VARIATIONAL QUANTUM MONTE CARLO CALCULATIONS INCLUDING SPIN-ORBIT COUPLING

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Electron correlation and relativistic effects play an important role in the chemistry and physics of heavy elements. Relativistic pseudopotentials do not only offer a possibility to reduce the computational effort by means of elimination of the core electrons, but also represent an efficient and reliable way to incorporate scalar relativistic as well as spin-orbit dependent terms in the Hamiltonian. Using this type of valence-only model Hamiltonian we performed variational Quantum Monte-Carlo calculations for atoms and small molecules of heavy elements. Electron correlation was accounted for by Jastrow factors which depend explicitly on the inter-electronic distances. The influence of dynamical correlation on the fine-structure of heavy atoms was investigated. In order to check the accuracy of our valence-only approach, we compare the results to those of fully relativistic all-electron configuration interaction calculations.