Beyond Born-Oppenheimer: Electronic Nonadiabatic Coupling Terms and Conical Intersections

Michael Baer

DESCRIPTION

INTRODUCING A POWERFUL APPROACH TO DEVELOPING RELIABLE QUANTUM MECHANICAL TREATMENTS OF A LARGE VARIETY OF PROCESSES IN MOLECULAR SYSTEMS.

The Born-Oppenheimer approximation has been fundamental to calculation in molecular spectroscopy and molecular dynamics since the early days of quantum mechanics. This is despite well-established fact that it is often not valid due to conical intersections that give rise to strong nonadiabatic effects caused by singular nonadiabatic coupling terms (NACTs). In Beyond Born-Oppenheimer, Michael Baer, a leading authority on molecular scattering theory and electronic nonadiabatic processes, addresses this deficiency and introduces a rigorous approach--diabatization--for eliminating troublesome NACTs and deriving well-converged equations to treat the interactions within and between molecules.

Concentrating on both the practical and theoretical aspects of electronic nonadiabatic transitions in molecules, Professor Baer uses a simple mathematical language to rigorously eliminate the singular NACTs and enable reliable calculations of spectroscopic and dynamical cross sections. He presents models of varying complexity to illustrate the validity of the theory and explores the significance of the study of NACTs and the relationship between molecular physics and other fields in physics, particularly electrodynamics.

The first book of its kind Beyond Born-Oppenheimer:

* Presents a detailed mathematical framework to treat electronic NACTs and their conical intersections
Describes the Born-Oppenheimer treatment, including the concepts of adiabatic and diabatic frameworks

Introduces a field-theoretical approach to calculating NACTs, which offers an alternative to time-consuming ab initio procedures

Discusses various approximations for treating a large system of diabatic Schrödinger equations

Presents numerous exercises with solutions to further clarify the material being discussed

Beyond Born-Oppenheimer is required reading for physicists, physical chemists, and all researchers involved in the quantum mechanical study of molecular systems.

ABOUT THE AUTHOR

Michael Baer is one of the foremost authorities on molecular scattering theory. He wrote the seminal paper in the field of electronic nonadiabatic molecular collisions in 1975 and has continued to make fundamental contributions to electronic nonadiabatic processes in molecular systems. He also contributed significantly to developing numerical methods to treat, quantum mechanically, reactive-exchange processes and is a co-author of the negative imaginary potential approach to decoupling the dynamics in different arrangement channels, which is now used worldwide. Dr. Baer, who received his M.Sc. and Ph.D from the Hebrew University of Jerusalem, is currently associated with the Fritz Haber Center for Molecular Dynamics at the Hebrew University in Jerusalem. Before that he was a theoretical physicist and an applied mathematician for almost 40 years at the Soreq Nuclear Research Center, Israel. The author was a visiting scientist in many foreign universities and scientific institutes, among them Harvard University and the University of Oxford. He has published more than 300 scientific articles and edited several books. In 1993 he was awarded the (Senior) Meitner-Humboldt Prize in Germany for Theoretical Chemistry and in 2003 he was nominated as a Szent-Györgyi professor for physics by the National Academy of Sciences in Hungary.

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