

Contents

	<i>Preface</i>	<i>page</i> xv
	<i>List of symbols</i>	xvii
1	Linear transformations	
1.1	Vectors	1
1.2	Linear transformations and matrices	2
	1.2.1 Functions of a matrix	5
	1.2.2 Special matrices	6
	1.2.3 Direct products of matrices	6
	1.2.4 Direct sums of matrices	7
1.3	Similarity transformations	8
	1.3.1 Functions of a matrix (revisited)	8
1.4	The characteristic equation of a matrix	9
	1.4.1 Diagonalizability and projection operators	10
1.5	Unitary transformations and normal matrices	12
	1.5.1 Examples of normal matrices	13
1.6	Exercises	14
2	The theory of matrix transformations	
2.1	Involutorial transformations	17
2.2	Application to the Dirac theory of the electron	20
	2.2.1 The Dirac γ -matrices	20
	2.2.2 The Dirac plane waves	21
	2.2.3 The symmetric Dirac plane waves	23
2.3	Intertwining matrices	24
	2.3.1 Idempotent matrices	26
2.4	Matrix diagonalizations	27
2.5	Basic properties of the characteristic transformation matrices	30
2.6	Construction of a transformation matrix	31
2.7	Illustrative examples	34
3	Elements of abstract group theory	
3.1	Group axioms	37
	3.1.1 The criterion for a finite group	38
	3.1.2 Examples of groups	38
3.2	Group generators for a finite group	40
	3.2.1 Examples	42
3.3	Subgroups and coset decompositions	43
	3.3.1 The criterion for subgroups	44

vi	<i>Contents</i>	
	3.3.2 Lagrange's theorem	44
3.4	Conjugation and classes	45
	3.4.1 Normalizers	45
	3.4.2 The centralizer	46
	3.4.3 The center	47
	3.4.4 Classes	47
3.5	Isomorphism and homomorphism	48
	3.5.1 Examples	49
	3.5.2 Factor groups	50
3.6	Direct products and semidirect products	51
4	Unitary and orthogonal groups	
4.1	The unitary group $U(n)$	53
	4.1.1 Basic properties	53
	4.1.2 The exponential form	54
4.2	The orthogonal group $O(n, c)$	55
	4.2.1 Basic properties	55
	4.2.2 Improper rotation	56
	4.2.3 The real orthogonal group $O(n, r)$	57
	4.2.4 Real exponential form	58
4.3	The rotation group in three dimensions $O(3, r)$	58
	4.3.1 Basic properties of rotation	58
	4.3.2 The conjugate rotations	62
	4.3.3 The Euler angles	63
5	The point groups of finite order	
5.1	Introduction	66
	5.1.1 The uniaxial group C_n	67
	5.1.2 Multiaxial groups. The equivalence set of axes and axis-vectors	67
	5.1.3 Notations and the multiplication law for point operations	68
5.2	The dihedral group D_n	73
5.3	Proper polyhedral groups P_o	75
	5.3.1 Proper cubic groups, T and O	77
	5.3.2 Presentations of polyhedral groups	79
	5.3.3 Subgroups of proper point groups	82
	5.3.4 Theorems on the axis-vectors of proper point groups	83
5.4	The Wyle theorem on proper point groups	85
5.5	Improper point groups	86
	5.5.1 General discussion	86
	5.5.2 Presentations of improper point groups	88
	5.5.3 Subgroups of point groups of finite order	90
5.6	The angular distribution of the axis-vectors of rotation for regular polyhedral groups	91
	5.6.1 General discussion	91
	5.6.2 Icosahedral group Y	93
	5.6.3 Buckminsterfullerene C_{60} (buckyball)	97
5.7	Coset enumeration	98

<i>Contents</i>		vii
6	Theory of group representations	
6.1	Hilbert spaces and linear operators	102
	6.1.1 Hilbert spaces	102
	6.1.2 Linear operators	103
	6.1.3 The matrix representative of an operator	105
6.2	Matrix representations of a group	107
	6.2.1 Homomorphism conditions	107
	6.2.2 The regular representation	109
	6.2.3 Irreducible representations	110
6.3	The basis of a group representation	112
	6.3.1 The carrier space of a representation	112
	6.3.2 The natural basis of a matrix group	114
6.4	Transformation of functions and operators	115
	6.4.1 General discussion	115
	6.4.2 The group of transformation operators	117
	6.4.3 Transformation of operators under $G = \{\hat{R}\}$	119
6.5	Schur's lemma and the orthogonality theorems on irreducible representations	120
6.6	The theory of characters	125
	6.6.1 Orthogonality relations	125
	6.6.2 Frequencies and irreducibility criteria	126
	6.6.3 Group functions	127
6.7	Irreducible representations of point groups	128
	6.7.1 The group C_n	129
	6.7.2 The group D_n	129
	6.7.3 The group T	131
	6.7.4 The group O	133
	6.7.5 The improper point groups	135
6.8	Properties of irreducible bases	135
	6.8.1 The orthogonality of basis functions	135
	6.8.2 Application to perturbation theory	136
6.9	Symmetry-adapted functions	138
	6.9.1 Generating operators	138
	6.9.2 The projection operators	141
6.10	Selection rules	144
7	Construction of symmetry-adapted linear combinations based on the correspondence theorem	
7.1	Introduction	149
7.2	The basic development	150
	7.2.1 Equivalent point space $S^{(n)}$	150
	7.2.2 The correspondence theorem on basis functions	152
	7.2.3 Mathematical properties of bases on $S^{(n)}$	153
	7.2.4 Illustrative examples of the SALCs of equivalent scalars	155
7.3	SALCs of equivalent orbitals in general	158
	7.3.1 The general expression of SALCs	158
	7.3.2 Two-point bases and operator bases	160
	7.3.3 Notations for equivalent orbitals	161

viii	<i>Contents</i>	
	7.3.4 Alternative elementary bases	161
	7.3.5 Illustrative examples	162
7.4	The general classification of SALCs	166
	7.4.1 $D^{(A)}$ SALCs from the equivalent orbitals $\in D^{(A)} \times \Delta^{(n)}$	167
7.5	Hybrid atomic orbitals	170
	7.5.1 The σ -bonding hybrid AOs	171
	7.5.2 General hybrid AOs	173
7.6	Symmetry coordinates of molecular vibration based on the correspondence theorem	174
	7.6.1 External symmetry coordinates of vibration	175
	7.6.2 Internal vibrational coordinates	177
	7.6.3 Illustrative examples	179
8	Subduced and induced representations	
8.1	Subduced representations	188
8.2	Induced representations	189
	8.2.1 Transitivity of induction	191
	8.2.2 Characters of induced representations	191
	8.2.3 The irreducibility condition for induced representations	191
8.3	Induced representations from the irreps of a normal subgroup	193
	8.3.1 Conjugate representations	193
	8.3.2 Little groups and orbits	194
	8.3.3 Examples	195
8.4	Irreps of a solvable group by induction	197
	8.4.1 Solvable groups	197
	8.4.2 Induced representations for a solvable group	198
	8.4.3 Case I (reducible)	199
	8.4.4 Case II (irreducible)	201
	8.4.5 Examples	202
8.5	General theorems on induced and subduced representations and construction of unirreps via small representations	203
	8.5.1 Induction and subduction	203
	8.5.2 Small representations of a little group	205
	8.5.3 Induced representations from small representations	206
9	Elements of continuous groups	
9.1	Introduction	209
	9.1.1 Mixed continuous groups	210
9.2	The Hurwitz integral	211
	9.2.1 Orthogonality relations	215
9.3	Group generators and Lie algebra	215
9.4	The connectedness of a continuous group and the multivalued representations	219
10	The representations of the rotation group	
10.1	The structure of $SU(2)$	224
	10.1.1 The generators of $SU(2)$	224
	10.1.2 The parameter space Ω' of $SU(2)$	226

<i>Contents</i>		ix
10.1.3	Spinors	228
10.1.4	Quaternions	228
10.2	The homomorphism between $SU(2)$ and $SO(3, r)$	229
10.3	Unirreps $D^{(j)}(\boldsymbol{\theta})$ of the rotation group	232
10.3.1	The homogeneity of $D^{(j)}(S)$	233
10.3.2	The unitarity of $D^{(j)}(S)$	234
10.3.3	The irreducibility of $D^{(j)}(\boldsymbol{\theta})$	234
10.3.4	The completeness of the unirreps $\{D^{(j)}(\boldsymbol{\theta}); j = 0, \frac{1}{2}, 1, \dots\}$	235
10.3.5	Orthogonality relations of $D^{(j)}(\boldsymbol{\theta})$	235
10.3.6	The Hurwitz density function for $SU(2)$	236
10.4	The generalized spinors and the angular momentum eigenfunctions	237
10.4.1	The generalized spinors	237
10.4.2	The transformation of the total angular momentum eigenfunctions under the general rotation U_J	238
10.4.3	The vector addition model	240
10.4.4	The Clebsch–Gordan coefficients	241
10.4.5	The angular momentum eigenfunctions for one electron	245
11	Single- and double-valued representations of point groups	
11.1	The double-valued representations of point groups expressed by the projective representations	247
11.1.1	The projective set of a point group	247
11.1.2	The orthogonality relations for projective unirreps	248
11.2	The structures of double point groups	250
11.2.1	Defining relations of double point groups	250
11.2.2	The structure of the double dihedral group D'_n	251
11.2.3	The structure of the double octahedral group O'	253
11.3	The unirreps of double point groups expressed by the projective unirreps of point groups	257
11.3.1	The uniaxial group C_∞	257
11.3.2	The group C_n	258
11.3.3	The group D_∞	258
11.3.4	The group D_n	260
11.3.5	The group O	261
11.3.6	The tetrahedral group T	263
12	Projective representations	
12.1	Basic concepts	266
12.2	Projective equivalence	268
12.2.1	Standard factor systems	269
12.2.2	Normalized factor systems	270
12.2.3	Groups of factor systems and multipliers	271
12.2.4	Examples of projective representations	272
12.3	The orthogonality theorem on projective irreps	274
12.4	Covering groups and representation groups	276
12.4.1	Covering groups	276
12.4.2	Representation groups	278

x	<i>Contents</i>	
12.5	Representation groups of double point groups	279
	12.5.1 Representation groups of double proper point groups P'	279
	12.5.2 Representation groups of double rotation–inversion groups P'_i	281
12.6	Projective unirreps of double rotation–inversion point groups P'_i	283
	12.6.1 The projective unirreps of $C'_{2r,i}$	285
	12.6.2 The projective unirreps of $D'_{n,i}$	286
	12.6.3 The projective unirreps of O'_i	287
13	The 230 space groups	
13.1	The Euclidean group in three dimensions $E^{(3)}$	289
13.2	Introduction to space groups	293
13.3	The general structure of Bravais lattices	295
	13.3.1 Primitive bases	295
	13.3.2 The projection operators for a Bravais lattice	298
	13.3.3 Algebraic expressions for the Bravais lattices	299
13.4	The 14 Bravais lattice types	302
	13.4.1 The hexagonal system H (D_{6i})	302
	13.4.2 The tetragonal system Q (D_{4i})	303
	13.4.3 The rhombohedral system RH (D_{3i})	306
	13.4.4 The orthorhombic system O (D_{2i})	307
	13.4.5 The cubic system C (O_i)	308
	13.4.6 The monoclinic system M (C_{2i})	309
	13.4.7 The triclinic system T (C_i)	311
	13.4.8 Remarks	311
13.5	The 32 crystal classes and the lattice types	313
13.6	The 32 minimal general generator sets for the 230 space groups	315
	13.6.1 Introduction	315
	13.6.2 The space groups of the class D_4	316
13.7	Equivalence criteria for space groups	318
13.8	Notations and defining relations	321
	13.8.1 Notations	321
	13.8.2 Defining relations of the crystal classes	322
13.9	The space groups of the cubic system	323
	13.9.1 The class T	326
	13.9.2 The class T_i ($=T_h$)	327
	13.9.3 The class O	329
	13.9.4 The class T_p ($=T_d$)	330
	13.9.5 The class O_i ($=O_h$)	331
13.10	The space groups of the rhombohedral system	332
	13.10.1 The class C_3	333
	13.10.2 The class C_{3i}	333
	13.10.3 The class D_3	333
	13.10.4 The class C_{3v}	334
	13.10.5 The class D_{3i} ($=D_{3d}$)	335
13.11	The hierarchy of space groups in a crystal system	336
	13.11.1 The cubic system	337
	13.11.2 The hexagonal system	337

<i>Contents</i>		xi
13.11.3	The rhombohedral system	337
13.11.4	The tetragonal system	338
13.12	Concluding remarks	338
14	Representations of the space groups	
14.1	The unirreps of translation groups	340
14.2	The reciprocal lattices	342
14.2.1	General discussion	342
14.2.2	Reciprocal lattices of the cubic system	344
14.2.3	The Miller indices	345
14.2.4	The density of lattice points on a plane	346
14.3	Brillouin zones	347
14.3.1	General construction of Brillouin zones	347
14.3.2	The wave vector point groups	348
14.3.3	The Brillouin zones of the cubic system	349
14.4	The small representations of wave vector space groups	352
14.4.1	The wave vector space groups \hat{G}_k	352
14.4.2	Small representations of \hat{G}_k via the projective representations of G_k	354
14.4.3	Examples of the small representations of \hat{G}_k	356
14.5	The unirreps of the space groups	358
14.5.1	The irreducible star	359
14.5.2	A summary of the induced representation of the space groups	360
15	Applications of unirreps of space groups to energy bands and vibrational modes of crystals	
15.1	Energy bands and the eigenfunctions of an electron in a crystal	362
15.2	Energy bands and the eigenfunctions for the free-electron model in a crystal	365
15.2.1	The notations for a small representation of \hat{G}_k	368
15.2.2	Example 1. A simple cubic lattice	368
15.2.3	Example 2. The diamond crystal	371
15.3	Symmetry coordinates of vibration of a crystal	377
15.3.1	General discussion	377
15.3.2	The small representations of the wave vector groups \hat{G}_k based on the equivalent Bloch functions	379
15.4	The symmetry coordinates of vibration for the diamond crystal	382
15.4.1	General discussion	382
15.4.2	Construction of the symmetry coordinates of vibration	385
16	Time reversal, anti-unitary point groups and their co-representations	
16.1	Time-reversal symmetry, classical	391
16.1.1	General introduction	391
16.1.2	The time correlation function	393
16.1.3	Onsager's reciprocity relation for transport coefficients	394

xii	<i>Contents</i>	
16.2	Time-reversal symmetry, quantum mechanical	396
16.2.1	General introduction	396
16.2.2	The properties of the time-reversal operator θ	400
16.2.3	The time-reversal symmetry of matrix elements of a physical quantity	401
16.3	Anti-unitary point groups	403
16.3.1	General discussion	403
16.3.2	The classification of ferromagnetics and ferroelectrics	407
16.4	The co-representations of anti-unitary point groups	409
16.4.1	General discussion	409
16.4.2	Three types of co-unirreps	410
16.5	Construction of the co-unirreps of anti-unitary point groups	413
16.5.1	G_s^e	414
16.5.2	C_n^e , C_n^q and C_n^u	415
16.5.3	D_n^e and D_n^q	417
16.5.4	The cubic groups	418
16.6	Complex conjugate representations	419
16.7	The orthogonality theorem on the co-unirreps	422
16.8	Orthogonality relations for the characters, the irreducibility condition and the type criteria for co-unirreps	424
16.8.1	Orthogonality relations for the characters of co-unirreps	424
16.8.2	Irreducibility criteria for co-unirreps	424
16.8.3	The type criterion for a co-unirrep	425
17	Anti-unitary space groups and their co-representations	
17.1	Introduction	428
17.2	Anti-unitary space groups of the first kind	430
17.2.1	The cubic system	432
17.2.2	The hexagonal system	433
17.2.3	The rhombohedral system	433
17.2.4	The tetragonal system	433
17.2.5	The orthorhombic system	433
17.2.6	The monoclinic system	435
17.2.7	The triclinic system	435
17.3	Anti-unitary space groups of the second kind	438
17.3.1	Illustrative examples	441
17.3.2	Concluding remarks	441
17.4	The type criteria for the co-unirreps of anti-unitary space groups and anti-unitary wave vector groups	442
17.5	The representation groups of anti-unitary point groups	445
17.6	The projective co-unirreps of anti-unitary point groups	450
17.6.1	Examples for the construction of the projective co-unirreps of H^2	458
17.7	The co-unirreps of anti-unitary wave vector space groups	460
17.7.1	Concluding remarks	463
17.8	Selection rules under an anti-unitary group	464
17.8.1	General discussion	464

Cambridge University Press

0521640628 - Group Theoretical Methods and Applications to Molecules and Crystals

Shoon K. Kim

Table of Contents

[More information](#)

<i>Contents</i>	xiii
17.8.2 Transitions between states belonging to different co-unirreps	465
17.8.3 Transitions between states belonging to the same co-unirrep	467
17.8.4 Selection rules under a gray point group	470
Appendix. Character tables for the crystal point groups	472
<i>References</i>	483
<i>Index</i>	487