M. Defranceschi   C. Le Bris

Mathematical Models and Methods for Ab Initio Quantum Chemistry

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Christophe Besse,Jean-Claude Garreau

Mathematical Models And Methods For Ab Initio Quantum Chemistry:

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    Lectures On Quantum Mechanics And Attractors 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with attractors of nonlinear Hamiltonian PDEs Featuring problem sets and accompanied by extensive contemporary and historical references this book could be used for the course on Quantum Mechanics and is also suitable for individual study   An Introduction to Mathematical Modeling J. Tinsley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

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Tröltzsch,2007-08-08 The international Conference on Optimal Control of Coupled Systems of partial Differential Equations was held at the Mathematisches Forschungs institut Oberwolfach from April 17 to 23 2005 The applications discussed during the conference includes the optimization and control of quantum mechanical systems   Control and Nonlinearity Jean-Michel Coron,2007 This book presents methods to study the controllability and the stabilization of nonlinear control systems in finite and infinite dimensions The emphasis is put on specific phenomena due to nonlinearities In particular many examples are given where nonlinearities turn out to be essential to get controllability or stabilization Various methods are presented to study the controllability or to construct stabilizing feedback laws The power of these methods is illustrated by numerous examples coming from such areas as celestial mechanics fluid mechanics and quantum mechanics The book is addressed to graduate students in mathematics or control theory and to mathematicians or engineers with an interest in nonlinear control systems governed by ordinary or partial differential equations   **Relativistic Theory of Atoms and Molecules III** Pekka Pyykkö,2013-06-29 Relativistic effects are of major importance for understanding the properties of heavier atoms and molecules Volumes I III of Relativistic Theory of Atoms and Molecules constitute the only available bibliography on related calculations In Volume III 3792 new references covering 1993 1999 are added to the database The material is characterized by an analysis of the respective papers The volume gives the user a comprehensive bibliography on relativistic atomic and molecular calculations including studies on the Dirac equation and related solid state work

   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   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

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