

PROGRESS IN THEORETICAL CHEMISTRY AND PHYSICS

Numerical Quantum Dynamics

Wolfgang Schweizer

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Fabio Bagarello



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Numerical Quantum Dynamics W. Schweizer, 2014-03-14

From Quantum to Classical Molecular Dynamics

Christian Lubich, 2008 Quantum dynamics of molecules poses a variety of computational challenges that are presently at the forefront of research efforts in numerical analysis in a number of application areas high dimensional partial differential equations multiple scales highly oscillatory solutions and geometric structures such as symplecticity and reversibility that are favourably preserved in discretizations This text addresses such problems in quantum mechanics from the viewpoint of numerical analysis illustrating them to a large extent on intermediate models between the Schrodinger equation of full many body quantum dynamics and the Newtonian equations of classical molecular dynamics The fruitful interplay between quantum dynamics and numerical analysis is emphasized

Numerical Quantum Dynamics W. Schweizer, 2005-12-27

It is an indisputable fact that computational physics form part of the essential landscape of physical science and physical education When writing such a book one is faced with numerous decisions e g Which topics should be included What should be assumed about the readers prior knowledge How should balance be achieved between numerical theory and physical application This book is not elementary The reader should have a background in quantum physics and computing On the other way the topics discussed are not addressed to the specialist This work bridges hopefully the gap between vanced students graduates and researchers looking for computational ideas beyond their fence and the specialist working on a special topic Many important topics and applications are not considered in this book The selection is of course a personal one and by no way exhaustive and the material presented obviously reflects my own interest What is Computational Physics During the past two decades computational physics became the third fundamental physical discipline Like the traditional partners experimental physics and theoretical physics computational physics is not restricted to a special area e g atomic physics or solid state physics Computational physics is a methodical ansatz useful in all subareas and not necessarily restricted to physics Of course this methods are related to computational aspects which means numerical and algebraic methods but also the interpretation and visualization of huge amounts of data

Quantum Dynamics for Classical Systems Fabio Bagarello, 2012-10-11

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 10⁻¹⁵s time regime for atomic motion to the atto 10⁻¹⁸s 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 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 *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 *Quantum Dynamics of Anharmonic Oscillators by Numerical Integration* Young Rang Lee Park,1970 Nuclear Science Abstracts ,1976

Theoretical Chemistry Accounts Christopher Cramer,D.G. Truhlar,2013-11-11 For the New Century Issue of the journal Theoretical Chemistry Accounts the advisory editors identified papers from the first century of theoretical chemistry and discussed their importance for the twentieth century with an eye towards the twenty first century Sixty six such perspectives are published in the New Century Issue To make this unique collection available to younger scientists for entertaining reading and re reading of the original publications the publisher decided to reprint a special edition of the issue

Electron Dynamics In Molecular Interactions: Principles And Applications Frank Hagelberg,2013-12-23 This volume provides a comprehensive introduction to the theory of electronic motion in molecular processes an increasingly relevant and rapidly expanding segment of molecular quantum dynamics Emphasis is placed on describing and interpreting transitions between electronic states in molecules as they occur typically in cases of reactive scattering between molecules photoexcitation or nonadiabatic coupling between electronic and nuclear degrees of freedom Electron Dynamics in Molecular Interactions aims at a synoptic presentation of some very recent theoretical efforts to solve the electronic problem in quantum molecular dynamics contrasting them with more traditional schemes The presented models are derived from their roots in basic quantum theory their interrelations are discussed and their characteristic applications to concrete chemical systems are outlined This volume also includes an assessment of the present status of electron dynamics and a report on novel developments to meet the current challenges in the field Further this monograph responds to a need for a systematic comparative treatise on nonadiabatic theories of quantum molecular dynamics which are of considerably higher complexity than the more traditional adiabatic approaches and are steadily gaining in importance This volume addresses a broad

readership ranging from physics or chemistry graduate students to specialists in the field of theoretical quantum dynamics

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.

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.

Numerical Simulations of Molecular Quantum Dynamics Reza Rajaie Khorasani, 2009

Advanced Partial Differential Equations Sameer Kulkarni, 2025-02-28 Embark on an in-depth exploration of partial differential equations (PDEs) with *Advanced Partial Differential Equations*. Our comprehensive guide provides a thorough overview of the theory, numerical methods, and practical applications of PDEs across various scientific and engineering fields. This resource is designed for both graduate-level students and professionals seeking to deepen their understanding of PDEs.

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Physics Of Clusters Gennady N Chuev,V D Lakhno,1998-08-25 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

Advances in Chemical Physics, Volume 163 K. Birgitta Whaley,2018-05-08 The Advances in Chemical Physics series provides the chemical physics field with a forum for critical authoritative evaluations of advances in every area of the discipline This is the only series of volumes available that presents the cutting edge of research in chemical physics Includes 10 contributions from leading experts in this field of research Contains a representative cross section of research in chemical reaction dynamics and state of the art quantum description of intramolecular and intermolecular dynamics Structured with an editorial framework that makes the book an excellent supplement to an advanced graduate class in physical chemistry chemical physics or molecular physics

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