

Semiclassical Methods in Molecular Scattering and Spectroscopy

edited by

M. S. CHILD

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Semiclabical Methods In Molecular Scattering And Spectroscopy

M S Child

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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

Quantum Molecular Dynamics David A. Micha,2025-10-31 Presents theoretical computational and practical aspects of collision induced phenomena with emphasis on the treatment of physical and chemical kinetics using quantum molecular dynamics Quantum Molecular Dynamics provides a state of the art overview of molecular collisions for energy transfer and reactivity phenomena in gases Grounded in the quantal theory of scattering and its semiclassical limits this comprehensive volume covers key concepts and theory computational approaches and various applications for specific physical systems Detailed chapters describe elastic inelastic and reactive collisions that lead to energy transfer electronic transitions chemical reactions and more Starting from the electronic structure and atomic conformation of molecules the text proceeds from introductory material to advanced modern treatments relevant to applications to new materials the environment biological phenomena and energy and fuels production Provides a thorough introduction to collision dynamics with realistic intermolecular forces Covers thermal rates and cross sections of molecular collisions phenomena Examines electronic excitation and relaxation phenomena mediated by molecular collisions Discusses many atom scattering theory as an introduction to more advanced descriptions Presents the computational aspects required to calculate and compare cross sections with experimental data Includes worked examples and applications to different physical systems Quantum Molecular

Dynamics is an important resource for researchers and advanced undergraduate and graduate students in physical theoretical and computational chemistry chemical physics materials science as well as chemists engineers and biologists working in the energy and pharmaceutical industries and the environment

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

[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

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