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SYMMETRY PRINCIPLES AND MAGNETIC SYMMETRY IN SOLID STATE PHYSICS

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Let each do as he pleases; but let there be symmetry

Joe Rosen

To Prema and to my girls
Asha, Anita, Sunita and Lalitha

PREFACE

This work arises from two sources and is therefore written in two parts. The first part has grown out of 20 lectures given to senior undergraduates and fresh graduate students of the University of the West Indies, Trinidad, and the University of Port Harcourt, Nigeria. A generous invitation to the first Caribbean Physics Meeting, sponsored by the Organization of American States and held at the Jamaica Campus of the University of the West Indies, was the motivating factor for adding the second part, which is based on a paper presented at the meeting.

The book is written at the level and style of lecture notes on the applications of group theory to solid state physics. The first part is intended for beginners in the field and as such a more complete treatment of the topics discussed here must be sought in the references given at the end of the text. This part is aimed at showing, via the extensive use of character tables, how symmetry arguments can be used to give a detailed insight into the physical properties of crystals closely linked with structures. An elementary course in solid state physics and quantum mechanics is considered a necessary prerequisite for this course.

Since the mathematical language of symmetry concepts is group theory, which is really a branch of pure mathematics, it is usually developed with reference to abstract entities. However, this is not the approach taken in Part I. All elegant proofs etc have been omitted. Experience has shown that for most beginners a better approach is to present first (as far as possible) the applications of symmetry and only afterwards should the formal aspects of the theory be introduced, if they need to be introduced at all at this stage!

Part I includes the following basic areas:

(i) introduction to group theoretical concepts and techniques;
(ii) basic symmetry operations present in the solid state;
(iii) illustrative examples.

I am sure that those who have the patience to go through this first part would acquire a workmanlike knowledge of group theory and would, with some determination and effort, be in a position to understand the second part of this book which deals with the more recent studies on the symmetry properties of magnetic crystals.

Part I contains a number of exercises at the end of each chapter. Most of these follow some derivation or development from within the text. All these problems have either detailed solutions or hints, given at the end of the book, which readers will find quite useful in understanding the subject matter.

It is hoped that this book will provide the necessary basis for further detailed courses on the subject and as such the selection of topics in Part I is deliberately restricted.

Part II is meant to be self-contained and can be read without reference to Part I by readers who are familiar with elementary group theory. It should also prove useful to graduate students and research workers beginning the study of magnetic crystals. It is hoped that it will provide a useful adjunct to any advanced course on the applications of symmetry principles in solid state physics.

S J Joshua
March 1990

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I am particularly grateful to Professor A P Cracknell whose lectures on applied group theory provided the initial stimulus to write this book. I am also grateful to him for the many valuable discussions and suggestions on the subject matter contained in Part II.

I should also like to express my sincere gratitude to Professor A F Gibson FRS, for having given me the opportunity and providing me with financial assistance to work in the Department of Physics at the University of Essex where most of this work was carried out. Furthermore, of the many members of the staff at the University who have aided and encouraged me during the course of this work, I wish to thank especially Professor R Loudon FRS, Professor David Tilley, the late Dr J A Reissland and Dr P Kapadia.

It is also with great pleasure that I acknowledge the invaluable comments and assistance provided by my students, especially S Deonarine and F D Morgan.

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Finally, I should like to thank Mrs Luigina Njuki, Secretary of the Department of Physics, Moi University, for her ceaseless assistance in typing and preparing the manuscript. The responsibility for any errors or shortcomings is of course entirely mine.

S J Joshua
March 1990

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PART II: SYMMETRY AND THE MAGNETIC STATE

PART I

INTRODUCTION TO SYMMETRY PRINCIPLES IN SOLID STATE PHYSICS

1

ELEMENTS OF SYMMETRY THEORY

1.1 Introduction

Crystals play a particularly important role in modern-day solid state electronic devices. In the study of the behaviour and properties of crystalline materials, one requires a good exposure to:

(i) quantum mechanics, which is needed to study the behaviour and properties of individual atoms;
(ii) statistical mechanics, which is needed to describe the average properties of a large ensemble of atoms; and
(iii) symmetry theory (or group theory), which is needed to describe and understand the properties arising from the symmetrical structure of the solid.

In this book we shall be concerned only with (iii). Group theory, however, is really a branch of pure mathematics and as such it is usually developed with reference to abstract entities. Nevertheless, this is not the course we shall adopt, as we shall be mainly concerned with the applications of the theory to problems in crystal physics.

1.2 The role of symmetry

Symmetry arguments not only greatly simplify calculations of the thermal, electrical, optical and magnetic properties of solids etc, but also often give a detailed insight into the physical situation. It is therefore a standard practice amongst research workers to carry out a symmetry analysis before undertaking any calculations or experimental investigations on problems in crystal physics.

Given any crystal system it is prudent to begin by considering what information may be gleaned from a symmetry analysis of the structure. As often happens, even when the empirical work has been done, a symmetry analysis is still very helpful in testing various models put forward.

The symmetry which we aim to exploit via group theory is, in most cases, the symmetry of the Hamiltonian operator. An operator will be a symmetry operator appropriate to a given Hamiltonian, if the Hamiltonian looks the same after applying the operation as it did before; in other words, the Hamiltonian is invariant or unchanged under the operation. Our studies of the symmetry of the Hamiltonian of the system will indicate the range of uses to which symmetry concepts can be put in quantum mechanics. To achieve our goal we must first develop the elements of group theory in a manner suitable for ready applications. Thus, we shall not spend time over fundamental theorems, axioms, proofs, etc which can be found in many excellent textbooks on group theory.

1.3 Symmetry concepts via group theory

1.3.1 Symmetry operations and symmetry elements

The symmetry possessed by a crystalline material is defined in terms of symmetry operations. An operation is said to be a symmetry operation if the body looks exactly the same after the operation as it did before the operation was carried out. The operation could be, for example, rotations through certain angles or reflections in various mirror planes. As an example, consider the equilateral triangle shown in figure 1.1. It is easy to see that if we performed an operation of rotating the triangle through 120° or 240° about the z axis, the triangle would be left in a position which is indistinguishable from the starting position. Such an operation or movement which transforms a body into itself or leaves it invariant is called a symmetry operation and the body is said to possess the appropriate symmetry element. A symmetry element is therefore a real geometrical part of the system and

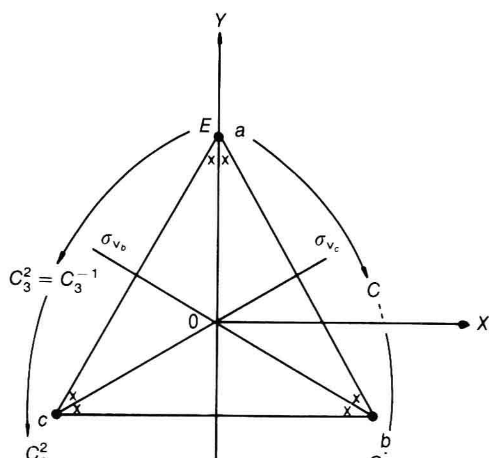

Figure 1.1 Symmetry operations corresponding to the crystal point group C_{3v}. The symbols have the following meanings (explained more fully in Chapter 4): C, cyclic group; σ, reflection plane; subscript 3, three-fold vertical rotation axes located at the central point 0; subscript v, vertical reflection planes.

also an identification symbol of the operation; for example, the symmetry element C_3 of the equilateral triangle implies the following symmetry operations: C_3^1, which corresponds to a clockwise rotation operation through 120° about the z axis; and C_3^2, which corresponds to a clockwise rotation operation through 240° about the z axis. The symbols are defined later on; for the moment it is important to note the difference between the terms symmetry elements and symmetry operations.

1.3.2 Basic types of symmetry elements

In dealing with crystal symmetry (point) groups we need to consider only the symmetry elements described and defined in table 1.1.

It is important to mention here briefly that suitable combinations of the symmetry elements given in table 1.1 define what is technically termed as a crystal point group. A crystal point group is defined as a collection of symmetry operations which, when applied about a point in the crystal, will leave the crystal structure invariant. Note that a crystal point group does not contain any translation operations. These are explained more fully in §4.5.

1.3.3 What is a symmetry group?

A symmetry group is a collection of symmetry elements $E, A, B, C, \ldots, X$ which satisfy the following group properties.

Table 1.1 The basic type of symmetry elements in Schoenflies notation.

No.	Symmetry element and symbol	Symmetry operation(s)
1	Identity element: E	Do nothing operation; like multiplying by 1
2	Mirror plane: σ	Reflection in a mirror
3	Centre of inversion or inversion symmetry: I	Inversion of all coordinates through the centre; I changes (x, y, z) to $(-x, -y, -z)$
4	Proper rotation axis: C_n	n-fold rotations about an appropriate axis. An n-fold axis generates n operations, e.g. the symmetry element C_6 implies the operations: C_6^1, C_6^2, C_6^3, C_6^4, C_6^5 and $C_6^6 = E$
5	Improper rotation axis: S_n	n-fold rotation about an axis followed by a reflection in a plane perpendicular to the axis of rotation, i.e. presence of S_n implies the independent existence of both C_n and σ elements