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# QUANTUM THEORY OF ANHARMONIC EFFECTS IN MOLECULES

KONSTANTIN V KAZAKOW

# **Quantum Theory Of Anharmonic Effects In Molecules**

Andrzej Horzela, Edward Kapuscik

#### **Quantum Theory Of Anharmonic Effects In Molecules:**

Quantum Theory of Anharmonic Effects in Molecules Konstantin V. Kazakov,2012-07-09 Presented in a clear and straightforward analysis this book explores quantum mechanics and the application of quantum mechanics to interpret spectral phenomena Specifically the book discusses the relation between spectral features in mid or rear infrared regions or in Raman scattering spectrum and interactions between molecules or molecular species such as molecular ions and their respective motions in gaseous or crystalline conditions Beginning with an overview of conventional methods and problems which arise in molecular spectroscopy the second half of the book suggests original techniques to investigate the area The treatment is based on rigorous quantum mechanical theories and procedures that are readily implemented in either manual methods or with symbolic computational software Offers a novel approach in its application to physical phenomena Concise and clear discussions of quantum mechanical theories and spectrum analysis Provides both theories and applications

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Uncommon Paths in Quantum Physics Konstantin V. Kazakov, 2014-06-26 Quantum mechanics is one of the most fascinating and at the same time most controversial branches of contemporary science Disputes have accompanied this science since its birth and have not ceased to this day Uncommon Paths in Quantum Physics allows the reader to contemplate deeply some ideas and methods that are seldom met in the contemporary literature Instead of widespread recipes of mathematical physics based on the solutions of integro differential equations the book follows logical and partly intuitional derivations of non commutative algebra Readers can directly penetrate the abstract world of quantum mechanics First book in the market that treats this newly developed area of theoretical physics the book will thus provide a fascinating overview of the prospective applications of this area strongly founded on the theories and methods that it describes Provides a solid foundation for the application of quantum theory to current physical problems arising in the interpretation of molecular spectra and important effects in quantum field theory New insight into the physics of anharmonic vibrations more feasible calculations with improved precision

Proceedings of the Second International Symposium on Quantum Theory

and Symmetries Edward Kapuścik, Andrzej Horzela, 2002 This book presents the up to date status of quantum theory and the outlook for its development in the 21st century The covered topics include basic problems of quantum physics with emphasis on the foundations of quantum theory quantum computing and control quantum optics coherent states and Wigner functions as well as on methods of quantum physics based on Lie groups and algebras quantum groups and noncommutative geometry

New Methods in Computational Quantum Mechanics Ilya Prigogine, Stuart A. Rice, 2009-09-09 The use of quantum chemistry for the quantitative prediction of molecular properties has long been frustrated by the technical difficulty of carrying out the needed computations In the last decade there have been substantial advances in the formalism and computer hardware needed to carry out accurate calculations of molecular properties efficiently These advances have been sufficient to make quantum chemical calculations a reliable tool for the quantitative interpretation of chemical phenomena and a guide to laboratory experiments However the success of these recent developments in computational quantum chemistry is not well known outside the community of practitioners In order to make the larger community of chemical physicists aware of the current state of the subject this self contained volume of Advances in Chemical Physics surveys a number of the recent accomplishments in computational quantum chemistry. This stand alone work presents the cutting edge of research in computational quantum mechanics Supplemented with more than 150 illustrations it provides evaluations of a broad range of methods including Quantum Monte Carlo methods in chemistry Monte Carlo methods for real time path integration The Redfield equation in condensed phase quantum dynamics Path integral centroid methods in quantum statistical mechanics and dynamics Multiconfigurational perturbation theory applications in electronic spectroscopy Electronic structure calculations for molecules containing transition metals And more Contributors to New Methods in Computational Quantum Mechanics KERSTIN ANDERSSON Department of Theoretical Chemistry Chemical Center Sweden DAVID M CEPERLEY National Center for Supercomputing Applications and Department of Physics University of Illinois at Urbana Champaign Illinois MICHAEL A COLLINS Research School of Chemistry Australian National University Canberra Australia REINHOLD EGGER Fakult t f r Physik Universit t Freiburg Freiburg Germany ANTHONY K FELTS Department of Chemistry Columbia University New York RICHARD A FRIESNER Department of Chemistry Columbia University New York MARKUS P F LSCHER Department of Theoretical Chemistry Chemical Center Sweden K M HO Ames Laboratory and Department of Physics Iowa State University Ames Iowa C H MAK Department of Chemistry University of Southern California Los Angeles California PER KE Malmqvist Department of Theoretical Chemistry Chemical Center Sweden MANUELA MERCH n Departamento de Qu mica F sica Universitat de Val ncia Spain LUBOS MITAS National Center for Supercomputing Applications and Materials Research Laboratory University of Illinois at Urbana Champaign Illinois STEFANO OSS Dipartimento di Fisica Universit di Trento and Istituto Nazionale di Fisica della Materia Unit di Trento Italy KRISTINE PIERLOOT Department of Chemistry University of Leuven Belgium W THOMAS POLLARD Department of

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Combining Quantum Mechanics and Molecular Mechanics. Some Recent Progresses in QM/MM Methods, 2010-06-14 Advances in Quantum Chemistry presents surveys of current developments in this rapidly developing field With invited reviews written by leading international researchers each presenting new results it provides a single vehicle for following progress in this interdisciplinary area Publishes articles invited reviews and proceedings of major international conferences and workshops Written by leading international researchers in quantum and theoretical chemistry Highlights important interdisciplinary developments Computational Chemistry David Young, 2004-04-07 A practical easily accessible guide for bench top chemists thisbook focuses on accurately applying computational chemistrytechniques to everyday chemistry problems Provides nonmathematical explanations of advanced topics incomputational chemistry Focuses on when and how to apply different computational techniques Addresses computational chemistry connections to biochemical systems and polymers Provides a prioritized list of methods for attacking difficult computational chemistry problems and compares advantages and disadvantages of various approximation techniques Describes how the choice of methods of software affects requirements for computer memory and processing time Vibrational-Rotational Excitations in Nonlinear Molecular Systems Alexander A. Ovchinnikov, Nikolai S. Erikhman, Kirill A. Pronin, 2012-12-06 If there would be no God then what a staff captain am I said one of the characters in a novel by Dostoevskii In a similar way we can exclaim If there would be no nonlinearity than what physics would that be Really the most interesting and exciting effects are described by non linear equations and vanish in the linear approximation For example the general theory of relativity by A Einstein comes to mind first one of the most beautiful physical theories which is in fact essentially nonlinear Next the phase transitions crystal liquid and liquid gas are due to the anhar monicity of interparticle interactions to dissociation and infinite motion Similarly transitions into the superconducting state or the superftuid would be impossible with purely harmonic interaction potentials Another bril liant achievement in nonlinear physics was the construction of a laser and the subsequent development of nonlinear optics. The latter describes the in teraction of the matter with light of super high intensity when multi quanta intra

molecular transitions become essential Last we should note here the very beautiful mathematical theory the theory of catastrophes Its subject is the study of invariant general properties of multi dimensional surfaces in the vicinity of bifurcation points with respect to continuous transformations *Physics and Chemistry at Low Temperatures* Leonid Khriachtchev,2019-05-08 Tunneling reactions in chemistry are characterized by the low temperature limit when the classical contribution is negligible Many practical applications benefit from the lack of heat and have a deep physical basis Interesting advantages of chemical synthesis at low temperatures have also been demonstrated This book covers fundamental and practical aspects of the processes and experimental and theoretical methods used in the field The chapters are written by leading scientists who have very strong experience in the selected topics and many practical recommendations can be found in this book

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