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On the evaluation of determinantal wave functions in open-shell Hartree-Fock theory

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Abstract: Slater method is modified for the evaluation of determinantal wave functions appearing in open-shell Hartree-Fock (HF) theory [1]. Using modified Slater method we have calculated, as an example, the orbital energies and the wave functions of terms obtained from the electronic configuration of a ground state of an N-atom system in the Hartree-Fock-Roothaan (HFR) approximation. The modified determinantal method introduced in this paper can be of considerable help and importance in the simplification and calculation of atomic and molecular electronic structure.

Key Words: Open-shell system; Hartree-Fock theory; Determinantal wave function.

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