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operators; 2.2.2 Spin operators; 2.2.3 Mixed operators; 2.3 Spin tensor operators; 2.3.1 Spin tensor operators; 2.3.2 Creation and annihilation operators; 2.3.3 Two-body creation operators; 2.3.4 Excitation operators; 2.3.5 Singlet excitation operators; 2.4 Spin properties of determinants; 2.4.1 General considerations; 2.4.2 Spin projection of determinants; 2.4.3 Total spin of determinants; 2.5 Configuration state functions; 2.6 The genealogical coupling scheme; 2.6.1 Representations of determinants and CSFs
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3.1.4 Orthogonal matrices3.1.5 Evaluation of matrix exponentials; 3.1.6 Nonunitary transformations; 3.2 Unitary spin-orbital transfonnations; 3.2.1 Unitary matrix expansions of creation and annihilation operators; 3.2.2 Exponential unitary transfonnations of the elementary operators; 3.2.3 Exponential unitary transfonnations of states in Fock space; 3.3 Symmetry-restricted unitary transfonnations; 3.3.1 The need for symmetry restrictions; 3.3.2 Symmetry restrictions in the spin-orbital basis; 3.3.3 Symmetry restrictions in the orbital basis; 3.4 The logarithmic matrix function
3.4.1 Definition of the logarithmic matrix function

Sommario/riassunto

Ab initio quantum chemistry has emerged as an important tool in chemical research and is appliced to a wide variety of problems in chemistry and molecular physics. Recent developments of computational methods have enabled previously intractable chemical problems to be solved using rigorous quantum-mechanical methods. This is the first comprehensive, up-to-date and technical work to cover all the important aspects of modern molecular electronic-structure theory. Topics covered in the book include:* Second quantization with spin adaptation* Gaussian basis sets and molecular-integral evaluation* H