

PROGRESS IN THEORETICAL CHEMISTRY AND PHYSICS

Numerical Quantum Dynamics

Wolfgang Schweizer

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Numerical Quantum Dynamics

W. Schweizer



Numerical Quantum Dynamics:

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, 2001-12-31 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 **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 meth ical ansatz useful in all subareas and not necessarily restricted to physics Of course this methods are related to computational aspects which means nume cal and algebraic methods but also the interpretation and visualization of huge amounts of data

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Numerical Quantum Dynamics ,2013 **Computational Strong-Field Quantum Dynamics** Dieter Bauer,2017-04-24 This graduate textbook introduces the com putational 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 Schr dinger 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.

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. **Applied**

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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

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Numerical Integration Young Rang Lee Park, 1970 *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 We cover a wide range of topics from classical PDEs and numerical methods to applications in physics engineering biology and finance Additionally we delve into advanced topics such as nonlinear equations and stochastic processes presenting each subject with rigorous mathematical treatment and clear explanations Our guide includes detailed discussions on numerical techniques for solving PDEs featuring finite difference finite element spectral and boundary integral methods Real world examples and case studies illustrate the

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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

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

Quantum Dynamics with Trajectories Robert E. Wyatt, 2005-05-20 This is a rapidly developing field to which the author is a leading contributor New methods in quantum dynamics and computational techniques with applications to interesting physical problems are brought together in this book Useful to both students and researchers

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

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