

PROGRESS IN THEORETICAL CHEMISTRY AND PHYSICS

Numerical Quantum Dynamics

Wolfgang Schweizer

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Numerical Quantum Dynamics

Fabio Bagarello



Numerical Quantum Dynamics:

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Quantum Dynamics for Classical Systems Fabio Bagarello, 2012-11-05 Introduces number operators with a focus on the relationship between quantum mechanics and social science Mathematics is increasingly applied to classical problems in finance biology economics and elsewhere Quantum Dynamics for Classical Systems describes how quantum tools the number operator in particular can be used to create dynamical systems in which the variables are operator valued functions and whose results explain the presented model The book presents mathematical results and their applications to concrete systems and discusses the methods used results obtained and techniques developed for the proofs of the results The central ideas of number operators are illuminated while avoiding excessive technicalities that are unnecessary for understanding and learning the various mathematical applications The presented dynamical systems address a variety of contexts and offer clear analyses and explanations of concluded results Additional features in Quantum Dynamics for Classical Systems include Applications across diverse fields including stock markets and population migration as well as a unique quantum perspective on these classes of models Illustrations of the use of creation and annihilation operators for classical problems Examples of the recent increase in research and literature on the many applications of quantum tools in applied mathematics Clarification on numerous misunderstandings and misnomers while shedding light on new approaches in the field Quantum Dynamics for Classical Systems is an ideal reference for researchers professionals and academics in applied mathematics economics physics biology and sociology The book is also excellent for courses in dynamical systems quantum mechanics and mathematical models

Numerical Quantum Dynamics, 2013

Computational Strong-Field Quantum Dynamics Dieter

Bauer, 2017-04-24 This graduate textbook introduces the computational techniques to study ultra fast quantum dynamics of matter exposed to strong laser fields Coverage includes methods to propagate wavefunctions according to the time dependent Schrödinger Klein Gordon or Dirac equation the calculation of typical observables time dependent density functional theory multi configurational time dependent Hartree Fock time dependent configuration interaction singles the strong field approximation and the microscopic particle in cell approach Contents How to propagate a wavefunction Calculation of typical strong field observables Time dependent relativistic wave equations Numerics of the Dirac and the Klein Gordon equation Time dependent density functional theory The multiconfiguration time dependent Hartree Fock method Time dependent configuration interaction singles Strong field approximation and quantum orbits Microscopic particle in cell approach

Numerical Methods for Complex Quantum Dynamics with Applications to Quantum Biology and Quantum Many-body Dynamics Robert Rosenbach, 2015

[Quantum Dynamic Imaging](#) Andre D

Bandrauk, Misha Ivanov, 2011-07-12 Studying and using light or photons to image and then to control and transmit molecular information is among the most challenging and significant research fields to emerge in recent years. One of the fastest growing areas involves research in the temporal imaging of quantum phenomena ranging from molecular dynamics in the femto to 10¹⁵s time regime for atomic motion to the atto to 10¹⁸s time scale of electron motion. In fact, the attosecond revolution is now recognized as one of the most important recent breakthroughs and innovations in the science of the 21st century. A major participant in the development of ultrafast femto and attosecond temporal imaging of molecular quantum phenomena has been theory and numerical simulation of the nonlinear non-perturbative response of atoms and molecules to ultrashort laser pulses. Therefore, imaging quantum dynamics is a new frontier of science requiring advanced mathematical approaches for analyzing and solving spatial and temporal multidimensional partial differential equations such as Time Dependent Schrödinger Equations (TDSE) and Time Dependent Dirac equations (TDDEs) for relativistic phenomena. These equations are also coupled to the photons in Maxwell's equations for collective propagation effects. Inversion of the experimental imaging data of quantum dynamics presents new mathematical challenges in the imaging of quantum wave coherences on subatomic, subnanometer spatial dimensions and multiple timescales from atto to femto and even nanoseconds. In Quantum Dynamic Imaging: Theoretical and Numerical Methods, leading researchers discuss these exciting state-of-the-art developments and their implications for R & D in view of the promise of quantum dynamic imaging science as the essential tool for controlling matter at the molecular level. Third International Conference on Mathematical and Numerical Aspects of Wave

Propagation Gary C. Cohen, 1995-01-01 This volume contains the papers presented at the title conference. Speakers from 13 different countries were represented at the meeting. A broad range of topics in theoretical and applied wave propagation is covered. Numerical Methods in Electromagnetics W.H.A. SCHILDERS, E.J.W. TER MATEN, 2005-04-04 This special volume provides a broad overview and insight in the way numerical methods are being used to solve the wide variety of problems in the electronics industry. Furthermore, its aim is to give researchers from other fields of application the opportunity to benefit from the results which have been obtained in the electronics industry. Complete survey of numerical methods used in the electronic industry. Each chapter is self-contained. Presents state-of-the-art applications and methods. Internationally recognised authors. **Numerical Grid Methods and Their Application to Schrödinger's Equation** C.

Cerjan, 1993-07-31 This book offers a unique perspective on the rapidly growing field of numerical grid methods applied to the solution of the Schrödinger equation. Several articles provide comprehensive reviews of the discrete variable and pseudo-spectral operator representation. The applications include sophisticated refinements of the basic approaches with emphasis on successful parallel implementation. The range of problems considered is broad, including reactive scattering, photoexcitation processes, mixed quantum-classical methodology and density functional electronic structure calculations. The book thus serves as a direct introduction to numerical grid methods and as a guide to future research. Numerical

Methods for Hyperbolic and Kinetic Problems Stéphane Cordier, 2005 Hyperbolic and kinetic equations arise in a large variety of industrial problems For this reason the Summer Mathematical Research Center on Scientific Computing and its Applications CEMRACS held at the Center of International Research in Mathematics CIRM in Luminy was devoted to this topic During a six week period junior and senior researchers worked full time on several projects proposed by industry and academia Most of this work was completed later on and the present book reflects these results The articles address modelling issues as well as the development and comparisons of numerical methods in different situations The applications include multi phase flows plasma physics quantum particle dynamics radiative transfer sprays and aeroacoustics The text is aimed at researchers and engineers interested in applications arising from modelling and numerical simulation of hyperbolic and kinetic problems

Physics of Clusters Viktor D. Lakhno, Gennady N. Chuev, 1998 The monograph is devoted to the relatively new and fast developing field of cluster physics It is based on talks given at the Cluster Workshops which were held in Pushchino in 1995 and 1996 The reports focus not only on the fundamental physical properties of clusters such as their geometric and electronic structure as well as optical thermal and magnetic properties but also on a broad spectrum of their potential applications These include nucleation and growth of small particles fabrication of new materials with predefined properties cluster assembled and nanostructures Some aspects of simulations and calculations of small particles and clusters are also discussed We hope that our monograph will be of interest to a broad range of readers who will be able to sense the excitement of the talks

Computational Methods in Photochemistry Andrei G. Kutateladze, 2005-05-05 Addressing critical aspects of computational modeling in photochemistry Molecular Methods in Photochemistry is designed to familiarize researchers and practitioners with state of the art computational methods to predict the reactivity of excited molecules It provides practical guidelines and examples for the modeling of excited states and describes

Quantum Dynamics of Simple Systems G.L Oppo, Stephen M. Barnett, E Riis, M Wilkinson, 1997-01-01 The present level of experimental sophistication in quantum physics allows physicists to explore domains unimaginable just a decade ago and to test the most fundamental laws of quantum mechanics This has led to renewed interest in devising new tests experiments and devices where it is possible to observe the interaction and localization of just a few atoms or photons These techniques have been used to reveal new nonclassical effects to question the limit of the principle of correspondence and to force quantum behavior in semiconductors With contributions from leading experts in quantum systems Quantum Dynamics of Simple Systems provides an overview of the present range of quantum dynamics exploring their use and exotic behaviors It covers specific subjects of quantum dynamics in a competent and detailed way with emphasis on simple systems where few atoms or electrons are involved This volume will prove to be a useful tool for graduate students as well as experienced physicists

Applied Linear Algebra Kartikeya Dutta, 2025-02-20 Applied Linear Algebra Core Principles is a comprehensive guide that delves into the principles methodologies and practical applications of linear algebra in various fields of science engineering

and technology Combining theoretical foundations computational techniques and real world examples this book offers a holistic approach to understanding and utilizing linear algebra concepts Covering a wide range of topics including vector spaces matrices eigenvalue problems singular value decomposition and numerical techniques readers will gain a thorough understanding of both fundamental and advanced principles Real world applications in data science machine learning signal processing control systems and image processing are integrated throughout demonstrating the practical relevance of linear algebra Complex mathematical concepts are presented in a clear and accessible manner making the book suitable for students researchers and practitioners with varying levels of mathematical background Detailed explanations illustrative examples and step by step solutions aid comprehension and retention An interdisciplinary approach connects theoretical concepts with practical applications highlighting the versatility of linear algebra in solving real world problems Extensive references to literature research papers and online resources enable readers to explore topics in greater depth This book is an invaluable resource for students researchers and professionals seeking to apply linear algebra techniques in their work across various domains

Photochemistry Stefano Crespi, Stefano Protti, 2024-12-18 Reviewing photo induced processes that have relevance to a wide number of academic and commercial disciplines this volume reflects the current interests in chemistry physics biology and technology Section one covers organic and computational aspects of photochemistry while Section two highlights topics like photomagnetism in organic dyes in silico photochemistry and delayed fluorescence in photosynthetic systems The final section covers the SPR lectures on photochemistry on photoredox catalysis in synthesis perfluoroalkylation of aliphatic substrates via photoinduced radical processes and photocycloadditions of aromatic compounds with alkenes The volume continues to provide essential reading for postgraduates academics and industrialists working in the field of photochemistry enabling them to keep on top of the literature

Numerical Methods for Non-Newtonian Fluids, 2010-12-20 Non Newtonian flows and their numerical simulations have generated an abundant literature as well as many publications and references to which can be found in this volume s articles This abundance of publications can be explained by the fact that non Newtonian fluids occur in many real life situations the food industry oil gas industry chemical civil and mechanical engineering the bio Sciences to name just a few Mathematical and numerical analysis of non Newtonian fluid flow models provide challenging problems to partial differential equations specialists and applied computational mathematicians alike This volume offers investigations Results and conclusions that will no doubt be useful to engineers and computational and applied mathematicians who are focused on various aspects of non Newtonian Fluid Mechanics New review of well known computational methods for the simulation viscoelastic and viscoplastic types Discusses new numerical methods that have proven to be more efficient and more accurate than traditional methods Articles that discuss the numerical simulation of particulate flow for viscoelastic fluids

Quantum Dynamics of Anharmonic Oscillators by Numerical Integration Young Rang Lee Park, 1970 Theoretical Femtosecond Physics Frank

Grossmann, 2008-07-24 This volume offers theoretical investigations of atoms and molecules interacting with pulsed or continuous wave lasers. Theoretical background is included and the text incorporates several exercises. Additional calculations are performed in the appendices.

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