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QUANTUM MONTE CARLO METHOD FOR HEAVY ATOMIC AND MOLECULAR SYSTEMS WITH SPIN-ORBIT INTERACTIONS[1] CODY MELTON, LUBOS MITAS, North Carolina State Univ — We present a new quantum Monte Carlo (QMC) method that can treat spin-orbit and other types of spin-depentent interactions explicitly. It is based on generalization of the fixed-phase and projection of the nonlocal operators with spinor trial wave functions. For testing the method we calculate several atomic and molecular systems such as Bi, W, Pb, PbH and PbO, some of them with both large- and small-core pseudopotentials. We validate the quality of the results against other correlated methods such as configuration interaction in two-component formalism. We find excellent agreement with extrapolated values for the total energies and we are able to reliably reproduce experimental values of excitation energies, electron affinity and molecular binding. We show that in order to obtain the agreement with experimental values the explicit inclusion of the spin-orbit interactions is crucial.

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