

CONTENTS

| | Page |
|---|--------|
| PREFACE | V |
| INTRODUCTION | 1—2 |
| 1. The Origin of the Brillouin Zone Concept | 1 |
| 2. The Single Electron Model | 2 |
| CHAPTER 1. THE ONE-DIMENSIONAL PERIODIC POTENTIAL | 4—28 |
| 3. Solutions of the Schrödinger Equation | 4 |
| 4. The Relation between the Eigenvalue and the Wave-Number . . | 7 |
| 5. General Properties of the Eigenvalues and the Wave Functions . | 9 |
| 6. The Kronig and Penney Model | 11 |
| 7. Boundary Conditions and the Enumeration of States | 17 |
| 8. Alternative Treatment Applicable to the Three-Dimensional Case | 18 |
| 9. Symmetry Properties | 23 |
| 10. Special Case: Nearly Free Electrons | 24 |
| 11. Effect of the Reality of $V(x)$ on the Symmetry of $\varepsilon(k)$ | 28 |
| References | 28 |
| CHAPTER 2. BRILLOUIN ZONES | 29—59 |
| 12. Bravais Lattices and the Translation Group | 29 |
| 13. The Reciprocal Lattice | 32 |
| 14. The Bloch Wave Functions | 34 |
| 15. The Symmetry of $\varepsilon(\mathbf{k})$ within the Brillouin Zone | 38 |
| 16. The Continuity of $\varepsilon(\mathbf{k})$ within the Brillouin Zone | 39 |
| 17. The Properties of Surfaces of Constant Energy. The Fermi Surface | 43 |
| 18. The Density of States with Respect to Energy | 49 |
| 19. Brillouin Zone for Rhombohedral Lattices | 55 |
| References | 59 |
| CHAPTER 3. THE CLASSIFICATION OF ELECTRONIC STATES. POINT GROUPS AND THEIR REPRESENTATIONS | 60—125 |
| 20. The Operations of the Point Group | 61 |
| 21. The Stereographic Projection | 66 |
| 22. The Hermann-Mauguin Notation for the Specification of Point Groups | 70 |
| 23. The Multiplication Table and the Group Classes | 72 |
| 23.1. The multiplication of classes | 75 |
| 24. The Regular Representation | 76 |
| 25. The Reduction of the Regular Representation. Group Characters . | 78 |
| 26. The Calculation of the Character Tables | 80 |
| 26.1. Point groups which contain the inversion | 86 |
| 27. Character Tables for the Principal Point Groups | 87 |
| 27.1. The cubic system. The holosymmetric point group m3m . . | 89 |
| 27.2. The cubic system. The point groups 432 and $\bar{4}3m$ | 92 |

| | Page |
|---|---------|
| 27.3. The trigonal system. The holosymmetric point group $\bar{3}m$ | 94 |
| 27.4. The orthorhombic system. The holosymmetric point group mmm | 96 |
| 27.5. The tetragonal system. The holosymmetric point group $\frac{4}{m} mm$ | 98 |
| 27.6. The hexagonal system. The point group $\bar{6}m2$ | 99 |
| 28. The Classification of States at Points of High Symmetry in the Bril- louin Zone | 101 |
| 28.1. The simple cubic lattice | 103 |
| 29. The Compatibility Relations | 108 |
| 30. The Energy Bands for Free Electrons | 111 |
| 30.1. The simple cubic lattice | 112 |
| 30.2. The body-centred cubic lattice | 116 |
| 30.3. Energy bands and symmetrized free electron wave functions | 118 |
| 30.4. The face-centred cubic lattice | 121 |
| 30.5. The symmetry point L | 121 |
| 30.6. The symmetry point W | 123 |
| 30.7. Energy bands and symmetrized wave functions | 123 |
| References | 125 |
| CHAPTER 4. ELECTRONIC STATES WHERE THE SPACE GROUPS CONTAIN GLIDES AND SCREW DISPLACEMENTS | 126—172 |
| 31. The Notation for the Space Groups | 127 |
| 32. The Space Group and the Wave-Vector Group | 131 |
| 33. The Close-Packed Hexagonal Structure | 135 |
| 33.1. Wave-vector groups and character tables | 135 |
| 33.2. The group of A and Γ | 138 |
| 33.3. The group of M and L | 141 |
| 33.4. The group of Σ | 142 |
| 33.5. Free electron wave functions and energy bands | 143 |
| 34. The Diamond Structure | 148 |
| 34.1. The group of the wave-vector X | 152 |
| 34.2. Symmetrized free electron wave functions at X | 155 |
| 34.3. The wave-vector L | 157 |
| 34.4. The states along the Δ -axis | 158 |
| 35. Electronic States in α -Uranium | 159 |
| 35.1. Wave-vector groups and character tables | 162 |
| 35.2. Energy bands and symmetrized free electron wave functions | 163 |
| 36. The Body-centred Cubic Lattice regarded as the Limit of the CsCl Structure | 170 |
| References | 172 |
| CHAPTER V. EXTENDED \mathbf{k} -SPACE. LARGE ZONES | 173—214 |
| 37. The Fourier Coefficients of the Potential Energy | 174 |
| 38. The Nearly Free Electron Approximation | 180 |

| | Page |
|---|----------------|
| 39. The Removal of Degeneracy in the Second Order | 183 |
| 40. The Structure Factor | 186 |
| 41. Reduction of \mathbf{k} -Space for a Two-Dimensional Square Lattice . . | 187 |
| 42. Reduction of Large Zones in Three Dimensions | 191 |
| 42.1. The close-packed hexagonal structure | 191 |
| 42.2. The large zone for the diamond structure | 193 |
| 42.3. The large zone for the bismuth structure. | 197 |
| 43. First Order Energies of Symmetrized Plane Waves | 200 |
| 44. Large Zones of Alloy Phases | 205 |
| 44.1. The geometry of large zones | 206 |
| 44.2. The γ -brass structure | 207 |
| 44.3. The wave-vector groups of the γ -brass structure | 210 |
| 44.4. The density of states | 212 |
| References | 214 |
| CHAPTER 6. QUANTITATIVE ESTIMATES OF WAVE FUNCTIONS AND ENERGIES | 215—245 |
| 45. The LCAO Method | 216 |
| 45.1. Bands based on atomic s-states | 219 |
| 45.2. Bands based on atomic p-states | 220 |
| 45.3. Superposition of atomic orbitals of different symmetries . | 225 |
| 46. The Orthogonalised Plane Wave Method | 229 |
| 46.1. Difficulties of the OPW method | 232 |
| 47. The Cellular Method | 233 |
| 47.1. An alternative form of the boundary conditions | 235 |
| 47.2. Approximations in practical calculations | 239 |
| 47.3. A correction to the eigenvalue by means of a surface integral | 241 |
| References | 245 |
| CHAPTER 7. SPIN-ORBIT COUPLING EFFECTS | 246—263 |
| 48. The Double Group | 246 |
| 49. Spin-Orbit Fine Structure of Electronic Levels in Crystals . . | 254 |
| 50. Spin-Orbit Effects at a General Point in the Brillouin Zone . | 262 |
| References | 263 |
| Author and Subject Index | 264—268 |