

M. Defranceschi C. Le Bris

Mathematical Models and Methods for Ab Initio Quantum Chemistry



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M. Defranceschi, C. Le Bris



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Alexander Komech, 2022-02-18 This book gives a concise introduction to Quantum Mechanics with a systematic coherent and in depth explanation of related mathematical methods from the scattering theory and the theory of Partial Differential Equations The book is aimed at graduate and advanced undergraduate students in mathematics physics and chemistry as well as at the readers specializing in quantum mechanics theoretical physics and quantum chemistry and applications to solid state physics optics superconductivity and quantum and high frequency electronic devices The book utilizes elementary mathematical derivations The presentation assumes only basic knowledge of the origin of Hamiltonian mechanics Maxwell equations calculus Ordinary Differential Equations and basic PDEs Key topics include the Schr dinger Pauli and Dirac equations the corresponding conservation laws spin the hydrogen spectrum and the Zeeman effect scattering of light and particles photoelectric effect electron diffraction and relations of quantum postulates with attractors of nonlinear Hamiltonian PDEs Featuring problem sets and accompanied by extensive contemporary and historical references this book could be used for the course on Quantum Mechanics and is also suitable for individual study

Quantum Control:

Mathematical and Numerical Challenges André D. Bandrauk, Michel C. Delfour, Claude Le Bris, 2003 It brought together mathematicians theoretical chemists and physicists working in the area of control and optimization of systems to address the outstanding numerical and mathematical problems

Essential Computational Modeling in Chemistry Philippe G.

Ciarlet, 2010-12-07 Essential Computational Modeling in Chemistry presents key contributions selected from the volume in the Handbook of Numerical Analysis Computational Modeling in Chemistry Vol 10 2005 Computational Modeling is an active field of scientific computing at the crossroads between Physics Chemistry Applied Mathematics and Computer Science Sophisticated mathematical models are increasingly complex and extensive computer simulations are on the rise Numerical Analysis and scientific software have emerged as essential steps for validating mathematical models and simulations based on these models This guide provides a quick reference of computational methods for use in understanding chemical reactions

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Computational Chemistry Philippe G. Ciarlet, Jacques-Louis Lions, 1990 Aiming to provide the reader with a general overview of the mathematical and numerical techniques used for the simulation of matter at the microscopic scale this book lays the emphasis on the numerics but modelling aspects are also addressed The contributors come from different scientific communities physics theoretical chemistry mathematical analysis stochastic analysis numerical analysis and the text should be suitable for graduate students in mathematics sciences and engineering and technology

Quantum Mechanics: Genesis and Achievements Alexander Komech, 2012-10-24 The focus of the present work is nonrelativistic and relativistic quantum mechanics with standard applications to the hydrogen atom The author has aimed at presenting quantum mechanics in a comprehensive yet accessible for mathematicians and other non physicists The genesis of quantum mechanics its applications to basic quantum phenomena and detailed explanations of the corresponding mathematical methods are presented The exposition is formalized whenever possible on the basis of the coupled Schroedinger Dirac and Maxwell equations Aimed at upper graduate and graduate students in mathematical and physical science studies

An Introduction to Mathematical Modeling J. Tinsley Oden, 2012-02-23 A modern approach to mathematical modeling featuring unique applications from the field of mechanics An Introduction to Mathematical Modeling A Course in Mechanics is designed to survey the mathematical models that form the foundations of modern science and incorporates examples that illustrate how the most successful models arise from basic principles in modern and classical mathematical physics Written by a world authority on mathematical theory and computational mechanics the book presents an account of continuum mechanics electromagnetic field theory quantum mechanics and statistical mechanics for readers with varied backgrounds in engineering computer science mathematics and physics The author streamlines a comprehensive understanding of the topic in three clearly organized sections Nonlinear Continuum Mechanics introduces kinematics as well as force and stress in deformable bodies mass and momentum balance of linear and angular momentum conservation of energy and constitutive equations Electromagnetic Field Theory and Quantum Mechanics contains a brief account of electromagnetic wave theory and Maxwell s equations as well as an introductory account of quantum mechanics with related topics including ab initio methods and Spin and Pauli s principles Statistical Mechanics presents an introduction to statistical mechanics of systems in thermodynamic equilibrium as well as continuum mechanics quantum mechanics and molecular dynamics Each part of the book concludes with exercise sets that allow readers to test their understanding of the presented material Key theorems and fundamental equations are highlighted throughout and an extensive bibliography outlines

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Exact Methods in Low-dimensional Statistical Physics and Quantum Computing Stephane Ouvry, Vincent Pasquier, Didina Serban, Leticia Cugliandolo, 2010-04-22 Low dimensional statistical models are instrumental in improving our understanding of emerging fields such as quantum computing and cryptography complex systems and quantum fluids This book of lectures by international leaders in the field sets these issues into a larger and more coherent theoretical perspective than is currently available

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Methods in Reaction Dynamics W. Jakubetz, 2012-12-06 Methods in Reaction Dynamics is a collection of lectures given at the 1999 Mariapfarr Workshop in Theoretical Chemistry Arranged as a series of detailed reviews it provides an overview of quantum mechanical techniques used to describe and simulate the dynamics and kinetics of elementary chemical reactions The volume provides in depth discussions of selected topics in Theoretical Chemistry such as quantum methods in theoretical and computational reaction dynamics and kinetics time dependent time independent and mixed quantum classical techniques Some of the topics have not been reviewed before in detail

Control of Coupled Partial Differential Equations Karl Kunisch, Günter Leugering, Jürgen Sprekels, Fredi Tröltzsch, 2007-08-08 The international Conference on Optimal Control of Coupled Systems of partial Differential Equations was held at the Mathematisches Forschungsinstitut Oberwolfach from April 17 to 23 2005 The applications discussed during the conference includes the optimization and control of quantum mechanical systems

Computational Optimization of Systems Governed by Partial

Differential Equations Alfio Borzi, Volker Schulz, 2012-01-26 This book provides a bridge between continuous optimization and PDE modelling and focuses on the numerical solution of the corresponding problems Intended for graduate students in PDE constrained optimization it is also suitable as an introduction for researchers in scientific computing or optimization

Nonlinear Optical and Atomic Systems Christophe Besse, Jean-Claude Garreau, 2015-08-26 Focusing on the interface between mathematics and physics this book offers an introduction to the physics the mathematics and the numerical simulation of nonlinear systems in optics and atomic physics The text covers a wide spectrum of current research on the subject which is an extremely active field in physics and mathematical physics with a very broad range of implications both for fundamental science and technological applications light propagation in microstructured optical fibers Bose Einstein condensates disordered systems and the newly emerging field of nonlinear quantum mechanics Accessible to PhD students this book will also be of interest to post doctoral researchers and seasoned academics

Numerical Homogenization by Localized Decomposition Axel Målqvist, Daniel Peterseim, 2020-11-23 This book presents the first survey of the Localized Orthogonal Decomposition LOD method a pioneering approach for the numerical homogenization of partial differential equations with multiscale data beyond periodicity and scale separation The authors provide a careful error analysis including previously unpublished results and a complete implementation of the method in MATLAB They also reveal how the LOD method relates to classical homogenization and domain decomposition Illustrated with numerical experiments that demonstrate the significance of the method the book is enhanced by a survey of applications including eigenvalue problems and evolution problems Numerical Homogenization by Localized Orthogonal Decomposition is appropriate for graduate students in applied mathematics numerical analysis and scientific computing Researchers in the field of computational partial differential equations will find this self contained book of interest as will applied scientists and engineers interested in multiscale simulation

Reaction and Molecular Dynamics A. Lagana, A. Riganelli, 2000-11-27 The amazing growth of computational resources has made possible the modeling of complex chemical processes To develop these models one needs to proceed from rigorous theoretical methods to approximate ones by exploiting the potential of innovative architectural features of modern concurrent processors This book reviews some of the most advanced theoretical approaches in the field of molecular reaction dynamics in order to cope as rigorously as possible with the complexity of real systems

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