

Solid-State Sciences

R. A. Evarestov V. P. Smirnov

Site Symmetry in Crystals

Theory and Applications

Second Enlarged Edition



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Site Symmetry In Crystals Theory And Applications

Gerald Burns



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Site Symmetry in Crystals Robert A. Evarestov, Vyacheslav P. Smirnov, 2012-12-06 Site Symmetry in Crystals is the first comprehensive account of the group theoretical aspects of the site local symmetry approach to the study of crystalline solids. The efficiency of this approach which is based on the concepts of simple induced and band representations of space groups is demonstrated by considering newly developed applications to electron surface states, point defects, symmetry analysis in lattice dynamics, the theory of second order phase transitions and magnetically ordered and non rigid crystals. Tables of simple induced representations are given for the 24 most common space groups allowing the rapid analysis of electron and phonon states in complex crystals with many atoms in the unit cell. [Site Symmetry in Crystals](#) Robert A.

Evarestov, Vyacheslav P. Smirnov, 1997-01-16

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Smirnov, 2012-12-06 The history of applications of space group theory to solid state physics goes back more than five decades. The periodicity of the lattice and the definition of a k space were the corner stones of this application. Prof Volker Heine in Vol 35 of Solid State Physics 1980 noted that even in perfect crystals where k space methods are appropriate the local properties such as the charge density, bond order etc are defined by the local environment of one atom. Naturally k space methods are not appropriate for crystals with point defects, surfaces and interfaces or for amorphous materials. In such cases the real space approach favored by chemists to describe molecules has turned out to be very useful. To span the gulf between the k space and real space methods it is helpful to recall that atoms in crystalline solids possess a site symmetry defined by the symmetry of the local environment of the atom occupying the site. The site symmetry concept is familiar to crystallographers and commonly used by them in the description of crystalline structures. However in the application of group theory to solid state physics problems the site symmetry approach has been used only for the last ten to fifteen years. In our book *Methods of Group Theory in the Quantum Chemistry of Solids* published in Russian in 1987 by Leningrad University Press we gave the first results of this application to the theory of electronic structure of crystals.

Magnetism and the Electronic Structure of Crystals Vladimir A. Gubanov, Alexandr I. Liechtenstein, Andrei V. Postnikov, 2012-12-06 The quantum theory of magnetism is a well developed part of contemporary solid state physics. The basic concepts of this theory can be used to describe such important effects as ferromagnetic ordering of localized magnetic moments in crystals and ferromagnetism of metals produced by essentially delocalized electrons as well as various types of mutual orientation of atomic magnetic moments in solids possessing different crystal lattices and compositions. In recent years the spin fluctuational approach has been developed which can overcome some contradictions between localized and itinerant models in the quantum mechanics of magnetic crystals. These are only some of the principal achievements of quantum magnetic theory. Almost all of the known magnetic properties of solids can be qualitatively explained on the basis of its concepts. Further developments should open up the possibility of reliable quantitative description of magnetic properties of solids.

Unfortunately such calculations based on model concepts appear to be very complicated and quite often not definite enough. The rather small number of parameters of qualitative models are usually not able to take into account the very different types of magnetic interactions that appear in crystals. Further development of magnetic theory requires quantitative information on electronic wave function in the crystal considered. This can be proved by electronic band structure and cluster calculations. In many cases the latter can be a starting point for quantitative calculations of parameters used in magnetic theory.

Physical Properties of Quasicrystals Zbigniew M. Stadnik, 2012-12-06 Quasicrystals are a new form of the solid state which differ from the other two known forms crystalline and amorphous by possessing a new type of long range translational order called quasiperiodicity and a noncrystallographic orientational order. This book provides an up to date description of the unusual physical properties of these new materials. Emphasis is placed on the experimental results which are compared with those of the corresponding crystalline and amorphous systems and discussed in terms of modern theoretical models. Written by leading authorities in the field the book will be of great use both to experienced workers in the field and to uninitiated graduate students.

Symmetry and Condensed Matter Physics M. El-Batanouny, F. Wooten, 2008-03-13 Unlike existing texts this book blends for the first time three topics in physics: symmetry, condensed matter physics and computational methods into one pedagogical textbook. It includes new concepts in mathematical crystallography, experimental methods capitalizing on symmetry aspects, non conventional applications such as Fourier crystallography, color groups, quasicrystals and incommensurate systems as well as concepts and techniques behind the Landau theory of phase transitions. Adopting a computational approach to the application of group theoretical techniques to solving symmetry related problems it dramatically alleviates the need for intensive calculations usually found in the presentation of symmetry. Writing computer programs helps the student achieve a firm understanding of the underlying concepts and sample programs based on Mathematica are presented throughout the book. Containing over 150 exercises this textbook is ideal for graduate students in condensed matter physics, materials science and chemistry. Solutions and computer programs are available online at www.cambridge.org/9780521828451.

Space Group Representations Nikolai B. Melnikov, Boris I. Reser, 2023-01-01 This book is devoted to the construction of space group representations, their tabulation and illustration of their use. Representation theory of space groups has a wide range of applications in modern physics and chemistry including studies of electron and phonon spectra, structural and magnetic phase transitions, spectroscopy, neutron scattering and superconductivity. The book presents a clear and practical method of deducing the matrices of all irreducible representations including double valued and tabulates the matrices of irreducible projective representations for all 32 crystallographic point groups. One obtains the irreducible representations of all 230 space groups by multiplying the matrices presented in these compact and convenient to use tables by easily computed factors. A number of applications to the electronic band structure calculations are illustrated through real life examples of different crystal structures. The book's content is accessible to both graduate and advanced

undergraduate students with elementary knowledge of group theory and is useful to a wide range of experimentalists and theorists in materials and solid state physics *Introduction to Group Theory with Applications* Gerald Burns, 2014-05-10

Introduction to Group Theory with Applications covers the basic principles concepts mathematical proofs and applications of group theory This book is divided into 13 chapters and begins with discussions of the elementary topics related to the subject including symmetry operations and group concepts The succeeding chapters deal with the properties of matrix representations of finite groups the vibrations of molecular and crystals vibrational wave function selection rules and molecular approximations These topics are followed by reviews of the basic of quantum mechanics crystal field theory atomic physics hybrid functions and molecular orbital theory The last chapters describe the symmetry of crystal lattices the band theory of solids and the full rotation group This book will be of value to undergraduate mathematics and physics students

Correlation Effects in Low-Dimensional Electron Systems Ayao Okiji, Norio Kawakami, 2012-12-06 Correlation Effects in Low Dimensional Electron Systems describes recent developments in theoretical condensed matter physics emphasizing exact solutions in one dimension including conformal field theoretical approaches the application of quantum groups and numerical diagonalization techniques Various key properties are presented for two dimensional highly correlated electron systems Spectroscopy of Mott Insulators and Correlated Metals Atsushi Fujimori, Yoshinori Tokura, 2012-12-06 Extensive studies of high T_c cuprate superconductors have stimulated investigations into various transition metal oxides Mott transitions in particular provide fascinating problems and new concepts in condensed matter physics This book is a collection of overviews by well known active researchers in this field It deals with the latest developments with particular emphasis on the theoretical spectroscopic and transport aspects

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