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Semiclassical Mechanics with Molecular Applications

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Semiclassical Mechanics With Molecular Applications

Xueming Yang, Kopin Liu



Semiclassical Mechanics With Molecular Applications:

Semiclassical Mechanics with Molecular Applications M. S. Child, 2014-08-21 The second edition of an established graduate text this book complements the material for a typical advanced graduate course in quantum mechanics by showing how the underlying classical structure is reflected in quantum mechanical interference and tunnelling phenomena and in the energy and angular momentum distributions of quantum mechanical states in the moderate to large 10 100 quantum number regime Applications include accurate quantization techniques for a variety of tunnelling and curve crossing problems and of non separable bound systems direct inversion of molecular scattering and spectroscopic data wavepacket propagation techniques and the prediction and interpretation of elastic inelastic and chemically reactive scattering The main text concentrates less on the mathematical foundations than on the global influence of the classical phase space structures on the quantum mechanical observables Further mathematical detail is contained in the appendices and worked problem sets are included as an aid to the student

Semiclassical Mechanics with Molecular Applications Mark Sheard Child, 2023 Relates Newton s classical theory to modern quantum mechanics in a manner designed for the interpretation of experiments This book gives a comprehensive account of the application of the theory to molecular systems with particular attention paid to the problems of non separability

Theory and Application of Quantum Molecular Dynamics John Z. H. Zhang, 1999 This book gives an updated and detailed presentation of modern quantum mechanical treatments and practical computational methods for dynamical processes of small molecular systems The main emphasis is on the recent development of successful theories and computational methods for the reactive scattering process Specific applications are given in detail for a number of benchmark chemical reaction systems in the gas phase and gas surface Differing from traditional physics books focusing on abstract collision theory for elastic collisions the book has been written in a fashion in which the development of general reactive or rearrangement scattering theory is accompanied by practical applications for realistic reaction systems

Introduction to Quantum Mechanics David Tannor, 2008-02-01 Introduction to Quantum Mechanics is a completely original manifesto covering quantum mechanics from a time dependent perspective in a unified way from beginning to end This text will change the way people think about and teach about quantum mechanics in chemistry and physics departments This brilliant new text a completely original manifesto covers quantum mechanics from a time dependent perspective in a unified way from beginning to end Intended for upper level undergraduate and graduate courses in quantum mechanics this text will change the way people think about and teach about quantum mechanics in chemistry and physics departments

Nonlinear Hamiltonian Mechanics Applied to Molecular Dynamics Stavros C. Farantos, 2014-09-22 This brief presents numerical methods for describing and calculating invariant phase space structures as well as solving the classical and quantum equations of motion for polyatomic molecules Examples covered include simple model systems to realistic cases of molecules spectroscopically studied Vibrationally excited and reacting molecules are nonlinear dynamical

systems and thus nonlinear mechanics is the proper theory to elucidate molecular dynamics by investigating invariant structures in phase space Intramolecular energy transfer and the breaking and forming of a chemical bond have now found a rigorous explanation by studying phase space structures

Unimolecular Reaction Dynamics Tomas Baer, William L. Hase, 1996-06-27 This book provides a penetrating and comprehensive description of energy selected reactions from a theoretical as well as experimental view Three major aspects of unimolecular reactions involving the preparation of the reactants in selected energy states the rate of dissociation of the activated molecule and the partitioning of the excess energy among the final products are fully discussed with the aid of 175 illustrations and over 1 000 references most from the recent literature Examples of both neutral and ionic reactions are presented Many of the difficult topics are discussed at several levels of sophistication to allow access by novices as well as experts Among the topics covered for the first time in monograph form is a discussion of highly excited vibrational rotational states and intramolecular vibrational energy redistribution Problems associated with the application of RRKM theory are discussed with the aid of experimental examples Detailed comparisons are also made between different statistical models of unimolecular decomposition Both quantum and classical models not based on statistical assumptions are described Finally a chapter devoted to the theory of product energy distribution includes the application of phase space theory to the dissociation of small and large clusters The work will be welcomed as a valuable resource by practicing researchers and graduate students in physical chemistry and those involved in the study of chemical reaction dynamics

Theory of Chemical Reaction Dynamics Antonio Laganà, 2005

The Role of Degenerate States in Chemistry, Volume 124 Michael Baer, Gert Due Billing, 2003-03-31 Edited by Nobel Prize winner Ilya Prigogine and renowned authority Stuart A Rice the Advances in Chemical Physics series provides a forum for critical authoritative evaluations in every area of the discipline In a format that encourages the expression of individual points of view experts in the field present comprehensive analyses of subjects of interest This stand alone special topics volume edited by Gert D Billing of the University of Copenhagen and Michael Baer of the Soreq Nuclear Research Center in Yavne Israel reports recent advances on the role of degenerate states in chemistry Volume 124 collects innovative papers on Complex States of Simple Molecular Systems Electron Nuclear Dynamics Conical Intersections and the Spin Orbit Interaction and many more related topics Advances in Chemical Physics remains the premier venue for presentations of new findings in its field

Modern Trends in Chemical Reaction Dynamics Xueming Yang, Kopin Liu, 2004 The field of chemical reaction dynamics has made huge progress during the last decade or so The aim of these volumes is to provide graduate students and experts in the field with a picture of the current status of advanced experimental and theoretical research in chemical reaction dynamics

Modern Methods for Multidimensional Dynamics Computations in Chemistry Donald Leo Thompson, 1998 This volume describes many of the key practical theoretical techniques that have been developed to treat chemical dynamics problems in many atom systems It contains thorough treatments of fundamental theory and prescriptions

for performing computations The selection of methods ranging from gas phase bimolecular reactions to complex processes in condensed phases reflects the breadth of the field The book is an excellent reference for proven and accepted methods as well as for theoretical approaches that are still being developed It is appropriate for graduate students and other novices who wish to begin working in chemical dynamics as well as active researchers who wish to acquire a wider knowledge of the field

Vibronic Interactions: Jahn-Teller Effect in Crystals and Molecules Michael D. Kaplan, George O. Zimmerman, 2012-12-06 This book is based mostly on the reports presented at the XVth International Jahn Teller Symposium on Vibronic Interactions in Crystals and Molecules and NATO Advanced Research Workshop Colossal Magnetoresistance and Vibronic Interactions that took place at Boston on August 16-22 of the year 2000 This is the first time the Symposium took place in the USA where recently the giant splash of the attention to the Jahn Teller effect occurred This tremendous interest to the field all over the world is reflected not only in the numerous publications in many American and European journals but of the leading scientists from additionally in the Symposium's participation the well known Universities National Laboratories and industrial companies which was the largest in the history of the Symposium The renaissance of the Jahn Teller physics is closely related to the three fundamental discoveries in science The most significant among them is the discovery of high T_c superconductivity by K A Muller and G Bednorz for whom the Jahn Teller idea was the motivation in their search The result of this search is well known a wide spectrum of the Jahn Teller ion based materials with T_c between 24K and 135K were found The second discovery is the existence of a new polymorph of carbon the C60 The microscopic analysis of all physical chemical and biological properties of the buckyballs is based on Jahn Teller type of interactions The third is colossal magnetoresistance

Molecular Quantum Mechanics Peter W. Atkins, Ronald S. Friedman, 2011 This text unravels those fundamental physical principles which explain how all matter behaves It takes us from the foundations of quantum mechanics through quantum models of atomic molecular and electronic structure and on to discussions of spectroscopy and the electronic and magnetic properties of molecules

Theory of Molecular Collisions Gabriel G Balint-Kurti, Alexander Palov, 2015-07-02 Almost 100 years have passed since Trautz and Lewis put forward their collision theory of molecular processes Today knowledge of molecular collisions forms a key part of predicting and understanding chemical reactions This book begins by setting out the classical and quantum theories of atom atom collisions Experimentally observable aspects of the scattering processes their relationship to reaction rate constants and the experimental methods used to determine them are described The quantum mechanical theory of reactive scattering is presented and related to experimental observables The role of lasers in the measurement and analysis of reactive molecular collisions is also discussed Written with postgraduates and newcomers to the field in mind mathematics is kept to a minimum and readers are guided to appendices and further reading to gain a deeper understanding of the mathematics involved

Advances in Chemical Physics, Volume 138 Stuart A. Rice, 2008-04-30 This series provides the chemical physics field with a forum for critical authoritative

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