

Introduction	1
From Thermal Activation to Tunneling	15
One-dimensional Models	55
Two-dimensional Tunneling	97
CHEMICAL DYNAMICS IN THE PRESENCE OF A HEAT BATH	117
Hydrogen Transfer	151
Tunneling Rotation	209
VIBRATION-ROTATION TUNNELING SPECTROSCOPY OF MOLECULES AND DIMERS	261
HEAVY PARTICLE TRANSFER	309
Conclusion	336
References	341
Author Index	359
Subject Index	371



INTRODUCTION

- 1.1. Historical Background
- 1.2. The Routes of Simplifying the Problem



FROM THERMAL ACTIVATION TO TUNNELING

- 2.1. Crossover Temperature
- 2.2. Tunneling and Dissipation
- 2.3. Coherent Versus Incoherent Tunneling
- 2.4. Vibronic Relaxation and Electron Transfer
- 2.5. Vibration-assisted Tunneling
- 2.6. Is There an Alternative to Tunneling?



ONE-DIMENSIONAL MODELS

CONTENTS

- 3.1. The Main Path Integral Relations
- 3.2. Numerical Path Integral Methods
- 3.3. Tunneling Trajectories for a One-Dimensional Barrier
- 3.4. Decay of a Metastable State
- 3.5. The Im F Method
- 3.6. Tunneling Splitting in a Double Well
- 3.7. Nonadiabatic Tunneling
- 3.8. Quantum Transition State Theory

Appendix A: Decay of a Metastable State and Tunneling Splitting in Terms of the One-Dimensional WKB Approximation

Appendix B: Equivalence of the Instanton Approach to Semiclassical TST



TWO-DIMENSIONAL TUNNELING

- 4.1. Decay of a Metastable State
- 4.2. Tunneling Splitting
- 4.3. Periodic Orbits in a Symmetric Double Well

CHEMICAL DYNAMICS IN THE PRESENCE OF A HEAT BATH

CONTENTS

- 5.1. The Quasienergy Method
 - 5.1.1. Adiabatic Approximation
 - 5.1.2. Classical Low-Frequency Heat Bath
- 5.2. Bath of Harmonic Oscillators
- 5.3. Dynamics of a Dissipative Two-Level system
- 5.4. Dissipative Nonadiabatic Tunneling

Appendix C: Dissipative Nonadiabatic Tunneling at T=0

HYDROGEN TRANSFER

- 6.1. Semiempirical Two-Dimensional Potential of a Hydrogen Bond
- 6.2. Hydrogen Bond and Tunneling Splitting
- 6.3. Tautomerization in Excited Electronic States
- 6.4. Two-Proton Transfer
- 6.5. Free Radical Conversion in Solids
- 6.6. Quantum Diffusion of Hydrogen
- 6.7. Exchange Reactions in Hydrogen Crystals



TUNNELING ROTATION

- 7.1. Splitting of Torsion Vibrational Levels
- 7.2. Potential for Hindered Rotation
- 7.3. Interaction Between Rotation and Lattice Vibrations
- 7.4. Coupled Tunneling Rotation
- 7.5. Cooperative Rotation



VIBRATION-ROTATION TUNNELING SPECTROSCOPY OF MOLECULES AND DIMERS

8.1.	Superson	nic	Cool	ling
CHARGO TO CAR		74. COM		0

- 8.2. Inversion Splitting
- 8.3. Pseudorotation
- 8.4. Interconversion of Hydrogen-bonded Dimers of Diatomic Molecules
- 8.5. Coupled Tunneling Motions in Hydrogen-Bonded Dimers
- 8.6. Large-Amplitude Motions in van der Waals Complexes

HEAVY PARTICLE TRANSFER

- 9.1. Tunneling Impurity States in Solids
- 9.2. Chemical Reactions
- 9.3. Chain Reactions