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7.5 Behavior at Small r -- 7.6 Nuclear Models -- 8 Properties of Relativistic Mean-Field Theory -- 8.1 Mean-Field Formalism in Second Quantization -- 8.2 Structure of the Spinor Rotation Operator -- 8.3 Relativistic Stationarity Conditions -- 8.4 Projection and Bounds -- 8.5 Many-Electron Theory -- III: Four-Component Methodology -- 9 Operators, Matrix Elements, and Wave Functions under Time-Reversal Symmetry -- 9.1 Time Reversal and Kramers-Restricted Representation of Operators -- 9.2 Matrix Elements under Time Reversal -- 9.3 Many-Particle States and Time Reversal -- 10 Matrices and Wave Functions under Double-Group Symmetry -- 10.1 Time-Reversal and Point-Group Symmetry -- 10.2 Time-Reversal Symmetry and Matrix Block Structure -- 10.3 Symmetry of Spinor Components -- 10.4 Symmetries of Two-Particle States -- 10.5 Matrix Elements and Symmetry -- 10.6 Time Reversal and Symmetry in the Many-Electron Hamiltonian -- 11 Basis-Set Expansions of Relativistic Electronic Wave Functions -- 11.1 The Dirac Equation in 2-Spinor Form -- 11.2 Kinetic Balance -- 11.3 Variational Bounds -- 11.4 Matrix Dirac-Hartree-Fock Equations in a 2-Spinor Basis -- 11.5 Kramers-Restricted 2-Spinor Matrix Dirac-Hartree-Fock Equations -- 11.6 Symmetry in the Kramers-Restricted Fock Matrix -- 11.7 Kramers-Restricted Open-Shell Methods -- 11.8 Expansion in Scalar Basis Sets -- 11.9 Basis Set Choice and Design -- 11.10 Comparison of Nonrelativistic and Relativistic SCF Methods -- 12 Correlation Methods -- 12.1 The Reference State -- 12.2 The No-Pair Approximation -- 12.3 Integral Transformations -- 12.4 Kramers-Restricted Møller-Plesset Perturbation Theory -- 12.5 Kramers-Restricted Coupled-Cluster Expansions -- 12.6 Open-Shell Kramers-Restricted Coupled-Cluster Expansions -- 12.7 Configuration Interaction Expansions -- 12.8 The Cost of Configuration Interaction Methods.
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Sommario/riassunto

This book introduces relativistic methods in quantum chemistry to non-experts and students. Its five sections cover classical relativity background; the Dirac equation; four-component methods, including symmetry, correlation, and properties; approximate methods, including perturbation theory, transformed Hamiltonians, regular approximations, matrix approximations, and pseudopotential methods; and an overview of relativistic effects on bonding.