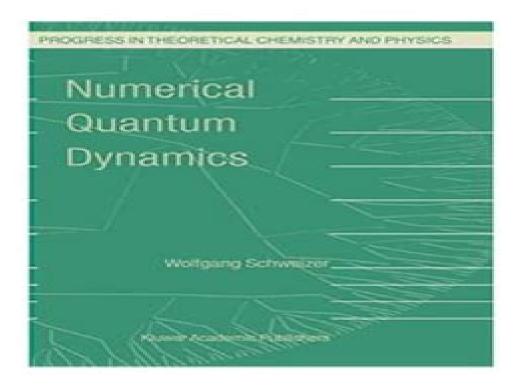
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Bandrauk, Misha Ivanov, 2011-07-12 Studying and using light or photons to image and then to control and transmit molecular information is among the most challenging and significant research fields to emerge in recent years One of the fastest growing 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 Schroedinger 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 Quantum Dynamics of Anharmonic Oscillators by Numerical Integration Young Rang Lee matter at the molecular level Quantum Dynamics of Simple Systems G.L Oppo, Stephen M. Barnett, E. Riis, M. Wilkinson, 1997-01-01 The Park.1970 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 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 Schroedinger 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

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Phillip L. Casamento, 2016
Numerical Simulations of Molecular Quantum Dynamics Reza Rajaie Khorasani, 2009

Elements of Photoionization Quantum Dynamics Methods Lampros A A Nikolopoulos, 2019-03-29 The dynamics of quantum systems exposed to ultrafast at the femtosecond time scale and strong laser radiation has a highly non linear character leading to a number of new phenomena outside the reach of traditional spectroscopy The current laser technology makes feasible the probing and control of quantum scale systems with fields that are as strong as the interatomic Coulombic interactions and time resolution that is equal to or less than typical atomic evolution times It is indispensable that any theoretical description of the induced physical processes should rely on the accurate calculation of the atomic structure and a realistic model of the laser radiation as pulsed fields This book aims to provide an elementary introduction of theoretical and computational methods and by no means is anywhere near to complete The selection of the topics as well as the particular viewpoint is best suited for early stage students and researchers the included material belongs in the mainstream of theoretical approaches albeit using simpler language without sacrificing mathematical accuracy Therefore subjects such as the Hilbert vector state density matrix operators amplitude equations Liouville equation coherent laser radiation free electron laser Dyson chronological operator subspace projection perturbation theory stochastic density matrix equations time dependent Schr dinger equation partial wave analysis spherical harmonics expansions basis and grid wavefunction expansions ionization electron kinetic energy and angular distributions are presented within the context of laser atom quantum dynamics Numerical Analysis and Computational Methods for Non-adiabatic Quantum Dynamics and Biological Models Di Fang, 2019 Focused on the numerical analysis and computational methods this dissertation consists of two independent parts quantum dynamics Part I and biological models Part II Non adiabatic phenomena are ubiquitous in

quantum systems where the excited states come into the play and hence the commonly applied Born Oppenheimer approximation is no longer valid In this dissertation efficient algorithms are proposed a for the quantum classical mixed Ehrenfest dynamics and b in diabatic representations respectively The former provides an efficient algorithm for mean field dynamics that has the form of a nonlinear Schr odinger system in low dimension while the latter proposes an embarrassingly parallel algorithm compatible for high dimensional problems near the transition zone which even works when adiabatic coupling terms appearing in traditional methods are not defined Here both multiscale and stochastic techniques are used Part II of this thesis discusses the two biological phenomena the formation adaptation and bifurcation of biological transport networks such as leaf venations and blood vessels and the subdiffusion observed in bio molecular systems and their corresponding models described by either nonlinear partial differential equations or stochastic differential equations To understand the model behaviors and predict phenomena numerical simulations are desired Unfortunately the computations are expensive for both cases due to the nonlinearity of the former and memory effects in the latter In this part we propose efficient algorithms for both models and provide numerical analysis to our schemes to illustrate the accuracy and efficiency Third International Conference on Mathematical and Numerical Aspects of Wave Propagation Gary C. of the methods 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 wich have been obtained in the electronics industry Complete survey of numerical methods used in the electronic industry Each chapter is selfcontained Presents state of the art applications and methods Internationally Numerical Grid Methods and Their Application to Schrödinger's Equation C. Cerjan, 1993-07-31 This recognised authors book offers a unique perspective on the rapidly growing field of numerical grid methods applied to the solution of the Schr dinger 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.

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