5  |
| 1.2.2    | Field Quantization and Casimir Effect .....                           | 7  |
| 1.2.3    | Fermions .....  | 9  |
| 1.2.4    | Basis Change in Second Quantization and Field<br>Operators .....      | 11 |
| 1.2.5    | Hubbard Model for the Hydrogen Molecule .....                         | 13 |
| 1.3      | Schrieffer-Wolff Canonical Transformation .....                       | 15 |
| 1.4      | Variational Principle .....   | 16 |
| 1.5      | Variational Approximations .....                                      | 18 |
| 1.6      | Non-degenerate Perturbation Theory .....                              | 18 |
| <b>2</b> | <b>Adiabatic Switching and Time-Ordered series</b> .....              | 19 |
| 2.1      | Time-dependent is Better: start from the <i>Golden Age</i> .....      | 19 |
| 2.2      | Evolution in Complex Time .....                                       | 21 |
| 2.2.1    | Heisenberg Picture .....  | 21 |
| 2.2.2    | Thermal Averages .....  | 23 |
| 2.3      | The Interaction Picture and the Viable Expansion .....                | 25 |
|          | Problems .....  | 26 |
| <b>3</b> | <b>Atomic Shells and Multiplets</b> .....                             | 29 |
| 3.1      | Shell Structure of Atoms .....  | 29 |
| 3.2      | Hartree-Fock Method .....   | 29 |
| 3.2.1    | Physical Meaning of Exchange: the Cohesion of a<br>Simple Metal ..... | 35 |
| 3.3      | Virial Theorem .....  | 37 |
| 3.4      | Hellmann-Feynman Theorem .....  | 38 |
| 3.5      | Central Field .....   | 38 |
| 3.5.1    | L-S Multiplets ( $H'_{rel} \rightarrow 0$ Limit) .....                | 40 |

|          |   |           |
|----------|---|-----------|
| 3.5.2    | Hund's First Rule .....   | 42        |
| 3.6      | Atomic Coulomb Integrals .....  | 43        |
| 3.6.1    | Hund's Second Rule .....  | 46        |
| 3.6.2    | J-J Coupling .....  | 46        |
| 3.6.3    | Intermediate Coupling .....   | 46        |
| 3.7      | Meitner-Auger Effect and Spectroscopy .....                                 | 48        |
| 3.7.1    | Auger Selection Rules and Line Intensities .....                            | 50        |
| <b>4</b> | <b>Green's Functions as Thought Experiments .....</b>                       | <b>55</b> |
| 4.1      | Green's Theorem for one-Body Problems .....                                 | 55        |
| 4.2      | How Many-Body Green's Functions Arise .....                                 | 55        |
| 4.2.1    | Correlation Functions .....   | 55        |
| 4.2.2    | Quantum Green's Functions .....   | 57        |
| 4.2.3    | Quantum Averages .....  | 58        |
| 4.2.4    | Green's functions at Finite Temperature .....                               | 59        |
| 4.3      | Non-interacting Propagators for Solids .....                                | 61        |
| 4.3.1    | Green's Functions for Tight-binding Hamiltonians ....                       | 66        |
| 4.3.2    | Lippmann-Schwinger Equation .....   | 70        |
| 4.3.3    | t matrix .....  | 70        |
| 4.3.4    | Inglesfield Embedding Method .....  | 71        |
| 4.4      | Kubo Formulae .....   | 73        |
| 4.5      | Vacuum Amplitudes .....   | 75        |
| 4.6      | Lehmann Representation .....  | 76        |
| 4.6.1    | Zero-Temperature Fermi Case .....   | 76        |
| 4.6.2    | Finite Temperatures, Fermi and Bose .....                                   | 78        |
| 4.6.3    | Fluctuation-Dissipation Theorem .....                                       | 79        |
| <b>5</b> | <b>Hopping Electron Models: an Appetizer .....</b>                          | <b>81</b> |
| 5.1      | Fano Resonances and Resolvents .....  | 81        |
| 5.1.1    | Resonances .....  | 81        |
| 5.1.2    | Fano Model .....  | 82        |
| 5.1.3    | One-body Treatment .....  | 82        |
| 5.1.4    | Many-Body Treatment .....   | 83        |
| 5.1.5    | The Resolvent .....   | 86        |
| 5.1.6    | Self-Energy Operator .....  | 89        |
| 5.2      | Magnetic Impurities and Chemisorption on Transition Metal<br>Surfaces ..... | 90        |
| 5.3      | Strong Coupling and the Kondo Peak .....                                    | 95        |
| 5.3.1    | Narrow-Band Anderson Model .....  | 95        |
| 5.3.2    | Anderson Model, s-d Model and Kondo Model .....                             | 98        |
| 5.3.3    | Fermi Level Singularity and Kondo Minimum .....                             | 100       |
| 5.4      | The $N_f \gg 1$ Expansion .....   | 101       |
| 5.4.1    | Kondo Temperature in the Spin-Fluctuation Case ....                         | 105       |
| 5.4.2    | Density of Occupied States .....  | 106       |
|          | Problems .....  | 107       |

|          |   |     |
|----------|---|-----|
| <b>6</b> | <b>Many-body Effects in Electron Spectroscopies</b> ..... | 109 |
| 6.1      | Electron Spectroscopy for Chemical Analysis (ESCA) .....  | 109 |
| 6.1.1    | Chemical Shifts .....                                     | 111 |
| 6.1.2    | Core-Level Splitting in Paramagnetic Molecules .....      | 111 |
| 6.1.3    | Shake-up, Shake-off, Relaxation .....                     | 113 |
| 6.1.4    | Lundqvist Model of Phonon and Plasmon Satellites ...      | 115 |
| 6.2      | Auger CVV Line Shapes: Two-Hole Resonances .....          | 118 |
| 6.2.1    | Desorption .....  | 122 |
| 6.3      | Two Interacting Fermions in a Lattice .....               | 123 |
| 6.4      | Quadratic Response Formalism and Spectroscopies .....     | 127 |
| 6.4.1    | One-Step Theory of Auger Spectra .....                    | 129 |
| 6.4.2    | Plasmon Gain .....  | 130 |
|          | Problems .....  | 130 |

---

## Part II Symmetry in Quantum Physics

---

|          |  |     |
|----------|--|-----|
| <b>7</b> | <b>Group Representations for Physicists</b> .....                    | 133 |
| 7.1      | Abstract Groups .....  | 133 |
| 7.2      | Point Symmetry in Molecules and Solids .....                         | 135 |
| 7.2.1    | Symmetry operators .....   | 135 |
| 7.2.2    | Dirac characters and Irreducible Representations .....               | 140 |
| 7.2.3    | Schur's lemma .....  | 143 |
| 7.2.4    | Continuous Groups .....  | 144 |
| 7.3      | Accidental degeneracy and hidden symmetries .....                    | 145 |
| 7.4      | Great Orthogonality Theorem (GOT) .....                              | 149 |
| 7.5      | Little Orthogonality Theorem (LOT) .....                             | 152 |
| 7.6      | Projection operators .....   | 154 |
| 7.7      | Regular representation .....   | 155 |
|          | Problems .....   | 156 |
| <b>8</b> | <b>Simpler Uses of Group Theory</b> .....                            | 157 |
| 8.1      | Molecular Orbitals .....   | 157 |
| 8.1.1    | Molecular Orbitals of $NH_3$ .....                                   | 157 |
| 8.1.2    | Molecular Orbitals of $CH_4$ .....                                   | 158 |
| 8.1.3    | Characters of Angular Momentum Eigenstates .....                     | 160 |
| 8.1.4    | Examples: $O_h$ Group, Ligand Group Orbitals, Crystal<br>Field ..... | 160 |
| 8.2      | Normal Modes of vibration .....                                      | 163 |
| 8.3      | Space-Time Symmetries of Bloch States .....                          | 169 |
| 8.4      | Space groups of solids .....   | 173 |
| 8.4.1    | Symmorphic and Nonsymmorphic Groups .....                            | 174 |
| 8.5      | Young Diagrams .....   | 177 |
|          | Problems .....   | 179 |

|          |   |     |
|----------|---|-----|
| <b>9</b> | <b>Product of Representations and Further Physical Applications</b> . . . . . | 181 |
| 9.1      | Irreducible Tensor Operators . . . . .  | 181 |
| 9.2      | Direct Product Representation . . . . .                                       | 183 |
| 9.2.1    | Selection Rules . . . . .   | 184 |
| 9.3      | Reduction of the Direct Product Representation . . . . .                      | 185 |
| 9.4      | Spin-Orbit Interaction and Double Groups . . . . .                            | 186 |
| 9.5      | Static and Dynamical Jahn-Teller Effect . . . . .                             | 188 |
| 9.5.1    | The Born-Oppenheimer (BO) Approximation . . . . .                             | 188 |
| 9.5.2    | The Jahn-Teller Theorem . . . . .   | 189 |
| 9.6      | Non-Adiabatic Operator . . . . .  | 193 |
| 9.6.1    | Dynamical Jahn-Teller Effect . . . . .  | 194 |
| 9.6.2    | How the $E \times \epsilon$ Hamiltonian arises . . . . .                      | 196 |
| 9.6.3    | Nuclear Wave Functions Cannot be Taken Real . . . . .                         | 197 |
| 9.7      | Wigner-Eckart Theorem with Applications . . . . .                             | 197 |
| 9.8      | The Symmetric Group and Many-Electron States . . . . .                        | 199 |
| 9.9      | Seniority Numbers in Atomic Physics . . . . .                                 | 201 |
|          | Problems . . . . .  | 204 |

---

### Part III More on Green Function Techniques

---

|           |  |     |
|-----------|--|-----|
| <b>10</b> | <b>Equations of Motion and Further Developments</b> . . . . .        | 207 |
| 10.1      | Equations of motion for the interacting propagator . . . . .         | 207 |
| 10.1.1    | Equations of Motion and Ground-State Energy . . . . .                | 208 |
| 10.2      | Time-Dependent Problems . . . . .                                    | 208 |
| 10.2.1    | Auger Induced Ionic Desorption: Knotek-Feibelman Mechanism . . . . . | 210 |
| 10.3      | Hierarchy of Greens Functions . . . . .                              | 212 |
| 10.4      | Composite Operator Method . . . . .                                  | 213 |
|           | Problems . . . . .   | 216 |
| <b>11</b> | <b>Feynman Diagrams for Condensed Matter Physics</b> . . . . .       | 217 |
| 11.1      | Diagrams for the Vacuum Propagator . . . . .                         | 217 |
| 11.1.1    | Wick's Theorem . . . . .   | 219 |
| 11.1.2    | Goldstone Diagrams . . . . .   | 221 |
| 11.1.3    | Diagram Rules for the Thermodynamic Potential . . . . .              | 224 |
| 11.2      | Linked Cluster Theorem . . . . .                                     | 225 |
| 11.2.1    | Valence Electron and Core Hole . . . . .                             | 227 |
| 11.2.2    | $H_2$ Model . . . . .  | 229 |
| 11.2.3    | The Linked Cluster Expansion and Green's Functions . . . . .         | 230 |
| 11.3      | Diagrams for the Dressed Propagator . . . . .                        | 231 |
| 11.3.1    | Adiabatic Switching and Perturbation Theory . . . . .                | 232 |
| 11.3.2    | Diagrams for the Propagator in frequency space . . . . .             | 235 |
| 11.4      | Dyson Equation . . . . .   | 238 |

|           |  |            |
|-----------|--|------------|
| 11.4.1    | External Potential . . . . .                                 | 241        |
| 11.5      | Self-Energy from Interactions . . . . .                      | 242        |
| 11.6      | Skeleton Diagrams . . . . .                                  | 245        |
| 11.7      | Two-body Green's Function: the Bethe-Salpeter Equation . . . | 245        |
| 11.8      | Self-Energy and Two-Body Green's Function . . . . .          | 247        |
| 11.9      | Functional Calculus and Diagrams . . . . .                   | 248        |
| 11.9.1    | The Self-Energy as a Functional . . . . .                    | 249        |
| 11.9.2    | Polarization Bubble . . . . .                                | 251        |
| 11.9.3    | The Vertex . . . . .   | 253        |
| 11.10     | Hedin's Equations . . . . .                                  | 254        |
| <b>12</b> | <b>Many-Body Effects and Further Theory . . . . .</b>        | <b>257</b> |
| 12.1      | High Density Electron Gas . . . . .                          | 257        |
| 12.1.1    | More Physical Insight about the RPA . . . . .                | 259        |
| 12.2      | Low Density Electron gas: Ladder Approximation . . . . .     | 263        |
| 12.3      | Ladder Approximations in Electron Spectroscopies . . . . .   | 264        |
| 12.3.1    | XPS and Auger Spectra from Metals . . . . .                  | 264        |
| 12.3.2    | The $U < 0$ Phenomenon . . . . .                             | 267        |
| 12.3.3    | Correlation in Early Transition Metals . . . . .             | 270        |
| 12.4      | Conserving Approximations . . . . .                          | 272        |
| 12.4.1    | Continuity Equation . . . . .                                | 272        |
| 12.4.2    | The $\Phi$ Functional . . . . .                              | 274        |
| 12.4.3    | Gauge Transformation . . . . .                               | 275        |
| 12.4.4    | Ground-State Energy and Grand Potential . . . . .            | 276        |
| 12.4.5    | Luttinger-Ward and ABL Variational Principles . . . . .      | 277        |
| 12.5      | Generalized Ward Identities . . . . .                        | 278        |
| 12.6      | Connection of Diagrams to D F T . . . . .                    | 279        |
| 12.6.1    | Highlights on Density Functional Theory . . . . .            | 279        |
| 12.6.2    | Sham - Schlüter Equation . . . . .                           | 282        |
|           | Problems . . . . .   | 283        |
| <b>13</b> | <b>Non-Equilibrium Theory . . . . .</b>                      | <b>285</b> |
| 13.1      | Time-Dependent Probes and Nonlinear Response . . . . .       | 285        |
| 13.2      | Kadanoff-Baym and Keldysh Methods . . . . .                  | 286        |
| 13.3      | Complex-Time Integrals by Langreth's Technique . . . . .     | 288        |
| 13.3.1    | Finite temperatures . . . . .                                | 290        |
| 13.4      | Keldysh-Dyson Equation on the Contour . . . . .              | 291        |
| 13.5      | Evolution on Keldysh Contour . . . . .                       | 294        |
| 13.5.1    | Contour Evolution of Bosons . . . . .                        | 298        |
| 13.6      | Selected Applications of the Keldysh Formalism . . . . .     | 298        |
| 13.6.1    | Atom-Surface Scattering . . . . .                            | 299        |
| 13.6.2    | Quantum Transport . . . . .                                  | 304        |
|           | Problems . . . . .   | 309        |

---

**Part IV Non-Perturbative Approaches and Applications**


---

|           |  |     |
|-----------|--|-----|
| <b>14</b> | <b>Some Recursion Techniques with Applications</b>         | 313 |
| 14.1      | Lanczos-Haydock Recursion                                  | 313 |
| 14.1.1    | Local Green's Function for a Chain                         | 313 |
| 14.1.2    | Green's Function of any System                             | 315 |
| 14.1.3    | Terminator   | 316 |
| 14.1.4    | Moments  | 322 |
| 14.2      | Spin-Disentangled Diagonalization                          | 323 |
| 14.3      | Method of Excitation Amplitudes                            | 326 |
| 14.4      | Feenberg Method  | 329 |
| 14.4.1    | Solving Linear Systems                                     | 332 |
| 14.4.2    | Homogeneous systems  | 333 |
|           | Problems   | 333 |
| <b>15</b> | <b>Aspects of Nonlinear Optics and Many-Photon Effects</b> | 335 |
| 15.1      | Diffusion of Radiation in Dipole Approximation             | 335 |
| 15.1.1    | Second-Order Processes                                     | 336 |
| 15.2      | Sum Frequency and Second-Harmonic Generation (SHG)         | 342 |
| 15.3      | Diffusion of Coherent Light                                | 343 |
| 15.3.1    | Effective mode   | 343 |
| 15.3.2    | Dynamical Stark Effect                                     | 346 |
|           | Problems   | 351 |

---

**Part V Selected Exact Results in Many-Body Problems**


---

|           |  |     |
|-----------|--|-----|
| <b>16</b> | <b>Quantum Phases</b>                                  | 355 |
| 16.0.3    | Gauge Transformations                                  | 355 |
| 16.0.4    | Spinor Rotations                                       | 356 |
| 16.0.5    | Galilean Transformations                               | 356 |
| 16.1      | Topologic phases                                       | 357 |
| 16.1.1    | Parametric Hamiltonians and Berry Phase                | 358 |
| 16.1.2    | Polarization of Solids                                 | 362 |
| <b>17</b> | <b>Pairing from repulsive interactions</b>             | 367 |
| 17.0.3    | $W = 0$ Pairing in Cu-O Clusters                       | 369 |
| 17.0.4    | Pairing Mechanism                                      | 373 |
| 17.0.5    | The $W = 0$ theorem                                    | 373 |
| 17.0.6    | Examples   | 375 |
| 17.1      | Superconducting flux quantization and Josephson effect | 378 |
|           | Problems   | 381 |

|  |     |
|--|-----|
| <b>18 Algebraic Methods</b> .....                            | 383 |
| 18.1 Lieb Theorems on the Half Filled Hubbard Model .....    | 383 |
| 18.2 Bethe Ansatz for the Heisenberg Chain .....             | 387 |
| 18.3 Bethe Ansatz for Interacting Fermions 1 Dimension ..... | 392 |
| 18.3.1 $\delta$ -Function Interaction .....                  | 392 |
| 18.3.2 The Hubbard Model in 1d .....                         | 396 |
| 18.3.3 The Periodic Boundary Conditions .....                | 401 |
| 18.3.4 Spin Chain Analogy .....                              | 403 |
| Problems .....   | 406 |

---

**Part VI Appendices**

---

|  |     |
|--|-----|
| <b>19 Appendix 1: Zero-point Energy in a Pillbox</b> ..... | 409 |
| <b>20 Appendix II-Character Tables</b> .....               | 411 |
| <b>21 Proof of the Wigner-Eckart Theorem</b> .....         | 413 |
| <b>Solutions</b> .....                                     | 415 |
| <b>References</b> .....                                    | 431 |
| <b>Index</b> .....   | 439 |