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Analytic Evaluation of two-electron Atomic Integrals involving Extended Hylleraas-CI functions with STO basis

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Abstract : Some typical overlap/potential energy integrals which occur in the use of extended Hylleraas-configuration interaction (E-Hy-CI) functions with Slater-type orbital (STO) basis for two-electron atomic structure calculations, have been evaluated analytically. The corresponding kinetic energy integrals have been simplified first by using formulas derived from Gauss′ divergence theorem in vector calculus, and then expressed in terms of overlap / potential energy matrix elements. Also closed-form expressions for such integrals which arise in the application of Hylleraas-CI functions, and CI functions have been obtained as special cases, and the calculated values are found to agree well with correct results published by other investigators.

Keywords : Exponentially correlated integrals, E-Hy-CI calculations, Two-electron atoms.

[Full Paper]