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Book review

Mukherjee, D (ed): Applied Many-Body Methods in Spectroscopy and Electronic Structure, Plenum Press, New York, 1992, 291 pages, US $79.50

This monograph contains a collection of ten articles on various aspects of many-body techniques applied to various problems of the atomic and molecular electronic structure, most of which were presented at the meeting of the same name in Calcutta in 1990. The opening article of a pedagogical nature entitled "The many-body perturbation theory (MBPT) of Brueckner and Goldstone" by Werner Kutzelnigg (33 pages) presents a discerning overview of theoretical foundations of the closed shell MBPT. It is intended as an easily accessible, modern day introduction to the MBPT in its both algebraic and diagrammatic forms and, at the same time, as a critical assessment providing new insights and a historical perspective on the many-body theory in general.

The second paper by Jean Paul Malrieu (21 pages) on "Dilemmas in the choice of model spaces supporting magnetic Hamiltonians" presents a critique of Heisenberg-type spin Hamiltonians, pointing out their limitations in describing the molecular electronic structure, even in high spin situations. The lack of transferability from the diatom to extended systems, serious intruder state problems as well as the limitations of the underlying model space are used as arguments for the intermediate Hamiltonian approaches.

An extensive article by Tarantelli et al. on "Recent developments in the calculation of molecular Auger spectra" (48 pages) presents a wealth of theoretical results on the spectra and dynamics of various doubly charged molecular cations, which are essential for the interpretation of broad-featured Auger spectral bands. Relying on the so-called algebraic diagrammatic construction, they exploit the second-order two-particle Green functions to address important aspects of molecular Auger spectroscopy, such as hole localization effects, vibrational structure and transition rates. The next contribution by I. Cacelli et al., entitled "Calculation of photoionization cross section: An Overview" (28 pages), deals with theoretical description of both one- and two-photon absorption processes. Invoking the clamped nuclei and dipole approximations, the authors discuss a plethora of methods for calculation of transition amplitudes that are essential for the determination of differential ionization cross sections. The paper by Danny L. Yeager on "Multiconfiguration Green's function (propagator) techniques for excitation energies, ionization potentials and electron affinities: An Overview" (29 pages), emphasizes the advantages of direct calculations of various energy differences using the appropriate one- or two-particle Green function formalism. A brief outline of the multiconfigurational spin tensor electron propagator (MCSTEP), MC linear response (MCTDHF/MCLR), as well as MC particle–particle (MCP2P) propagator methods is followed by illustrative examples.

The next paper on "MBPT and coupled cluster (CC) approaches to parity nonconservation (PNC) in atoms: A survey of recent developments" by Steven A. Blundell (30 pages) presents a very accessible account of the interplay between the theory and experiment enabling a precision testing of the standard model and of the new physics beyond this model. The author briefly outlines the underlying physics of a weak neutral current interaction that is responsible for PNC in atoms and illustrates both the MBPT and CC calculations of relevant quantities on the Cs atom. The paper is well written and reads like a detective story.

The contribution by Shih-I Chu on "Complex-scaling coupled-channel methods for atomic and molecular resonances in intense external fields" (20 pages), and that by Cleanthes A. Nicolaides on "Theory and computation of nonstationary states of polyelectronic atoms and molecules" (27 pages) employ Floquet theory based complex scaling techniques. While Chu's contribution focusses on resonant states induced by strong external fields as produced by modern lasers, Nicolaides explores

various auto-, multiphoton- and above threshold-ionizations as well as diabatic, quasidiabatic and other nonstationary states.

The last two contributions are devoted to various aspects of multireference (MR) CC approaches. That by Uzi Kaldor on "MRCC approach to spectroscopic constants: Molecular geometries and harmonic frequencies" (19 pages) addresses the capabilities of the valence universal or Fock space approach using an incomplete model space (IMS) for the computation of basic spectroscopic properties determining the rotational and vibrational structure of the molecular spectra. Following a very brief introduction, the author concentrates on a review of his earlier results for alkali dimers and nitrogen containing triatomics. The closing article "On the construction of size extensive effective Hamiltonians in general model spaces using quasi-Hilbert and quasi-Fock strategies" by Debasis Mukhopadhyay (Jr.) and the editor himself (25 pages) addresses the problem of complete vs. incomplete model spaces for the MRCC theories. Following a brief résumé of the Fock space CC theory with IMS, the authors formulate the so-called quasi-Hilbert and quasi-Fock space theories, in which the Fock space IMS is projected onto a single and several n-valence sectors, respectively, and discuss their size extensivity. The monograph is completed with a 3-page index.

On the whole, these proceedings offer an interesting selection of topics of various many-body techniques and of their application to various aspects of the atomic and molecular electronic structure that is both informative and timely.

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