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Nota di contenuto	Differential equations -- Propagators and second quantization -- The Huckel model -- Electron field operators -- Angular momentum -- Double-time Green's functions -- The electron propagator -- Electrons in a central potential -- Electron propagator -- The WKB propagator -- The atomic central field problem -- Electron propagator -- Hartree-Fock equations -- Complex spectra -- Single subshell approximation -- Approximate atomic transition amplitudes -- The hydrogen atom -- The carbon and nitrogen atoms -- The excitation propagator -- Antisymmetrized geminal power -- Interaction of radiation and matter -- A charged particle in an electromagnetic field -- Quantization of the radiation field -- Absorption spectroscopy -- RPA transition moments -- Optical rotatory dispersion and circular dichroism -- Temperature-Dependent theory -- Molecules in magnetic fields --

Nuclear spins -- Magnetic susceptibility -- NMR-Spectra -- Indirect nuclear Spin-Spin coupling constants -- Magnetic properties of molecules -- Diamagnetic molecules -- Units and magnitude of magnetic susceptibilities -- Paramagnetic molecules -- NMR spectra and shielding -- NMR spectra and Spin-Spin coupling -- The Origin Problem -- The Gauge Problem -- Calculation of magnetic properties -- An elementary example of NMR spectra -- Paramagnetic molecules -- Electron propagator in higher orders -- Renormalization of the electron propagator -- The 2p-h TDA and the diagonal 2p-h TDA self-energy -- Partitioning and inner projections -- Method of solution.

Sommario/riassunto

The only authoritative reference source on the propagator concept, now thoroughly revised and updated Much has changed in the study of quantum and theoretical chemistry since the publication of the first edition of Propagators in Quantum Chemistry. Advances in computer power and software packages now make it possible to calculate molecular structure, properties, spectra, and reactivity with greater predictive power. Chemical processes, especially under conditions not readily available in the laboratory, can also be much more easily studied via theory and computations. In this environment, the concept of propagators (or Green's functions) is emerging as an increasingly useful tool in the study of atomic and molecular processes. Propagators in Quantum Chemistry, Second Edition presents the theory and basic approximations of propagators in a unified manner as it provides: * A thorough introduction to propagators, and how they can be used to study atomic and molecular properties and spectra * Updated examples and technical details of the use of the propagator concept in various common approximate treatments * Problems that provide the opportunity to work out further details and applications of the theory Propagators, which are still gaining acceptance as tools in theoretical chemistry, have a long-demonstrated power and success in a number of areas including condensed matter physics. Propagators in Quantum Chemistry clearly describes the unprecedented utility and value of propagators, and explores how and why they are becoming increasingly important to scientists and researchers across the scientific spectrum.