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Autore	Ullrich Carsten
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Nota di contenuto	Cover; Contents; List of abbreviations; 1 Introduction; 1.1 A survey of time-dependent phenomena; 1.2 Preview of and guide to this book; 2 Review of ground-state density-functional theory; 2.1 The formal framework of DFT; 2.2 Exact properties; 2.3 Approximate functionals; PART I: THE BASIC FORMALISM OF TDDFT; 3 Fundamental existence theorems; 3.1 Time-dependent many-body systems; 3.2 The Runge-Gross theorem; 3.3 The van Leeuwen theorem; 4 The time-dependent Kohn-Sham scheme; 4.1 The time-dependent Kohn-Sham equation; 4.2 Spin-dependent systems; 4.3 The adiabatic approximation 4.4 The meaning of self-consistency in DFT and TDDFT4.5 Numerical time propagation; 5 Time-dependent observables; 5.1 Explicit density functionals; 5.2 Implicit density functionals; 5.3 The time-dependent energy; 6 Properties of the time-dependent xc potential; 6.1 What is the universal xc functional?; 6.2 Some exact conditions; 6.3 Galilean invariance and the harmonic potential theorem; 6.4 Memory and causality; 6.5 Initial-state dependence; 6.6 Time-dependent variational principles; 6.7 Discontinuity upon change of particle number; PART II: LINEAR RESPONSE AND EXCITATION ENERGIES

7 The formal framework of linear-response TDDFT 7.1 General linear-response theory; 7.2 Spectroscopic observables; 7.3 Linear density response in TDDFT; 7.4 Warm-up exercise: TDDFT for two-level systems; 7.5 Calculation of excitation energies: the Casida equation; 7.6 The Tamm-Dancoff approximation and other simplifications; 7.7 Excitation energies with time-dependent Hartree-Fock theory; 8 The frequency-dependent xc kernel; 8.1 Exact properties; 8.2 Approximations; 8.3 The xc kernels of the homogeneous electron liquid; 9 Applications to atomic and molecular systems 9.1 Excitation energies of small systems: basic trends and features 9.2 Molecular excited-state properties with TDDFT: an overview; 9.3 Double excitations; 9.4 Charge-transfer excitations; 9.5 The Sternheimer equation; 9.6 Optical spectra via time propagation schemes; PART III: FURTHER DEVELOPMENTS; 10 Time-dependent current-DFT; 10.1 The adiabatic approximation and beyond; 10.2 The failure of nonadiabatic local approximations in TDDFT; 10.3 The formal framework of TDCDFT; 10.4 The VK functional; 10.5 Applications of TDCDFT in the linear-response regime 10.6 Memory effects: elasticity and dissipation 11 The time-dependent optimized effective potential; 11.1 The static OEP approach for orbital functionals; 11.2 The TDOEP scheme; 11.3 TDOEP in the linear regime; 12 Extended systems; 12.1 Electronic structure and excitations of periodic solids; 12.2 Spectroscopy of density fluctuations: plasmons; 12.3 Optical absorption and excitons; 12.4 TDCDFT in periodic systems; 13 TDDFT and many-body theory; 13.1 Perturbation theory along the adiabatic connection; 13.2 Nonequilibrium Green's functions and the Keldysh action 13.3 xc kernels from many-body theory

Sommario/riassunto

Time-dependent density-functional theory (TDDFT) describes the quantum dynamics of interacting electronic many-body systems formally exactly and in a practical and efficient manner. TDDFT has become the leading method for calculating excitation energies and optical properties of large molecules, with accuracies that rival traditional wave-function based methods, but at a fraction of the computational cost. This book is the first graduate-level text on the concepts and applications of TDDFT, including many examples and exercises, and extensive coverage of the literature. The book begins with a s