

Semiclassical Methods in Molecular Scattering and Spectroscopy

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Semiclabical Methods In Molecular Scattering And Spectroscopy

Reinhard Schinke



Semiclabical Methods In Molecular Scattering And Spectroscopy:

Semiclassical Methods in Molecular Scattering and Spectroscopy M S Child,1980-02-29 *Semiclassical Methods in Molecular Scattering and Spectroscopy* M.S. Child,2012-12-06 Proceedings of the NATO Advanced Study Institute Cambridge England September 1979 *Semiclassical methods in molecular scattering and spectroscopy* Nato Advanced Study Institute,1980 *Semiclassical Methods in Molecular Scattering and Spectroscopy* M. S. Child,1980

Photodissociation Dynamics Reinhard Schinke,1995-05-11 Photodissociation induced by the absorption of single photons permits the detailed study of molecular dynamics such as the breaking of bonds internal energy transfer and radiationless transitions The availability of powerful lasers operating over a wide frequency range has stimulated rapid development of new experimental techniques which make it possible to analyse photodissociation processes in unprecedented detail This text elucidates the achievements in calculating photodissociation cross sections and fragment state distributions from first principles starting from multi dimensional potential energy surfaces and the Schr dinger equation of nuclear motion Following an extended introduction in which the various types of observables are outlined the book summarises the basic theoretical tools namely the time independent and the time dependent quantum mechanical approaches as well as the classical picture of photodissociation The discussions of absorption spectra diffuse vibrational structures the vibrational and rotational state distributions of the photofragments form the core of the book More specific topics such as the dissociation of vibrationally excited molecules emission during dissociation or nonadiabatic effects are also discussed It will be of interest to graduate students and senior scientists working in molecular physics spectroscopy molecular collisions and molecular kinetics

Equilibrium Molecular Structures Jean Demaison,James E. Boggs,Attila G. Csaszar,2016-04-19 Molecular structure is the most basic information about a substance determining most of its properties Determination of accurate structures is hampered in that every method applies its own definition of structure and thus results from different sources can yield significantly different results Sophisticated protocols exist to account for these

AFOSR Chemical & Atmospheric Sciences Program Review United States. Air Force. Directorate of Chemical and Atmospheric Sciences,

Airy Functions And Applications To Physics (2nd Edition) Olivier Vallee,Manuel Soares,2010-06-17 Addressed mainly to physicist and chemical physicist this textbook is the result of a broad compilation of current knowledge on analytical properties of Airy functions In particular the calculus implying the Airy functions is developed with care In the latter chapters examples are given to succinctly illustrate the use of Airy functions in classical and quantum physics The physicist for instance in fluid mechanics can find what he is looking for in the references for works of molecular physics or in physics of surfaces and vice versa The knowledge on Airy functions is frequently reviewed The reason may be found in the need to express a physical phenomenon in terms of an effective and comprehensive analytical form for the whole scientific community a

The Theory of Chemical Reaction Dynamics D.C. Clary,2012-12-06 The calculation of cross sections and rate

constants for chemical reactions in the gas phase has long been a major problem in theoretical chemistry. The need for reliable and applicable theories in this field is evident when one considers the significant recent advances that have been made in developing experimental techniques such as lasers and molecular beams to probe the microscopic details of chemical reactions. For example, it is now becoming possible to measure cross sections for chemical reactions state selected in the vibrational rotational states of both reactants and products. Furthermore, in areas such as atmospheric combustion and interstellar chemistry, there is an urgent need for reliable reaction rate constant data over a range of temperatures, and this information is often difficult to obtain in experiments. The classical trajectory method can be applied routinely to simple reactions, but this approach neglects important quantum mechanical effects such as tunnelling and resonances. For all these reasons, the quantum theory of reactive scattering is an area that has received considerable attention recently. This book describes the proceedings of a NATO Advanced Research Workshop held at CECAM Orsay, France, in June 1985. The Workshop concentrated on a critical examination and discussion of the recent developments in the theory of chemical reaction dynamics, with particular emphasis on quantum theories. Several papers focus on exact theories for reactions.

Physical Problems Solved by the Phase-Integral Method Nanny Fröman, Per Olof Fröman, 2002-06-13. This book provides a thorough introduction to one of the most efficient approximation methods for the analysis and solution of problems in theoretical physics and applied mathematics. It is written with practical needs in mind and contains a discussion of 50 problems with solutions of varying degrees of difficulty. The problems are taken from quantum mechanics, but the method has important applications in any field of science involving second order ordinary differential equations. The power of the asymptotic solution of second order differential equations is demonstrated, and in each case the authors clearly indicate which concepts and results of the general theory are needed to solve a particular problem. This book will be ideal as a manual for users of the phase integral method, as well as a valuable reference text for experienced research workers and graduate students.

Spectroscopic Properties of Inorganic and Organometallic Compounds D M Adams, E A V Ebsworth, 2007-10-31. *Spectroscopic Properties of Inorganic and Organometallic Compounds* provides a unique source of information on an important area of chemistry. Divided into sections mainly according to the particular spectroscopic technique used, coverage in each volume includes NMR with reference to stereochemistry, dynamic systems, paramagnetic complexes, solid state NMR, and Groups 13-18, nuclear quadrupole resonance spectroscopy, vibrational spectroscopy of main group and transition element compounds, and coordinated ligands and electron diffraction. Reflecting the growing volume of published work in this field, researchers will find this Specialist Periodical Report an invaluable source of information on current methods and applications. Specialist Periodical Reports provide systematic and detailed review coverage in major areas of chemical research. Compiled by teams of leading experts in their specialist fields, this series is designed to help the chemistry community keep current with the latest developments in their field. Each volume in the series is published either annually or

biennially and is a superb reference point for researchers www.rsc.org/spr *Molecules and Radiation* Jeffrey I. Steinfeld, 2012-11-09 This unified treatment introduces upper level undergraduates and graduate students to the concepts and methods of modern molecular spectroscopy and their applications to quantum electronics lasers and related optical phenomena Starting with a review of the prerequisite quantum mechanical background the text examines atomic spectra and diatomic molecules including the rotation and vibration of diatomic molecules and their electronic spectra A discussion of rudimentary group theory advances to considerations of the rotational spectra of polyatomic molecules and their vibrational and electronic spectra molecular beams masers and lasers and a variety of forms of spectroscopy including optical resonance spectroscopy coherent transient spectroscopy multiple photon spectroscopy and spectroscopy beyond molecular constants The text concludes with a series of useful appendixes **INIS Atomindex**, 1982 *Phase-Integral Method* Nanny Fröman, Per O. Fröman, 1998-02-18 The result of two decades spent developing and refining the phase integral method to a high level of precision the authors have applied this method to problems in various fields of theoretical physics The problems treated are of a mathematical nature but have important physical applications This book will thus be of great use to research workers in various branches of theoretical physics where the problems can be reduced to one dimensional second order differential equations of the Schrödinger type for which phase integral solutions are required Includes contributions from notable scientists who have already made use of the authors technique *Asymptotic and Computational Analysis* R. Wong, 2020-12-17 Papers presented at the International Symposium on Asymptotic and Computational Analysis held June 1989 Winnipeg Man sponsored by the Dept of Applied Mathematics University of Manitoba and the Canadian Applied Mathematics Society *Photodissociation and Photoionisation* K. P. Lawley, 2009-09-08 Experts in the field cover a wide range of theoretical and practical aspects of photodissociation and photoionization This complete survey covers everything from laser isotope separation at the applied end to current theories of the quantum mechanics of photodissociation **New Horizons of Quantum Chemistry** P.-O. Löwdin, A. Pullman, 2012-12-06 The Fourth International Congress in Quantum Chemistry under the auspices of the International Academy of Molecular Quantum Science in Menton France was arranged at Uppsala University Uppsala Sweden during the period June 14 19 1982 in close collaboration with the University of Florida The previous congresses were held in Menton 1973 New Orleans 1976 and Kyoto 1979 and the 1985 congress is tentatively planned to be held in the province of Quebec Canada The Congress consisted of six symposia in various areas of quantum chemistry solid state theory and quantum biology The meeting was attended by about 450 scientists from 45 different nations and a total of more than 300 scientific papers were presented Even the poster contributions were given some plenary time These proceedings contain the text of the plenary lectures as well as the chairmen's introductions whereas the contributed papers will be published in the International Journal of Quantum Chemistry John Wiley Sons New York in the regular January April 1983 issues **Theory of Slow Atomic Collisions** E.E. Nikitin, S.Y. Umanskii, 2012-12-06

The theory of atom molecule collisions is one of the basic fields in chemical physics. Its most challenging part, the dynamics of chemical reactions, is as yet unresolved but is developing very quickly. It is here a great help to have an analysis of those parts of collision theory which are already complete, a good example being the theory of atomic collisions in processes specific to chemical physics. It has long been observed that many notions of this theory can also be applied successfully to reactive and unreactive molecular collisions. Moreover, atomic collisions often represent a touchstone in testing approaches proposed for the solution of more complicated problems. Research on the theory of slow atomic collisions carried out at the Moscow Institute of Chemical Physics has been based on just these ideas. A general viewpoint concerning the setting up and representation of the theory came out of these studies and appeared to be useful in studying complicated systems as well. It underlies the representation of the theory of slow atomic collisions in this book.

Femtochemistry Ahmed H. Zewail, 1994

These two volumes on Femtochemistry present a timely contribution to a field central to the understanding of the dynamics of the chemical bond. This century has witnessed great strides in time and space resolutions down to the atomic scale, providing chemists, biologists, and physicists with unprecedented opportunities for seeing microscopic structures and dynamics. Femtochemistry is concerned with the time resolution of the most elementary motions of atoms during chemical change: bond breaking and bond making on the femtosecond (10⁻¹⁵ second) time scale. This atomic scale of time resolution has now reached the ultimate for the chemical bond, and as Lord George Porter puts it, chemists are near the end of the race against time. These two volumes cover the general concepts, techniques, and applications of femtochemistry. Professor Ahmed Zewail, who has made the pioneering contributions in this field, has from over 250 publications selected the articles for this anthology. These volumes begin with a commentary and a historical chronology of the milestones. He then presents a broad perspective of the current state of knowledge in femtochemistry by researchers around the world and discusses possible new directions. In the words of a colleague, it is a must on the reading list for all of my students; all readers will find this to be an informative and valuable overview. The introductory articles in Volume I provide reviews for both the non-experts as well as for experts in the field. This is followed by papers on the basic concepts. For applications, elementary reactions are studied first, and then complex reactions. Volume I is complete with studies of solvation dynamics, non-reactive systems, ultrafast electron diffraction, and the control of chemical reactions. Volume II continues with reaction rates, the concept of elementary intramolecular vibrational energy redistribution (IVR), and the phenomena of rotational coherence, which has become a powerful tool for the determination of molecular structure via time resolution. The second volume ends with an extensive list of references according to topics based on work by Professor Zewail and his group at Caltech. These collected works by Professor Zewail will certainly be indispensable to both experts and beginners in the field. The author is known for his clarity and for his creative and systematic contributions. These volumes will be of interest and should prove useful to chemists, biologists, and physicists. As noted by Professor J. Manz, Berlin, and Professor A. W. Castleman Jr., Penn State, femtochemistry is

yielding exciting new discoveries from analysis to control of chemical reactions with applications in many domains of chemistry and related fields e g physical organic and inorganic chemistry surface science molecular biology etc *Advances in Atomic, Molecular, and Optical Physics* ,1993-03-05 Advances in Atomic Molecular and Optical Physics

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