2nd Edition

NONADIABATIC TRANSITION

**Concepts, Basic Theories
and Applications**

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Concepts, Basic Theories
and Applications

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Preface to the Second Edition

The range of possible applications of the theory of nonadiabatic transition has been widely expanded since the printing of the first edition of this book, reflecting the importance of the transitions in various fields of physics and chemistry, and even in biology. Especially in chemical dynamics, not only proper theoretical understanding of various nonadiabatic chemical dynamics occurring in Nature has become possible, but also control of chemical dynamics and manifestation of molecular functions are not just simple dreams any more. Thanks to the remarkable developments of laser technology, nonadiabatic transitions induced by lasers can be controlled by appropriately designing lasers. A new field of *nonadiabatic chemical dynamics* is thus emerging as a futuristic subject.

Three new chapters 14–16 are added in this second edition. Chapter 14 is entitled “Comprehension of Nonadiabatic Chemical Dynamics” and is devoted mainly to the applications of the Zhu–Nakamura formulas to chemical reaction dynamics, photo-induced dynamics, and electron transfer. Realistic large chemical and biological systems can now be treated properly. “Control of Chemical Dynamics” and “Manifestation of Molecular Functions” are discussed in Chapters 15 and 16, respectively. Theoretical possibilities of controlling chemical dynamics are demonstrated by numerical examples of efficient excitation/de-excitation by the periodic chirping, utilization of the complete reflection phenomenon, and control of wave packet motion. Molecular function is an important futuristic subject and Chapter 16 contains the discussions about molecular switching, hydrogen transmission through carbon ring, photo-conversion of cyclohexadiene to hexatriene, and molecular motors. These just represent some simple examples of various future possibilities. In accordance with these new chapters, some other chapters are reorganized. Main changes are as follows: Two

new sections are created in Chapter 7: “Time-Dependent Nonlinear Equations Related to Bose–Einstein Condensate Problems” and “Wave Packet Dynamics in a Linearly Chirped Laser Field”. The title of Chapter 8 is changed to “Effects of Coupling to Phonons and Quantum Devices”, considering the recent progress of the investigation of quantum devices with use of the nonadiabatic transitions. In Chapter 10 more space is allocated to explain the semiclassical propagation methods in more detail (Section 10.3). The treatment of three-dimensional chemical reactions is moved to the new Chapter 14, and a new Section 10.4 is created as “Nonadiabatic Transition State Theory”. Chapter 13 is largely reorganized. Explanations of the optimal control theories are added and the numerical applications in Section 13.3 are moved to Section 15.1 of a new Chapter 15.

Most of the new contents added in this second edition are the results of collaborations with my many co-workers. Taking this opportunity, I would like to thank them.

I would also like to express my hearty thanks to National Science Council of Taiwan, National Chiao Tung University in Hsinchu, Taiwan, and people at The Institute of Molecular Science, Department of Applied Chemistry, Faculty of Science of the University for providing me this very nice opportunity to work on this second edition. Especially, I am deeply indebted to Professor S.H. Lin and Professor Y.P. Lee.

Acknowledgment is also due to the following publishers for permission to reproduce various copyright materials: the societies listed in the first edition, Springer publisher, and World Scientific Publishing.

Finally, I would like to thank my wife, Suwako, for her continuous support in my life. This work could not be finished without her support in Taiwan.

I really hope that the field of *nonadiabatic chemical dynamics* will flourish in future by establishing collaborations among dynamics theory, quantum chemistry, physical and organic chemistry, and laser science.

Hiroki Nakamura

Okazaki, Japan and Hsinchu, Taiwan

August 2011

Preface to the First Edition

“Nonadiabatic transition” is a very multi-disciplinary concept and phenomenon which constitutes a fundamental mechanism of state and phase changes in various dynamical processes in physics, chemistry, and biology. This book has been written on the opportunity that the complete solutions of the basic problem have been formulated for the first time since the pioneering works done by Landau, Zener, and Stueckelberg in 1932. It not only contains this new theory, but also surveys the history and theoretical works in the related subjects without going into much details of mathematics. Both time-independent and time-dependent phenomena are discussed. Since the newly completed theory is useful for various applications, the final recommended formulas are summarized in Appendix in directly usable forms. Discussions are also devoted to intriguing phenomena of complete reflection and bound states in the continuum, and further to possible applications of the theory such as molecular switching and control of molecular processes by external fields.

This book assumes the background knowledge of the level of graduate students and is basically intended as a standard reference for practical uses in various research fields of physics and chemistry.

The writing of this book was suggested and recommended by Professor Kazuo Takayanagi and Professor Phil G. Burke. My thanks are also due to my many collaborators with whose help a lot of works written in this book have been accomplished.

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Hiroki Nakamura
Okazaki, Japan
February 2001

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