

Contents

Acronyms	xxi
1 Introduction	1
1.1 What Is $k \cdot p$ Theory?	1
1.2 Electronic Properties of Semiconductors	1
1.3 Other Books	3
Part I Homogeneous Crystals	
2 One-Band Model	7
2.1 Overview	7
2.2 $k \cdot p$ Equation	7
2.3 Perturbation Theory	9
2.4 Canonical Transformation	9
2.5 Effective Masses	12
2.5.1 Electron	12
2.5.2 Light Hole	13
2.5.3 Heavy Hole	14
2.6 Nonparabolicity	14
2.7 Summary	15
3 Perturbation Theory – Valence Band	17
3.1 Overview	17
3.2 Dresselhaus–Kip–Kittel Model	17
3.2.1 Hamiltonian	17
3.2.2 Eigenvalues	21
3.2.3 L, M, N Parameters	22
3.2.4 Properties	30
3.3 Six-Band Model for Diamond	32
3.3.1 Hamiltonian	32
3.3.2 DKK Solution	40
3.3.3 Kane Solution	43

3.4	Wurtzite	45
3.4.1	Overview	45
3.4.2	Basis States	46
3.4.3	Chuang–Chang Hamiltonian	46
3.4.4	Gutsche–Jahne Hamiltonian	52
3.5	Summary	54
4	Perturbation Theory – Kane Models	55
4.1	Overview	55
4.2	First-Order Models	55
4.2.1	Four-Band Model	56
4.2.2	Eight-Band Model	57
4.3	Second-Order Kane Model	61
4.3.1	Löwdin Perturbation	61
4.3.2	Four-Band Model	62
4.4	Full-Zone $k \cdot p$ Model	64
4.4.1	15-Band Model	64
4.4.2	Other Models	69
4.5	Wurtzite	69
4.5.1	Four-Band: Andreev-O’Reilly	70
4.5.2	Eight-Band: Chuang–Chang	71
4.5.3	Eight-Band: Gutsche–Jahne	71
4.6	Summary	77
5	Method of Invariants	79
5.1	Overview	79
5.2	DKK Hamiltonian – Hybrid Method	79
5.3	Formalism	84
5.3.1	Introduction	84
5.3.2	Spatial Symmetries	84
5.3.3	Spinor Representation	88
5.4	Valence Band of Diamond	88
5.4.1	No Spin	89
5.4.2	Magnetic Field	90
5.4.3	Spin–Orbit Interaction	93
5.5	Six-Band Model for Diamond	114
5.5.1	Spin–Orbit Interaction	115
5.5.2	k -Dependent Part	115
5.6	Four-Band Model for Zincblende	116
5.7	Eight-Band Model for Zincblende	117
5.7.1	Weiler Hamiltonian	117
5.8	14-Band Model for Zincblende	120
5.8.1	Symmetrized Matrices	121
5.8.2	Invariant Hamiltonian	123

5.8.3	<i>T</i> Basis Matrices	125
5.8.4	Parameters	128
5.9	Wurtzite	132
5.9.1	Six-Band Model	132
5.9.2	Quasi-Cubic Approximation	136
5.9.3	Eight-Band Model	137
5.10	Method of Invariants Revisited	140
5.10.1	Zincblende	140
5.10.2	Wurtzite	146
5.11	Summary	151
6	Spin Splitting	153
6.1	Overview	153
6.2	Dresselhaus Effect in Zincblende	154
6.2.1	Conduction State	154
6.2.2	Valence States	154
6.2.3	Extended Kane Model	156
6.2.4	Sign of Spin-Splitting Coefficients	160
6.3	Linear Spin Splittings in Wurtzite	161
6.3.1	Lower Conduction-Band <i>e</i> States	163
6.3.2	<i>A, B, C</i> Valence States	164
6.3.3	Linear Spin Splitting	165
6.4	Summary	166
7	Strain	167
7.1	Overview	167
7.2	Perturbation Theory	167
7.2.1	Strain Hamiltonian	167
7.2.2	Löwdin Renormalization	170
7.3	Valence Band of Diamond	170
7.3.1	DKK Hamiltonian	171
7.3.2	Four-Band Bir–Pikus Hamiltonian	171
7.3.3	Six-Band Hamiltonian	172
7.3.4	Method of Invariants	174
7.4	Strained Energies	177
7.4.1	Four-Band Model	177
7.4.2	Six-Band Model	179
7.4.3	Deformation Potentials	179
7.5	Eight-Band Model for Zincblende	180
7.5.1	Perturbation Theory	181
7.5.2	Method of Invariants	182
7.6	Wurtzite	183
7.6.1	Perturbation Theory	183
7.6.2	Method of Invariants	184

7.6.3	Examples	186
7.7	Summary	186

Part II Nonperiodic Problem

8	Shallow Impurity States	189
8.1	Overview	189
8.2	Kittel–Mitchell Theory	190
8.2.1	Exact Theory	191
8.2.2	Wannier Equation	193
8.2.3	Donor States	194
8.2.4	Acceptor States	197
8.3	Luttinger–Kohn Theory	198
8.3.1	Simple Bands	199
8.3.2	Degenerate Bands	210
8.3.3	Spin-Orbit Coupling	213
8.4	Baldereschi–Lipari Model	214
8.4.1	Hamiltonian	216
8.4.2	Solution	217
8.5	Summary	219
9	Magnetic Effects	221
9.1	Overview	221
9.2	Canonical Transformation	222
9.2.1	One-Band Model	222
9.2.2	Degenerate Bands	230
9.2.3	Spin-Orbit Coupling	232
9.3	Valence-Band Landau Levels	235
9.3.1	Exact Solution	235
9.3.2	General Solution	239
9.4	Extended Kane Model	240
9.5	Landé g -Factor	240
9.5.1	Zinblende	241
9.5.2	Wurtzite	243
9.6	Summary	244
10	Electric Field	245
10.1	Overview	245
10.2	One-Band Model of Stark Effect	245
10.3	Multiband Stark Problem	246
10.3.1	Basis Functions	246
10.3.2	Matrix Elements of the Coordinate Operator	248
10.3.3	Multiband Hamiltonian	249
10.3.4	Explicit Form of Hamiltonian Matrix Contributions	253

10.4	Summary	255
11	Excitons	257
11.1	Overview	257
11.2	Excitonic Hamiltonian	258
11.3	One-Band Model of Excitons	259
11.4	Multiband Theory of Excitons	261
11.4.1	Formalism	261
11.4.2	Results and Discussions	266
11.4.3	Zincblende	267
11.5	Magnetoexciton	268
11.6	Summary	270
12	Heterostructures: Basic Formalism	273
12.1	Overview	273
12.2	Bastard's Theory	274
12.2.1	Envelope-Function Approximation	274
12.2.2	Solution	276
12.2.3	Example Models	277
12.2.4	General Properties	279
12.3	One-Band Models	280
12.3.1	Derivation	280
12.4	Burt–Foreman Theory	282
12.4.1	Overview	283
12.4.2	Envelope-Function Expansion	283
12.4.3	Envelope-Function Equation	287
12.4.4	Potential-Energy Term	294
12.4.5	Conventional Results	299
12.4.6	Boundary Conditions	305
12.4.7	Burt–Foreman Hamiltonian	306
12.4.8	Beyond Burt–Foreman Theory?	316
12.5	Sercel–Vahala Theory	318
12.5.1	Overview	318
12.5.2	Spherical Representation	319
12.5.3	Cylindrical Representation	324
12.5.4	Four-Band Hamiltonian in Cylindrical Polar Coordinates	329
12.5.5	Wurtzite Structure	336
12.6	Arbitrary Nanostructure Orientation	350
12.6.1	Overview	350
12.6.2	Rotation Matrix	350
12.6.3	General Theory	352
12.6.4	[1 $\bar{1}$ 0] Quantum Wires	353
12.7	Spurious Solutions	360
12.8	Summary	361

- 13 Heterostructures: Further Topics** 363
 - 13.1 Overview 363
 - 13.2 Spin Splitting 363
 - 13.2.1 Zincblende Superlattices 363
 - 13.3 Strain in Heterostructures 367
 - 13.3.1 External Stress 367
 - 13.3.2 Strained Heterostructures 369
 - 13.4 Impurity States 371
 - 13.4.1 Donor States 371
 - 13.4.2 Acceptor States 372
 - 13.5 Excitons 373
 - 13.5.1 One-Band Model 373
 - 13.5.2 Type-II Excitons 376
 - 13.5.3 Multiband Theory of Excitons 377
 - 13.6 Magnetic Problem 378
 - 13.6.1 One-Band Model 379
 - 13.6.2 Multiband Model 382
 - 13.7 Static Electric Field 384
 - 13.7.1 Transverse Stark Effect 384
 - 13.7.2 Longitudinal Stark Effect 386
 - 13.7.3 Multiband Theory 388

- 14 Conclusion** 391

- A Quantum Mechanics and Group Theory** 393
 - A.1 Löwdin Perturbation Theory 393
 - A.1.1 Variational Principle 393
 - A.1.2 Perturbation Formula 394
 - A.2 Group Representation Theory 397
 - A.2.1 Great Orthogonality Theorem 397
 - A.2.2 Characters 398
 - A.3 Angular-Momentum Theory 399
 - A.3.1 Angular Momenta 399
 - A.3.2 Spherical Tensors 399
 - A.3.3 Wigner-Eckart Theorem 400
 - A.3.4 Wigner $3j$ Symbols 400

- B Symmetry Properties** 401
 - B.1 Introduction 401
 - B.2 Zincblende 401
 - B.2.1 Point Group 402
 - B.2.2 Irreducible Representations 403
 - B.3 Diamond 406
 - B.3.1 Symmetry Operators 406
 - B.3.2 Irreducible Representations 407

B.4 Wurtzite 407
 B.4.1 Irreducible Representations..... 410

C Hamiltonians 413

C.1 Basis Matrices 413
 C.1.1 $s = \frac{1}{2}$ 413
 C.1.2 $l = 1$ 413
 C.1.3 $J = \frac{3}{2}$ 413

C.2 $|JM_J\rangle$ States 414

C.3 Hamiltonians 414
 C.3.1 Notations 416
 C.3.2 Diamond 416
 C.3.3 Zincblende 416
 C.3.4 Wurtzite 416
 C.3.5 Heterostructures 416

C.4 Summary of $k \cdot p$ Parameters 416

References 431

Index 443