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Diffusion quantum Monte Carlo for atomic spin-orbit interactions[1] MINYI ZHU, SHI GUO, LUBOS MITAS, North Carolina State University — We present a generalization of the quantum Monte Carlo methods (QMC) for dealing with the spin-orbit (SO) effects in heavy atom systems. For heavy elements, the spin-orbit interaction plays an important role in electronic structure calculation and becomes comparable to the exchange, correlations and other effects. We implement relativistic lj-dependent effective core potentials for valence-only calculations. Due to the spin-dependent Hamiltonian, the antisymmetric trial wave functions are constructed from two-component spinors in jj-coupling so that the states are labeled by its total angular momentum J. A new spin representation is proposed which is based on summation over all possible spin states without generating large fluctutations and the fixed-phase approximation is used to avoid the sign problem. Our approach is different from the recent idea based on rotating (sampling) the spinors according to the action of the spin-orbit operator. We demonstrate the approach on heavy atom and small molecular systems in both variational and diffusion Monte Carlo methods and we calculate both ground and excited states. The results show very good agreement with independent methods and experimental results within the accuracy of the used effective core potentials.

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