SELECTED TOPICS IN SOLID STATE PHYSICS

Editor E. P. Wohlfarth

Volume X

GROUP THEORY AND ELECTRONIC ENERGY BANDS IN SOLIDS

BY J. F. CORNWELL

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J. F. CORNWELL

Lecturer in Theoretical Physics,
University of St. Andrews

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Group theory and electronic energy bands in solids

To my wife Elizabeth

PREFACE

This book has three main aims. Firstly, it is intended to provide a thorough and self-contained introduction to the use of group theory in the calculation and classification of electronic energy bands in solids. It is hoped that this will be useful both for those who intend to calculate energy bands and for those who have to interpret calculations and relate them to the experimental situation. The book has been laid out in such a way as to assist in making the subject more accessible to this latter group. In particular, the theory of groups and its role in quantum mechanics is developed from scratch. Moreover, in the first five chapters only the absolutely essential group theoretical concepts needed for symmorphic space groups are introduced, the more difficult concepts being treated later. To dispel the slightly abstract air which sometimes surrounds this subject, a number of concrete examples are treated in detail. The second aim has been to make a close study of the more advanced aspects of the subject, again treating all the more difficult points in some detail. These aspects include non-symmorphic space groups, time-reversal symmetry, and double groups and spin–orbit coupling. The third and final aim has been to give a summary of the considerable recent work on the subject.

It is a pleasure to acknowledge the fruitful discussions the author has had with Professor E. P. Wohlfarth both concerning this book and topics dealt with in it, and also the careful typing by Mrs C. G. MacArthur of the manuscript.

J. F. CORNWELL

LIST OF MOST IMPORTANT SYMBOLS

Only the symbols that are very frequently used are listed here. The brief descriptions of them are supplemented by a note of the section or equation in which they are defined. Many other symbols are used from time to time, and are defined as they occur. The notation for matrices is described in appendix 4.

$\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$	Basic lattice vectors of the crystal (ch. 1 § 3.1)
$\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3$	Basic lattice vectors of the reciprocal lattice [eq. (4.6)]
C_{ni}	Proper rotation through $2\pi/n$ about the axis Oi (ch. 1 § 1)
$\bar{C}_{ni}$	Generalized proper rotation through $2\pi/n$ about the axis Oi (ch. 8 § 3, appendix 2)
$\mathscr{C}_i$	ith class of a group (ch. 1 § 2.4)
E	Identity transformation (ch. 1 § 1)
$\bar{E}$	Generalized identity transformation (ch. 8 § 3, appendix 2)
$E_n(\boldsymbol{k})$	nth energy level at point $\boldsymbol{k}$ (ch. 4 § 6). (The suffix n is sometimes omitted)
$\mathscr{G}$	In purely group theoretical developments, such as in ch. 1 (except § 3), ch. 2 and ch. 6, merely denotes a group. In ch. 3 $\mathscr{G}$ denotes the group of the Schrödinger equation, and in all other places $\mathscr{G}$ denotes more specifically the space group of the crystal
$\mathscr{G}_o$	The point group of the space group $\mathscr{G}$ (ch. 1 § 3)
$\mathscr{G}(\boldsymbol{k})$	The group of the wave vector $\boldsymbol{k}$ (ch. 7 § 1)
$\mathscr{G}_o(\boldsymbol{k})$	The point group of the wave vector $\boldsymbol{k}$ (ch. 5 § 1)

$H(\boldsymbol{r})$	Hamiltonian operator
I	Inversion operator (ch. 1 § 1)
$\bar{I}$	Generalized inversion operator (ch. 8 § 3, appendix 2)
$\boldsymbol{K}_m$	Reciprocal lattice vector [eq. (4.13)]
$\boldsymbol{k}$	Allowed wave vector [eq. (4.8)]
$\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots$	Vectors of the star of $\boldsymbol{k}$ (ch. 5 § 1, ch. 7 § 1)
$M(\boldsymbol{k})$	Number of vectors in the star of $\boldsymbol{k}$
$O(T), O(\bar{T})$	Spinor transformation operators (ch. 8 § 3)
$P(T)$	Scalar transformation operator (ch. 3 § 2)
$\mathscr{P}^p_{mn}$	Projection operator [eq. (3.22)]
$\boldsymbol{R}, \boldsymbol{R}(T)$	Transformation matrix [eq. (1.1)]
$\boldsymbol{R}_1, \boldsymbol{R}_2, \ldots$	Transformation matrices generating star of $\boldsymbol{k}$ (ch. 5 § 1, ch. 7 § 1)
$\mathscr{S}$	Subgroup of $\mathscr{G}$
T	A transformation (ch. 1 § 1)
$\bar{T}$	A generalized transformation (ch. 8 § 3)
$\boldsymbol{t}$	A translation. (This symbol frequently appears with subscripts or superscripts attached)
$\boldsymbol{t}_n$	Lattice vector of the crystal [eq. (1.9)]
$\mathscr{T}$	The subgroup of pure primitive translations of the space group $\mathscr{G}$ (ch. 1 § 3.1, ch. 4 § 2)
$\mathscr{T}(\boldsymbol{k})$	Subgroup of $\mathscr{T}$ corresponding to $\boldsymbol{k}$ (ch. 7 § 2, ch. 9 § 9.1)
$\boldsymbol{u}, \boldsymbol{u}(\boldsymbol{R})$	SU_2 matrix corresponding to proper rotation $\boldsymbol{R}$ (ch. 8 § 2)
$\boldsymbol{\Gamma}$	Matrix of a representation (ch. 2 § 1). (This symbol frequently appears with superscripts attached)
χ	Character of representation (ch. 2 § 5). (This symbol frequently appears with superscripts attached)

CONTENTS

CHAPTER 1

BASIC CONCEPTS

§ 1. COORDINATE TRANSFORMATIONS

This book is concerned with the study of the symmetry properties of functions having physical significance. These can be described by stating how the functions transform under coordinate transformations.

Consider the following example of such a transformation. Suppose that Ox, Oy, Oz are three mutually perpendicular axes, and Ox', Oy', Oz' are another set of mutually perpendicular axes with the same origin O, which could, for example, be obtained from the first set by a rotation about some axis through O. Suppose that (x, y, z) and (x', y', z') are the coordinates of any point with respect to these two sets of axes. (That is, both sets of coordinates represent the *same* point.) Then the relationship between the two sets of coordinates can be written in the form

$$\boldsymbol{r}' = \boldsymbol{R}(T)\,\boldsymbol{r}, \tag{1.1}$$

where $\boldsymbol{r}=(x, y, z)$ and $\boldsymbol{r}'=(x', y', z')$, all such vectors being treated as 3×1 column matrices in matrix expressions unless otherwise indicated, and $\boldsymbol{R}(T)$ is a 3×3 matrix with real coefficients which depend *only* on the rotation, and not on the particular point under consideration. (The definitions, notations and properties of matrices used in this book are summarized in appendix 4.) $\boldsymbol{R}(T)$ will be called the transformation matrix corresponding to the transformation or symmetry operation T. It will sometimes be written merely as $\boldsymbol{R}$. As an example, suppose that Oz and Oz'

coincide, and Ox', Oy' are obtained from Ox, Oy by a rotation through an angle ϕ in the right-hand screw sense about Oz, as shown in figs. 1.1 and 1.2. Then

$$
\begin{aligned}
x' &= x\cos\phi + y\sin\phi \\
y' &= -x\sin\phi + y\cos\phi\,, \\
z' &= z
\end{aligned}
$$

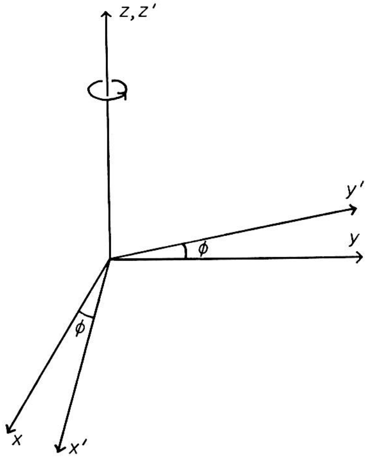

Fig. 1.1

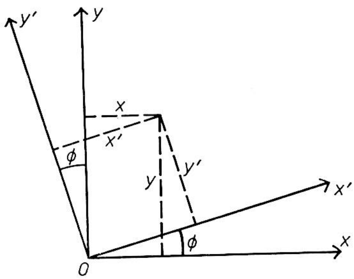

Fig. 1.2