Complete Single−Center Basis Sets in Atomic Calculations[1]

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Single particle orbitals centered on the nucleus are the most commonly used basis in large-scale calculations of atomic structure. The convergence towards a complete basis set, with respect to both the number and angular momenta of the orbitals included in a configuration interaction (CI) expansion, has been investigated using the ground and excited states of the helium atom [1,2,3]. This enabled energies to be determined to within 10^{-8} Hartree, whilst the convergence of the electron-electron δ-function and other relativistic corrections have been examined in detail. Unusual convergence patterns in the CI-Kohn variational scattering method have been observed and, however, high-precision calculations of elastic positron scattering from atoms are achievable [4].

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