

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

**Andrea Crisanti, Giovanni
Paladin, Angelo Vulpiani**



Site Symmetry In Crystals Theory And Applications:

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

Site Symmetry in Crystals Robert A. Evarestov, Vyacheslav P.

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

Structural Analysis of Point Defects in Solids Johann-Martin Spaeth, Jürgen R. Niklas, Ralph H.

Bartram, 2012-12-06 Structural Analysis of Point Defects in Solids introduces the principles and techniques of modern electron paramagnetic resonance EPR spectroscopy essential for applications to the determination of microscopic defect structures Investigations of the microscopic and electronic structure and also correlations with the magnetic properties of solids require various multiple magnetic resonance methods such as ENDOR and optically detected EPR or ENDOR This book discusses experimental technological and theoretical aspects of these techniques comprehensively from a practical viewpoint with many illustrative examples taken from semiconductors and other solids The nonspecialist is informed about the potential of the different methods while the researcher faced with the task of determining defect structures is provided with the necessary tools together with much information on computer aided methods of data analysis and the principles of modern spectrometer design

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

Electronic Properties of High-T_c Superconductors Hans Kuzmany, Michael Mehring, Jörg Fink, 2012-12-06 The International Winter School on

Electronic Properties of High Temperature Superconductors held between March 7 14 1992 in Kirchberg Tyrol Austria was the sixth in a series of meetings to be held at this venue Four of the earlier meetings were dedicated to issues in the field of

conducting polymers while the winter school held in 1990 was devoted to the new discipline of high T_c superconductivity. This year's meeting constituted a forum not only for the large number of scientists engaged in high T_c research but also for those involved in the new and exciting field of fullerenes. Many of the issues raised during the earlier winter schools on conducting polymers and the last one on high T_c superconductivity have taken on a new significance in the light of the discovery of superconducting C materials. 60 The Kirchberg meetings are organized in the style of a school where experienced scientists from universities, research laboratories and industry have the opportunity to discuss their most recent results and where students and young scientists can learn about the present status of research and applications from some of the most eminent workers in their field. In common with the previous winter school on high T_c superconductors, the of the cuprate superconductors present one focused on the electronic properties. In addition, consideration was given to related compounds which are relevant to the understanding of the electronic structure of the cuprates in the normal state to other oxide superconductors and to fulleride superconductors.

Low-Dimensional Electronic Systems Guenther Neubauer, Friedemar Kuchar, Helmut Heinrich, 2013-03-13. Owing to new physical technological and device concepts of low dimensional electronic systems the physics and fabrication of quasi zero one and two dimensional systems are rapidly growing fields. The contributions presented in this volume cover results of nanostructure fabrication including recently developed techniques for example tunneling probe techniques and molecular beam epitaxy quantum transport including the integer and fractional quantum Hall effect optical and transport studies of the two dimensional Wigner solid phonon studies of low dimensional systems and Si/SiGe heterostructures and superlattices. To the readers new in the field this volume gives a comprehensive introduction and for the experts it is an update of their knowledge and a great help for decisions about future research activities.

Products of Random Matrices Andrea Crisanti, Giovanni Paladin, Angelo Vulpiani, 2012-12-06. At the present moment after the success of the renormalization group in providing a conceptual framework for studying second order phase transitions we have a nearly satisfactory understanding of the statistical mechanics of classical systems with a non random Hamiltonian. The situation is completely different if we consider the theory of systems with a random Hamiltonian or of chaotic dynamical systems. The two fields are connected in fact in the latter the effects of deterministic chaos can be modelled by an appropriate stochastic process. Although many interesting results have been obtained in recent years and much progress has been made we still lack a satisfactory understanding of the extremely wide variety of phenomena which are present in these fields. The study of disordered or chaotic systems is the new frontier where new ideas and techniques are being developed. More interesting and deep results are expected to come in future years. The properties of random matrices and their products form a basic tool whose importance cannot be underestimated. They play a role as important as Fourier transforms for differential equations. This book is extremely interesting as far as it presents a unified approach for the main results which have been obtained in the study of random matrices. It will become a reference book for

people working in the subject The book is written by physicists uses the language of physics and I am sure that many physicists will read it with great pleasure

Interatomic Potential and Structural Stability Kiyoyuki Terakura, Hisazumi Akai, 2013-03-08 Structural stability is of fundamental importance in materials science Up to date information on the theoretical aspects of phase stability of materials is contained in this volume Most of the first principles calculations are based on the local density approximation LDA In contrast this volume contains very recent results of going beyond LDA such as the density gradient expansion and the quantum Monte Carlo method Following the recently introduced theoretical methods for the calculation of interatomic potentials forces acting on atoms and total energies such as the Car Parrinello the effective medium and the bond order method attempts have been made to develop even more sophisticated methods such as the order N method in electronic structure calculations The present status of these methods and their application to real systems are described In addition in order to study the phase stability at finite temperatures the microscopic calculations have to be combined with statistical treatment of the systems to describe e g order disorder transitions on the Si 001 surface or alloy phase diagrams This book contains examples for this type of calculations

Phonon Scattering in Condensed Matter VII Michael Meissner, Robert O. Pohl, 2012-12-06 This volume contains the proceedings of the Seventh International Conference on Phonon Scattering in Condensed Matter held August 3-7 1992 at Cornell University in Ithaca NY USA The preceding conferences were held at St Maxime and Paris France 1972 Nottingham UK 1975 Providence USA 1979 Stuttgart Germany 1983 Urbana USA 1986 and Heidelberg Germany 1989 The Heidelberg conference was held jointly with the Third International Conference on Phonon Physics The next conference to be held in August 1995 in Sapporo Japan and hosted by Professor T Nakayama and his colleagues will also be such a joint conference This conference was attended by 227 scientists from 27 countries and covered all aspects of phonon scattering in condensed matter ranging from the more traditional topics of thermal conductivity Kapitza resistance and ballistic phonon propagation to the recently added topics such as electron phonon interaction in high T_c superconductors the use of phonons in particle detection and phonons in confined geometries The 207 papers arranged in 11 chapters in this volume are a cross section of the present activities in the quite obviously vibrant field of phonons and their interactions

The Quantum Hall Effects Tapash Chakraborty, Pekka Pietiläinen, 2013-03-12 The experimental discovery of the fractional quantum Hall effect FQHE at the end of 1981 by Tsui Stormer and Gossard was absolutely unexpected since at this time no theoretical work existed that could predict new structures in the magnetotransport coefficients under conditions representing the extreme quantum limit It is more than thirty years since investigations of bulk semiconductors in very strong magnetic fields were begun Under these conditions only the lowest Landau level is occupied and the theory predicted a monotonic variation of the resistivity with increasing magnetic field depending sensitively on the scattering mechanism However the experimental data could not be analyzed accurately since magnetic freeze out effects and the transitions from a degenerate to a nondegenerate system complicated the

interpretation of the data For a two dimensional electron the positive background charge is well separated from the two gas where dimensional system magnetic freeze out effects are barely visible and an analysis of the data in the extreme quantum limit seems to be easier First measurements in this magnetic field region on silicon field effect transistors were not successful because the disorder in these devices was so large that all electrons in the lowest Landau level were localized Consequently models of a spin glass and finally of a Wigner solid were developed and much effort was put into developing the technology for improving the quality of semi conductor materials and devices especially in the field of two dimensional electron systems

Fundamentals of Semiconductors Peter YU,Manuel Cardona,2007-05-08 This third updated edition of Fundamentals of Semiconductors attempts to fill the gap between a general solid state physics textbook and research articles by providing detailed explanations of the electronic vibrational transport and optical properties of semiconductors The approach is physical and intuitive rather than formal and pedantic Theories are presented to explain experimental results This textbook has been written with both students and researchers in mind Its emphasis is on understanding the physical properties of Si and similar tetrahedrally coordinated semiconductors The explanations are based on physical insights Each chapter is enriched by an extensive collection of tables of material parameters figures and problems Many of these problems lead the student by the hand to arrive at the results

Fundamentals of Semiconductor Peter YU,Manuel Cardona,2013-11-11 Fundamentals of Semiconductors attempts to fill the gap between a general solid state physics textbook and research articles by providing detailed explanations of the electronic vibrational transport and optical properties of semiconductors The approach is physical and intuitive rather than formal and pedantic Theories are presented to explain experimental results This textbook has been written with both students and researchers in mind Its emphasis is on understanding the physical properties of Si and similar tetrahedrally coordinated semiconductors The explanations are based on physical insights Each chapter is enriched by an extensive collection of tables of material parameters figures and problems Many of these problems lead the student by the hand to arrive at the results

Physics of Zero- and One-Dimensional Nanoscopic Systems Sachindra Nath Karmakar,Santanu Kumar Maiti,Chowdhury Jayeeta,2007-09-04 In recent years submicron and nanoscale systems have featured strongly on the research agenda due to the technological progress and new physics that have emerged from studies of ultra small systems A fundamental understanding of basic physical phenomena on the mesoscopic and nanoscopic scales is required to exploit the technological potential offered by these exotic materials The present book contains review like chapters by some of the leading experts in the field covering topics such as the Kondo effect electron transport disorder and quantum coherence with electron electron interaction persistent current thermoelectric phenomena etc in quantum dots quantum wires carbon nanotubes and more This book will be valuable to researchers and students in condensed matter physics

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