Finite Element and Boundary Element Applications in Quantum Mechanics

L. Ramdas Ram-Mohan

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Isaac Elishakoff,Yongjian Ren

Finite Element And Boundary Element Applications In Quantum Mechanics:

Finite Element and Boundary Element Applications in Quantum Mechanics L. Ramdas Ram-Mohan,2002 This book introduces the finite element and boundary element methods FEM and BEM for applications to quantum mechanical systems A discretization of the action integral with finite elements followed by application of variational principles brings a very general approach to the solution of Schroedinger s equation for physical systems in arbitrary geometries with complex mixed boundary conditions The variational approach is a common thread through the book and is used for the improvement of solutions to spectroscopic accuracy to adaptively improve finite element meshs to develop a time dependent theory and also to generate the solution of large sparse matrix eigenvalue problems A thorough introduction to BEM is given using the modelling of surface plasmons quantum electron waveguides and quantum scattering as illustrative examples The book should be useful to graduate students and researchers in basic quantum theory quantum semiconductor modeling computational physics mathematics and chemistry   Theoretical Methods, Algorithms, and Applications of Quantum Systems in Chemistry, Physics, and Biology Sourav Pal,Vipin Srivastava,Vidya Avasare,Jean Maruani,2025-08-21 This volume contains peer reviewed contributions based on talks presented at the 26th International Workshop on Quantum Systems in Chemistry Physics and Biology held in Jaipur India in October 2023 It provides an in depth discussion of methodological approaches that are relevant across various length scales elucidating their applications in diverse chemical and biological systems such as catalysis and materials Authored by experts in their respective fields each chapter showcases recent developments and offers insights into the latest research trends This book is aimed at advanced graduate students academics and researchers both in university and corporation laboratories interested in state of the art and novel trends in quantum chemistry physics and biology and their applications   Finite Element Methods for Structures with Large Stochastic Variations Isaac Elishakoff,Yongjian Ren,2003 The finite element method FEM can be successfully applied to various field problems in solid mechanics fluid mechanics and electrical engineering This text discusses finite element methods for structures with large stochastic variations   Optics and Its Applications David Blaschke,Dmitry Firsov,Aram Papoyan,Hayk A. Sarkisyan,2022-10-05 This book features selected articles based on contributions presented at the 9th International Symposium on Optics and Its Applications OPTICS 2022 in Yerevan Ashtarak Armenia The annual OPTICS symposium brings together renowned experts from all over the world working in the fields of atomic optics plasmonics optics of nanostructures as well as the optics of condensed matter and provides a perfect setting for their discussions of the most recent developments in this area The 9th iteration in this series dedicated to the 80th birthday of Academician Eduard Kazaryan focuses on topics dealing with the spectroscopy of real and artificial atoms linear and nonlinear optical characteristics of quantum wells and two dimensional materials The book highlights recent results of few particle optical characteristics of artificial atoms in the framework of the exactly solvable Moshinsky model as well as an electro optical analog of the magneto

optical Faraday effect In addition a detailed study of the nucleation process its characterization as well as electronic and optical properties of graded composition quantum dots in the Stranski Krastanov growth mode is presented **Finite Element Methods for Maxwell's Equations** Peter Monk,2003-04-17 Finite Element Methods For Maxwell s Equations is the first book to present the use of finite elements to analyse Maxwell s equations This book is part of the Numerical Analysis and Scientific Computation Series Handbook of Nanostructured Materials and Nanotechnology, Five-Volume Set Hari Singh Nalwa,1999-10-29 Nanostructured materials is one of the hottest and fastest growing areas in today s materials science field along with the related field of solid state physics Nanostructured materials and their based technologies have opened up exciting new possibilites for future applications in a number of areas including aerospace automotive x ray technology batteries sensors color imaging printing computer chips medical implants pharmacy and cosmetics The ability to change properties on the atomic level promises a revolution in many realms of science and technology Thus this book details the high level of activity and significant findings are available for those involved in research and development in the field It also covers industrial findings and corporate support This five volume set summarizes fundamentals of nano science in a comprehensive way The contributors enlisted by the editor are at elite institutions worldwide Key Features Provides comprehensive coverage of the dominant technology of the 21st century Written by 127 authors from 16 countries making this truly international First and only reference to cover all aspects of nanostructured materials and nanotechnology

Compound Semiconductors 2004 J.C. Woo,H. Hasegawa,Y.S. Kwon,T. Yao,K.H. Yoo,2005-04-01 Compound Semiconductors 2004 was the 31st Symposium in this distinguished international series held at Hoam Convention Center of Seoul National University Seoul Korea from September 12 to September 16 2004 It attracted over 180 submissions from leading scientists in academic and industrial research institutions and remains a major forum for the compound semiconductor research community since the first one held in 1966 at Edinburgh UK under the name of International Symposium on Gallium Arsenide and related Compounds These proceedings provide an international perspective on the latest research and an overview of recent important developments in III V compounds II VI compounds and IV IV compounds In the total of 106 papers notable progress was reported in the development of zinc oxide and spintronics Steady advances were seen in traditional topics such as III V based electronic and optoelectronic devices growth and processing and characterization Novel research trends were observed in quantum structures such as quantum wires and dots which are promising for future developments in nanotechnology As the primary forum for research into these materials and their device applications the book is an essential reference for researchers working on compound semiconductors in semiconductor physics device physics materials science chemistry and electronic and electrical engineering Handbook of Materials Modeling Sidney Yip,2007-11-17 This Handbook contains a set of articles introducing the modeling and simulation of materials from the standpoint of basic methods and studies The intent is to provide a compendium that is foundational to an

emerging eld of computational research a new discipline that may now be called Compu tional Materials This area has become suf ciently diverse that any attempt to cover all the pertinent topics would be futile Even with a limited scope the present undertaking has required the dedicated efforts of 13 Subject Editors to set the scope of nine chapters solicit authors and collect the manuscripts The contributors were asked to target students and non specialists as the primary audience to provide an accessible entry into the eld and to offer references for further reading With no precedents to follow the editors and authors were only guided by a common goal to produce a volume that would set a standard toward de ning the broad community and stimulating its growth The idea of a reference work on materials modeling surfaced in conver tions with Peter Bin eld then the Reference Works Editor at Kluwer Academic Publishers in the spring of 1999 The rationale at the time already seemed quite clear the eld of computational materials research was t ing off powerful computer capabilities were becoming increasingly available and many sectors of the scienti c community were getting involved in the enterprise

Bands and Photons in III-V Semiconductor Quantum Structures Igor Vurgaftman,Matthew P. Lumb,Jerry R. Meyer,2020-11-22 Semiconductor quantum structures are at the core of many photonic devices such as lasers photodetectors solar cells etc To appreciate why they are such a good fit to these devices we must understand the basic features of their band structure and how they interact with incident light Many books have taken on this task in the past but their treatments tend either to pluck results from the literature and present them as received truths or to rely on unrealistically simple models Bands and Photons in III V Semiconductor Quantum Structures takes the reader from the very basics of III V semiconductors some preparation in quantum mechanics and electromagnetism is helpful and shows how seemingly obscure results such as detailed forms of the Hamiltonian optical transition strengths and recombination mechanisms follow The reader would not need to consult other references to fully understand the material although a few handpicked sources are listed for those who would like to deepen their knowledge further Connections to the properties of novel materials such as graphene and transition metal dichalcogenides are pointed out to help prepare the reader for contributing at the forefront of research in those fields The book also supplies a complete up to date database of the band parameters that enter into the calculations along with tables of optical constants and interpolation schemes for alloys From these foundations the book goes on to derive the characteristics of photonic semiconductor devices with a focus on the mid infrared using the same principles of building all concepts from the ground up explaining all derivations in detail giving quantitative examples and laying out dimensional arguments whenever they can help the reader s understanding **Multi-Band Effective Mass Approximations** Matthias Ehrhardt,Thomas Koprucki,2014-07-17 This book addresses several mathematical models from the most relevant class of kp Schr dinger systems Both mathematical models and state of the art numerical methods for adequately solving the arising systems of differential equations are presented The operational principle of modern semiconductor nano structures such as quantum wells quantum wires or quantum dots relies on quantum mechanical effects The goal of numerical simulations using

quantum mechanical models in the development of semiconductor nano structures is threefold First they are needed for a deeper understanding of experimental data and of the operational principle Secondly they allow us to predict and optimize in advance the qualitative and quantitative properties of new devices in order to minimize the number of prototypes needed Semiconductor nano structures are embedded as an active region in semiconductor devices Thirdly and finally the results of quantum mechanical simulations of semiconductor nano structures can be used with upscaling methods to deliver parameters needed in semi classical models for semiconductor devices such as quantum well lasers This book covers in detail all these three aspects using a variety of illustrative examples Readers will gain detailed insights into the status of the multiband effective mass method for semiconductor nano structures Both users of the kp method as well as advanced researchers who want to advance the kp method further will find helpful information on how to best work with this method and use it as a tool for characterizing the physical properties of semiconductor nano structures The book is primarily intended for graduate and Ph D students in applied mathematics mathematical physics and theoretical physics as well as all those working in quantum mechanical research or the semiconductor opto electronic industry who are interested in new mathematical aspects *Computer Methods and Experimental Measurements for Surface Effects and Contact Mechanics VIII* J. T. M. de Hosson,2007 The importance of contact and surface problems in modern engineering and their combined effects has led to the Eighth International Conference on Computer Methods and Experimental Measurements for Surface and Contact Mechanics Nowadays the importance of contact and surface problems in many technological fields is well understood they are complex and inherently non linear due to their moving boundaries and the different properties of materials particularly along the contact surfaces Structural components fail from wear corrosion high cycle fatigue etc that is to say affected and initiated by the surface conditions The use of surface treatments can reduce the cost of components and extend the life of the elements Their effect is of particular importance in the case of surfaces undergoing contact a problem which is addressed throughout the book Topics featured Surface Treatment Surface problems in Contact Mechanics Fracture Mechanics Coupled analysis and experiments Thin Coatings Thick Coatings Contact Mechanics Material Surface in Contact Applications and Case Studies *Introduction to Monte Carlo Methods for Transport and Diffusion Equations* Bernard Lapeyre,Etienne Pardoux,Rémi Sentis,2003 This text is used by for the resolution of partial differential equations trasnport equations the Boltzmann equation and the parabolic equations of diffusion <u>Introduction to Parallel Computing</u> Wesley Petersen,Peter Arbenz,2004-01-08 In the last few years courses on parallel computation have been developed and offered in many institutions in the UK Europe and US as a recognition of the growing significance of this topic in mathematics and computer science There is a clear need for texts that meet the needs of students and lecturers and this book based on the author s lecture at ETH Zurich is an ideal practical student guide to scientific computing on parallel computers working up from a hardware instruction level to shared memory machines and finally to distributed memory machines Aimed at

advanced undergraduate and graduate students in applied mathematics computer science and engineering subjects covered include linear algebra fast Fourier transform and Monte Carlo simulations including examples in C and in some cases Fortran This book is also ideal for practitioners and programmers **Quantum Transport** Supriyo Datta,2005-06-16 This book presents the conceptual framework underlying the atomistic theory of matter emphasizing those that relate to current flow This includes some of the most advanced concepts of non equilibrium quantum statistical mechanics No prior acquaintance with quantum mechanics is assumed Many numerical examples are used to provide concrete illustrations and the corresponding MATLAB codes can be downloaded from the web Videostreamed lectures keyed to specific sections of the book are also available through the web Written for senior and graduate students **Physical Properties of Nanorods** Roman Krahne,Liberato Manna,Giovanni Morello,Albert Figuerola,Chandramohan George,Sasanka Deka,2013-06-12 Inorganic nanoparticles are among the most investigated objects nowadays both in fundamental science and in various technical applications In this book the physical properties of nanowires formed by nanoparticles with elongated shape i e rod like or wire like are described The transition in the physical properties is analyzed for nanorods and nanowires consisting of spherical and rod like nanoparticles The physical properties of nanowires and elongated inorganic nanoparticles are reviewed too The optical electrical magnetic mechanical and catalytic properties of nanowires consisting of semiconductors noble and various other metals metal oxides properties and metal alloys are presented The applications of nanorods and nanowires are discussed in the book **Numerical methods for scientists and engineers** H. M. Antia,2012-11-15 This book presents an exhaustive and in depth exposition of the various numerical methods used in scientific and engineering computations It emphasises the practical aspects of numerical computation and discusses various techniques in sufficient detail to enable their implementation in solving a wide range of problems The main addition in the third edition is a new Chapter on Statistical Inferences There is also some addition and editing in the next chapter on Approximations With this addition 12 new programs have also been added **Maple in Mathematics Education and Research** Robert M. Corless,Jürgen Gerhard,Ilias S. Kotsireas,2021-07-19 This book constitutes refereed proceedings of the 4th Maple Conference MC 2020 held in Waterloo Ontario Canada in November 2020 The 25 revised full papers and 3 short papers were carefully reviewed and selected out of 75 submissions one invited paper is also presented in the volume The papers included in this book cover topics in education algorithms and applciations of the mathematical software Maple *The Inclusion-Based Boundary Element Method (iBEM)* Huiming Yin,Gan Song,Liangliang Zhang,Chunlin Wu,2022-04-14 The Inclusion Based Boundary Element Method iBEM is an innovative numerical method for the study of the multi physical and mechanical behaviour of composite materials linear elasticity potential flow or Stokes fluid dynamics It combines the basic ideas of Eshelby s Equivalent Inclusion Method EIM in classic micromechanics and the Boundary Element Method BEM in computational mechanics The book starts by explaining the application and extension of the EIM from elastic problems to the

Stokes fluid and potential flow problems for a multiphase material system in the infinite domain It also shows how switching the Green s function for infinite domain solutions to semi infinite domain solutions allows this method to solve semi infinite domain problems A thorough examination of particle particle interaction and particle boundary interaction exposes the limitation of the classic micromechanics based on Eshelby s solution for one particle embedded in the infinite domain and demonstrates the necessity to consider the particle interactions and boundary effects for a composite containing a fairly high volume fraction of the dispersed materials Starting by covering the fundamentals required to understand the method and going on to describe everything needed to apply it to a variety of practical contexts this book is the ideal guide to this innovative numerical method for students researchers and engineers The multidisciplinary approach used in this book drawing on computational methods as well as micromechanics helps to produce a computationally efficient solution to the multi inclusion problem The iBEM can serve as an efficient tool to conduct virtual experiments for composite materials with various geometry and boundary or loading conditions Includes case studies with detailed examples of numerical implementation   Reviews in Computational Chemistry, Volume 26 Kenny B. Lipkowitz,Thomas R. Cundari,Donald B. Boyd,2008-11-19 Computational chemistry is increasingly used in conjunction with organic inorganic medicinal biological physical and analytical chemistry biotechnology materials science and chemical physics This series is essential in keeping those individuals involved in these fields abreast of recent developments in computational chemistry   Polymer-based Nanocomposites for Energy and Environmental Applications Mohammad Jawaid,Mohammad Mansoob Khan,2018-01-03 Polymer Based Nanocomposites for Energy and Environmental Applications provides a comprehensive and updated review of major innovations in the field of polymer based nanocomposites for energy and environmental applications It covers properties and applications including the synthesis of polymer based nanocomposites from different sources and tactics on the efficacy and major challenges associated with successful scale up fabrication The chapters provide cutting edge up to date research findings on the use of polymer based nanocomposites in energy and environmental applications while also detailing how to achieve material s characteristics and significant enhancements in physical chemical mechanical and thermal properties It is an essential reference for future research in polymer based nanocomposites as topics such as sustainable recyclable and eco friendly methods for highly innovative and applied materials are current topics of importance Covers a wide range of research on polymer based nanocomposites Provides updates on the most relevant polymer based nanocomposites and their prodigious potential in the fields of energy and the environment Demonstrates systematic approaches and investigations from the design synthesis characterization and applications of polymer based nanocomposites Presents a useful reference and technical guide for university academics and postgraduate students Masters and Ph D

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