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Autore	Benjamin Scott
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Autore	May Volkhard
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Nota di contenuto	Charge and Energy Transfer Dynamics in Molecular Systems; Contents; Preface to the Third Edition; Preface to the Second Edition; Preface to the First Edition; 1 Introduction; 2 Electronic and Vibrational Molecular States; 2.1 Introduction; 2.2 Molecular Schrodinger Equation; 2.3 Born-Oppenheimer Separation; 2.3.1 Born-Oppenheimer Approximation; 2.3.2 Some Estimates; 2.4 Electronic Structure Methods; 2.4.1 The Hartree-Fock Equations; 2.4.2 Density Functional Theory; 2.5 Condensed Phase Approaches; 2.5.1 Dielectric Continuum Model; 2.5.2 Explicit Quantum-Classical Solvent Model 2.6 Potential Energy Surfaces2.6.1 Harmonic Approximation and Normal Mode Analysis; 2.6.2 Operator Representation of the Normal Mode Hamiltonian; 2.6.3 Reaction Paths; 2.7 Diabatic versus Adiabatic Representation of the Molecular Hamiltonian; 2.8 Supplement; 2.8.1 The Hartree-Fock Equations; 2.8.2 Franck-Condon Factors; 2.8.3 The

Two-Level System; 2.8.4 The Linear Molecular Chain and the Molecular Ring; References; Further Reading; 3 Dynamics of Isolated and Open Quantum Systems; 3.1 Introduction; 3.2 Time-Dependent Schrodinger Equation; 3.2.1 Wave Packets
3.2.2 The Interaction Representation3.2.3 Multidimensional Wave Packet Dynamics; 3.3 The Golden Rule of Quantum Mechanics; 3.3.1 Transition from a Single State into a Continuum; 3.3.2 Transition Rate for a Thermal Ensemble; 3.3.3 Green's Function Approach; 3.4 The Nonequilibrium Statistical Operator and the Density Matrix; 3.4.1 The Density Operator; 3.4.2 The Density Matrix; 3.4.3 Equation of Motion for the Density Operator; 3.4.4 Wigner Representation of the Density Operator; 3.4.5 Dynamics of Coupled Multilevel Systems in a Heat Bath
3.5 The Reduced Density Operator and the Reduced Density Matrix3.
5.1 The Reduced Density Operator; 3.5.2 Equation of Motion for the Reduced Density Operator; 3.5.3 Mean-Field Approximation; 3.5.4 The Interaction Representation of the Reduced Density Operator; 3.5.5 The Projection Superoperator; 3.5.6 Second-Order Equation of Motion for the Reduced Density Operator; 3.6 The Reservoir Correlation Function; 3.6.1 General Properties of $C_{uv}(t)$; 3.6.2 Harmonic Oscillator Reservoir; 3.6.3 The Spectral Density; 3.6.4 Linear Response Theory for the Reservoir; 3.6.5 Classical description of $C_{uv}(t)$
3.7 Quantum Master Equation3.7.1 Markov Approximation; 3.8 Reduced Density Matrix in Energy Representation; 3.8.1 The Quantum Master Equation in Energy Representation; 3.8.2 Multilevel Redfield Equations; 3.8.3 The Secular Approximation; 3.8.4 State Expansion of the System-Reservoir Coupling; 3.8.5 From Coherent to Dissipative Dynamics: A Simple Example; 3.8.6 Coordinate and Wigner Representation of the Reduced Density Matrix; 3.9 Generalized Rate Equations: The Liouville Space Approach; 3.9.1 Projection Operator Technique; 3.9.2 Generalized Rate Equations; 3.9.3 Rate Equations
3.9.4 The Memory Kernels

Sommario/riassunto

This 3rd edition has been expanded and updated to account for recent developments, while new illustrative examples as well as an enlarged reference list have also been added. It naturally retains the successful concept of its predecessors in presenting a unified perspective on molecular charge and energy transfer processes, thus bridging the regimes of coherent and dissipative dynamics, and establishing a connection between classic rate theories and modern treatments of ultrafast phenomena. Among the new topics are:- Time-dependent density functional theory- Heterogeneous electr
