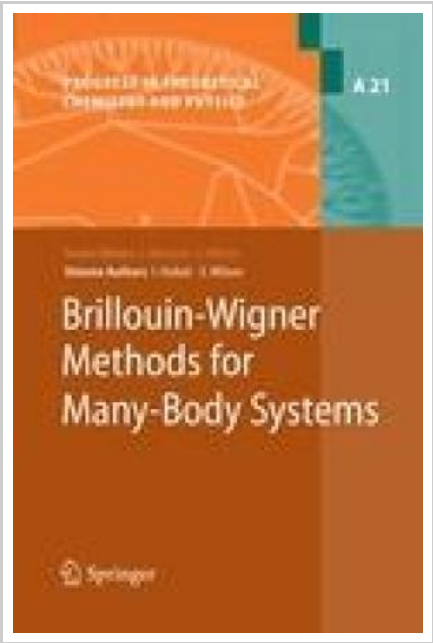

Brillouin-Wigner Methods for Many-Body Systems

By Ivan Hubac

Springer Mrz 2012, 2012. Taschenbuch. Book Condition: Neu. 235x155x13 mm. This item is printed on demand - Print on Demand Titel. - In twenty-first century science, computational modelling is a powerful tool for the study of matter on a nanoscale. It complements an increasing range of experimental probes providing new or more accurate measurements in nanoscience and nanotechnology. The theoretical apparatus upon which electronic structure models are built determines their computational tractability which in turn determines their utility in applications to systems of increasing complexity. The accurate description of the effects of electron correlation is of central importance in ab initio electronic structure theory of atomic and molecular systems. Many body methods, in particular many-body perturbation theory and various coupled cluster expansions, are firmly established as the methods of choice in calculating electron correlation energies. Second order, Moeller-Plesset perturbation theory is the most widely used ab initio quantum chemical technique. Coupled cluster theory with single and double excitations and a perturbative estimate of the contribution of triple excitations is often regarded as a best compromise of accuracy and computational tractability. Both of these methods employ a single reference formalism which is not adequate for studies of systems involving significant quasidegeneracy...

Reviews

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