

- | | |
|-------------------------|--|
| 1. Record Nr. | UNIORUON00062773 |
| Autore | YEGANE ARANI, Mohammad |
| Titolo | Bara-yi aghazi-i navin dar falsafah / bi-qalam-i Muammad Yagnah
rn |
| Pubbl/distr/stampa | Landan, : [s.n.], 1976-1978 |
| Descrizione fisica | 3 v. ; 29 cm. |
| Classificazione | IRA VII |
| Soggetti | Filosofia |
| Lingua di pubblicazione | Persiano |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| ----- | |
| 2. Record Nr. | UNINA9910962897603321 |
| Autore | Nitzan Abraham |
| Titolo | Chemical dynamics in condensed phases : relaxation, transfer and
reactions in condensed molecular systems // Abraham Nitzan |
| Pubbl/distr/stampa | Oxford ; ; New York, : Oxford University Press, 2006 |
| ISBN | 0191523879
9780191523878 |
| Edizione | [1st ed.] |
| Descrizione fisica | xxii, 719 p. : ill |
| Collana | Oxford graduate texts |
| Disciplina | 541/.394 |
| Soggetti | Molecular dynamics
Chemical reaction, Conditions and laws of |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Nota di bibliografia | Includes bibliographical references and index. |
| Nota di contenuto | Intro -- Contents -- PART I: BACKGROUND -- 1 Review of some
mathematical and physical subjects -- 1.1 Mathematical background --
1.2 Classical mechanics -- 1.3 Quantum mechanics -- 1.4
Thermodynamics and statistical mechanics -- 1.5 Physical observables |

as random variables -- 1.6 Electrostatics -- 2 Quantum dynamics using the time-dependent Schrödinger equation -- 2.1 Formal solutions -- 2.2 An example: The two-level system -- 2.3 Time-dependent Hamiltonians -- 2.4 A two-level system in a time-dependent field -- 2.5 A digression on nuclear potential surfaces -- 2.6 Expressing the time evolution in terms of the Green's operator -- 2.7 Representations -- 2.8 Quantum dynamics of the free particles -- 2.9 Quantum dynamics of the harmonic oscillator -- 2.10 Tunneling -- 2A: Some operator identities -- 3 An Overview of Quantum Electrodynamics and Matter-Radiation Field Interaction -- 3.1 Introduction -- 3.2 The quantum radiation field -- 3A: The radiation field and its interaction with matter -- 4 Introduction to solids and their interfaces -- 4.1 Lattice periodicity -- 4.2 Lattice vibrations -- 4.3 Electronic structure of solids -- 4.4 The work function -- 4.5 Surface potential and screening -- 5 Introduction to liquids -- 5.1 Statistical mechanics of classical liquids -- 5.2 Time and ensemble average -- 5.3 Reduced configurational distribution functions -- 5.4 Observable implications of the pair correlation function -- 5.5 The potential of mean force and the reversible work theorem -- 5.6 The virial expansion-the second virial coefficient -- PART II: METHODS -- 6 Time correlation functions -- 6.1 Stationary systems -- 6.2 Simple examples -- 6.3 Classical time correlation functions -- 6.4 Quantum time correlation functions -- 6.5 Harmonic reservoir -- 7 Introduction to stochastic processes -- 7.1 The nature of stochastic processes. 7.2 Stochastic modeling of physical processes -- 7.3 The random walk problem -- 7.4 Some concepts from the general theory of stochastic processes -- 7.5 Harmonic analysis -- 7A: Moments of the Gaussian distribution -- 7B: Proof of Eqs (7.64) and (7.65) -- 7C: Cumulant expansions -- 7D: Proof of the Wiener-Khintchine theorem -- 8 Stochastic equations of motion -- 8.1 Introduction -- 8.2 The Langevin equation -- 8.3 Master equations -- 8.4 The Fokker-Planck equation -- 8.5 Passage time distributions and the mean first passage time -- 8A: Obtaining the Fokker-Planck equation from the Chapman-Kolmogorov equation -- 8B: Obtaining the Smoluchowski equation from the overdamped Langevin equation -- 8C: Derivation of the Fokker-Planck equation from the Langevin equation -- 9 Introduction to quantum relaxation processes -- 9.1 A simple quantum-mechanical model for relaxation -- 9.2 The origin of irreversibility -- 9.3 The effect of relaxation on absorption lineshapes -- 9.4 Relaxation of a quantum harmonic oscillator -- 9.5 Quantum mechanics of steady states -- 9A: Using projection operators -- 9B: Evaluation of the absorption lineshape for the model of Figs 9.2 and 9.3 -- 9C: Resonance tunneling in three dimensions -- 10 Quantum mechanical density operator -- 10.1 The density operator and the quantum Liouville equation -- 10.2 An example: The time evolution of a two-level system in the density matrix formalism -- 10.3 Reduced descriptions -- 10.4 Time evolution equations for reduced density operators: The quantum master equation -- 10.5 The two-level system revisited -- 10A: Analogy of a coupled 2-level system to a spin $\frac{1}{2}$ system in a magnetic field -- 11 Linear response theory -- 11.1 Classical linear response theory -- 11.2 Quantum linear response theory -- 11A: The Kubo identity -- 12 The Spin-Boson Model -- 12.1 Introduction -- 12.2 The model. 12.3 The polaron transformation -- 12.4 Golden-rule transition rates -- 12.5 Transition between molecular electronic states -- 12.6 Beyond the golden rule -- PART III: APPLICATIONS -- 13 Vibrational energy relaxation -- 13.1 General observations -- 13.2 Construction of a model Hamiltonian -- 13.3 The vibrational relaxation rate -- 13.4

Evaluation of vibrational relaxation rates -- 13.5 Multi-phonon theory of vibrational relaxation -- 13.6 Effect of supporting modes -- 13.7 Numerical simulations of vibrational relaxation -- 13.8 Concluding remarks -- 14 Chemical reactions in condensed phases -- 14.1 Introduction -- 14.2 Unimolecular reactions -- 14.3 Transition state theory -- 14.4 Dynamical effects in barrier crossing-The Kramers model -- 14.5 Observations and extensions -- 14.6 Some experimental observations -- 14.7 Numerical simulation of barrier crossing -- 14.8 Diffusion-controlled reactions -- 14A: Solution of Eqs (14.62) and (14.63) -- 14B: Derivation of the energy Smoluchowski equation -- 15 Solvation dynamics -- 15.1 Dielectric solvation -- 15.2 Solvation in a continuum dielectric environment -- 15.3 Linear response theory of solvation -- 15.4 More aspects of solvation dynamics -- 15.5 Quantum solvation -- 16 Electron transfer processes -- 16.1 Introduction -- 16.2 A primitive model -- 16.3 Continuum dielectric theory of electron transfer processes -- 16.4 A molecular theory of the nonadiabatic electron transfer rate -- 16.5 Comparison with experimental results -- 16.6 Solvent-controlled electron transfer dynamics -- 16.7 A general expression for the dielectric reorganization energy -- 16.8 The Marcus parabolas -- 16.9 Harmonic field representation of dielectric response -- 16.10 The nonadiabatic coupling -- 16.11 The distance dependence of electron transfer rates -- 16.12 Bridge-mediated long-range electron transfer. -- 16.13 Electron transport by hopping -- 16.14 Proton transfer -- 16A: Derivation of the Mulliken-Hush formula -- 17 Electron transfer and transmission at molecule-metal and molecule-semiconductor interfaces -- 17.1 Electrochemical electron transfer -- 17.2 Molecular conduction -- 18 Spectroscopy -- 18.1 Introduction -- 18.2 Molecular spectroscopy in the dressed-state picture -- 18.3 Resonance Raman scattering -- 18.4 Resonance energy transfer -- 18.5 Thermal relaxation and dephasing -- 18.6 Probing inhomogeneous bands -- 18.7 Optical response functions -- 18A: Steady-state solution of Eqs (18.58): the Raman scattering flux -- Index -- A -- B -- C -- D -- E -- F -- G -- H -- I -- J -- K -- L -- M -- N -- O -- P -- Q -- R -- S -- T -- V -- W -- X.

Sommario/riassunto

Graduate level textbook presenting some of the most fundamental processes that underlie physical, chemical and biological phenomena in complex condensed phase systems. Includes in-depth descriptions of relevant methodologies, and provides ample introductory material for readers of different backgrounds.
