APPLICATIONS OF GROUP THEORY TO ATOMS, MOLECULES, AND SOLIDS

The majority of all knowledge concerning atoms, molecules, and solids has been derived from applications of group theory. Taking a unique, applications-oriented approach, this book gives readers the tools needed to analyze any atomic, molecular, or crystalline solid system.

Using a clearly defined, eight-step program, this book helps readers to understand the power of group theory, what information can be obtained from it, and how to obtain it. The book takes in modern topics, such as graphene, carbon nanotubes, and isotopic frequencies of molecules, as well as more traditional subjects: the vibrational and electronic states of molecules and solids, crystal-field and ligand-field theory, transition-metal complexes, space groups, time-reversal symmetry, and magnetic groups.

With over a hundred end-of-chapter exercises, this book is invaluable for graduate students and researchers in physics, chemistry, electrical engineering, and materials science.

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CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE
UNIVERSITY PRESS

University Printing House, Cambridge CB2 8BS, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314-321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi - 110025, India

103 Penang Road, #05-06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of the University of Cambridge.

It furthers the University's mission by disseminating knowledge in the pursuit of education, learning and research at the highest international levels of excellence.

www.cambridge.org
Information on this title: www.cambridge.org/9781107028524

First published 2014

A catalogue record for this publication is available from the British Library

Library of Congress Cataloging in Publication data
Wolfram, Thomas, 1936–
Applications of group theory to atoms, molecules, and solids / Thomas Wolfram, Şinasi Ellialtıoğlu.
pages cm
ISBN 978-1-107-02852-4 (hardback)
1. Solids – Mathematical models. 2. Molecular structure. 3. Atomic structure. 4. Group theory.
I. Title.
QC176.W65 2013
530.4´1015122–dc23
2013008434

ISBN 978-1-107-02852-4 Hardback

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Preface

The majority of all knowledge accumulated in physics and chemistry concerning atoms, molecules, and solids has been derived from applications of group theory to quantum systems.

My (T.W.) first encounter with group theory was as an undergraduate in physics, struggling to understand Wigner's *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra* (1959). I felt there was something magical about the subject. It was amazing to me that it was possible to analyze a physical system knowing only the symmetry and obtain results that were absolute, independent of any particular model. To me it was a miracle that it was possible to find some exact eigenvectors of a Hamiltonian by simply knowing the geometry of the system or the symmetry of the potential.

Many books devote the initial chapters to deriving abstract theorems before discussing any of the applications of group theory. We have taken a different approach. The first chapter of this book is devoted to finding the molecular vibration eigenvalues, eigenvectors, and force constants of a molecule. The theorems required to accomplish this task are introduced as needed and discussed, but the proofs of the theorems are given in the appendices. (In later chapters the theorems needed for the analysis are derived within the discussions.) By means of this applications-oriented approach we are able to immediately give a general picture of how group theory is applied to physical systems. The emphasis is on the process of applying group theory. The various steps needed to analyze a physical system are clearly delineated. By the end of the first chapter the reader should have an appreciation for the power of group theory, what information can be obtained, and how to obtain it. That is, the "magic" of group theory should already be apparent.

In addition to the essential, traditional topics, there are new topics, including the electronic and vibrational properties of graphene and nanotubes, the vibrations of isotopically substituted molecules, localized vibrations, and discussions of the axially symmetric lattice dynamics model. The energy bands and vibrational

normal modes of crystals with the perovskite structure are also discussed in detail.

The material in this book was developed in part from group-theory courses and from a series of lectures presented in courses on special topics at the University of Missouri-Columbia. It is appropriate for science and engineering graduate students and advanced undergraduate seniors. The ideal reader will have had a course in quantum mechanics and be familiar with eigenvalue problems and matrix algebra. However, no prerequisite knowledge of group theory is necessary.

This book may be employed as a primary text for a first course in group theory or as an auxiliary book for courses in quantum mechanics, solid-state physics, physical chemistry, materials science, or electrical engineering. It is intended as a self-teaching tool and therefore the analyses in the early chapters are given in some detail. Each chapter includes a set of exercises designed to reinforce and extend the material discussed in the chapter.

Thomas Wolfram
and
Şinasi Ellialtıoğlu