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Titolo	An Algebraic Approach to the Many-Electron Problem // by Jaroslav Zamastil, Tereza Uhlíková
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Disciplina	530.12
Soggetti	Quantum theory Quantum electrodynamics Mathematical physics Materials science - Data processing Electronic structure Quantum chemistry - Computer programs Solid state physics Quantum Physics Quantum Electrodynamics, Relativistic and Many-body Calculations Mathematical Methods in Physics Electronic Structure Calculations Electronic Devices
Lingua di pubblicazione	Inglese
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Nota di contenuto	Chapter 1: Quantized electron field -- Chapter 2: Hartree-Fock approximation -- Chapter 3: Coupled cluster method -- Chapter 4: Further developments.
Sommario/riassunto	This book presents an algebraic approach to the coupled cluster method for many-electron systems, pioneered by Josef Paldus. Using field methods along with an algebraic, rather than diagrammatic, approach facilitates a way of deriving the coupled cluster method which is readily understandable at the graduate level. The book begins with the notion of the quantized electron field and shows how the N-electron Hamiltonian can be expressed in its language. This is followed by introduction of the Fermi vacuum and derivation of the Hartree-Fock

equations along with conditions for stability of their solutions. Following this groundwork, the book discusses a method of configuration interaction to account for dynamical correlations between electrons, pointing out the size-extensivity problem, and showing how this problem is solved with the coupled cluster approach. This is followed by derivation of the coupled cluster equations in spin-orbital form. Finally, the book explores practical aspects, showing how one may take advantage of permutational and spin symmetries, and how to solve coupled-cluster equations, illustrated by the Hubbard model of benzene, the simplest quasi-realistic model of electron correlation.
