

Lecture Notes in Physics

Founding Editors: W. Beiglböck, J. Ehlers, K. Hepp, H. Weidenmüller

Editorial Board

R. Beig, Vienna, Austria
W. Beiglböck, Heidelberg, Germany
W. Domcke, Garching, Germany
B.-G. Englert, Singapore
U. Frisch, Nice, France
F. Guinea, Madrid, Spain
P. Hänggi, Augsburg, Germany
W. Hillebrandt, Garching, Germany
R. L. Jaffe, Cambridge, MA, USA
W. Janke, Leipzig, Germany
H. v. Löhneysen, Karlsruhe, Germany
M. Mangano, Geneva, Switzerland
J.-M. Raimond, Paris, France
D. Sornette, Zurich, Switzerland
S. Theisen, Potsdam, Germany
D. Vollhardt, Augsburg, Germany
W. Weise, Garching, Germany
J. Zittartz, Köln, Germany

The Lecture Notes in Physics

The series Lecture Notes in Physics (LNP), founded in 1969, reports new developments in physics research and teaching – quickly and informally, but with a high quality and the explicit aim to summarize and communicate current knowledge in an accessible way. Books published in this series are conceived as bridging material between advanced graduate textbooks and the forefront of research and to serve three purposes:

- to be a compact and modern up-to-date source of reference on a well-defined topic
- to serve as an accessible introduction to the field to postgraduate students and nonspecialist researchers from related areas
- to be a source of advanced teaching material for specialized seminars, courses and schools

Both monographs and multi-author volumes will be considered for publication. Edited volumes should, however, consist of a very limited number of contributions only. Proceedings will not be considered for LNP.

Volumes published in LNP are disseminated both in print and in electronic formats, the electronic archive being available at springerlink.com. The series content is indexed, abstracted and referenced by many abstracting and information services, bibliographic networks, subscription agencies, library networks, and consortia.

Proposals should be sent to a member of the Editorial Board, or directly to the managing editor at Springer:

Christian Caron
Springer Heidelberg
Physics Editorial Department I
Tiergartenstrasse 17
69121 Heidelberg / Germany
christian.caron@springer.com

Richard C. Powell

Symmetry, Group Theory, and the Physical Properties of Crystals

 Springer

Richard C. Powell
Professor Emeritus
University of Arizona
Tucson, AZ
USA
rcpowell@u.arizona.edu

ISSN 0075-8450 e-ISSN 1616-6361
ISBN 978-1-4419-7597-3 e-ISBN 978-1-4419-7598-0
DOI 10.1007/978-1-4419-7598-0
Springer New York Dordrecht Heidelberg London

© Springer Science+Business Media, LLC 2010

All rights reserved. This work may not be translated or copied in whole or in part without the written permission of the publisher (Springer Science+Business Media, LLC, 233 Spring Street, New York, NY 10013, USA), except for brief excerpts in connection with reviews or scholarly analysis. Use in connection with any form of information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed is forbidden.

The use in this publication of trade names, trademarks, service marks, and similar terms, even if they are not identified as such, is not to be taken as an expression of opinion as to whether or not they are subject to proprietary rights.

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

Why do we look at some things and think they are beautiful while other things do not appear esthetically pleasing to us? This is a question that has always interested mankind. One answer is given by the following quotation from an early president of the College of New Jersey (now Princeton University):

“Beauty is found in immaterial things like proportion or uniformity. . . . called by various names of regularity, order, uniformity, symmetry, proportion, harmony, etc.”. . . Jonathan Edwards¹

Symmetry not only provides the natural harmony that makes something appear beautiful to us, but also is of great value to science because it dictates the physical traits of many objects. Nature itself seems to love beauty since atoms tend to self-assemble into shapes with specific symmetry and crystals grow in geometric lattices. In many cases, if we know the symmetry of something we can predict some of its important properties without having to resort to experimentation or complicated calculations.

One area where the concept of symmetry plays an important role is that of crystalline solids. Crystals, by their very nature, exhibit specific symmetries. Crystalline materials have many important applications in devices based on their electronic, optical, thermal, magnetic, and mechanical properties. Solid state physicists and chemists, as well as material scientists and engineers, have developed rigorous quantum theoretical models to describe these properties and sophisticated measurement techniques to verify these models.

Many times, however, in screening materials for a new application it is useful to be able to quickly and easily determine if a specific material will have the appropriate properties without making detailed calculations or experiments. This can be done by analyzing the symmetry properties of the material. The mathematical formalism that has been developed to accomplish this is called group theory. The symmetry properties of a crystal can be described by a group of mathematical

¹J. Edwards, *Works of Jonathan Edwards* (Banner of Truth Trust, Edinburgh, 1979)

operations. Then using simple group theory procedures, the physical properties of the crystal can be determined.

During the 45 years I have been involved in teaching and research in various areas of solid state physics, I have made extensive use of the concepts of group theory. Yet I have been surprised at how little emphasis this topic receives in any formal educational curriculum. Generally, a student studying solid state physics or chemistry will be exposed to crystal structures early in the semester and then have no further exposure to crystal symmetry until some special topic such as nonlinear optics is discussed. This book focuses on the symmetry of crystals and the description of this symmetry through the use of group theory. Although specific examples are provided of using this formalism to determine both the microscopic and macroscopic properties of materials, the emphasis is on the comprehensive, pervasive nature of symmetry in all areas of solid state science.

The intent of the book is to be a reference source for those doing research or teaching in solid state science and engineering, or a text for a specialty course in group theory applied to the properties of crystals.

Tucson, AZ
June 2010

Richard C. Powell

Contents

1	Symmetry in Solids	1
1.1	Symmetry	1
1.2	Crystal Structures	4
1.3	Symmetry in Reciprocal Space	15
1.4	Problems	24
	References	24
2	Group Theory	25
2.1	Basic Concepts of Group Theory	27
2.2	Character Tables	31
2.3	Group Theory Examples	40
	2.3.1 C_{3v} Point Group	40
	2.3.2 O_h Point Group	45
2.4	Group Theory in Quantum Mechanics	47
2.5	Problems	52
	References	53
3	Tensor Properties of Crystals	55
3.1	First-Rank Matter Tensors	57
3.2	Second-Rank Matter Tensors	62
3.3	Third-Rank Matter Tensors	68
3.4	Fourth-Rank Matter Tensors	73
3.5	Problems	77
	References	77
4	Symmetry Properties of Point Defects in Solids	79
4.1	Energy Levels of Free Ions	79
4.2	Crystal Field Symmetry	85
4.3	Energy Levels of Ions in Crystals	87

4.4	Example: d-Electrons	95
4.5	Example: f-Electrons.....	100
4.6	Problems	104
	References	104
5	Symmetry and the Optical Properties of Crystals	105
5.1	Tensor Treatment of Polarization.....	105
5.2	Birefringence.....	114
5.3	Optical Activity	118
5.4	Electrooptical Effect	123
5.5	Photoelastic Effect	131
5.6	Problems	134
	References	134
6	Nonlinear Optics	137
6.1	Basic Concepts.....	138
6.2	Effective Nonlinear Optical Coefficient	145
6.3	Index Matching	150
6.4	Maximizing SHG Efficiency.....	153
6.5	Two-Photon Absorption	157
6.6	Problems	162
	References	163
7	Symmetry and Lattice Vibrations	165
7.1	Symmetry and Local Mode Vibrations	166
7.2	Symmetry and Lattice Vibrational Modes.....	173
7.3	Transitions Between Vibrational Energy Levels	180
	7.3.1 Radiationless Transitions	181
	7.3.2 Infrared Transitions	183
7.4	Raman Scattering	185
7.5	Jahn–Teller Effect.....	194
7.6	Problems	198
	References	198
8	Symmetry and Electron Energy Levels	201
8.1	Symmetry and Molecular Bonds	201
8.2	Character Tables for Space Groups.....	212
8.3	Electron Energy Bands.....	214
8.4	Symmetry Properties of Electron Energy Bands	220
8.5	Problems	223
	References	224
Errata	E1
Index	225