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Variational and diffusion quantum Monte Carlo methods for spin-orbit interactions in heavy element systems[1] LUBOS MITAS, RENE DERIAN, SHI GUO, North Carolina State University — In most electronic structure quantum Monte Carlo calculations spins of individual electrons have fixed values which are determined by the spin and spatial symmetries of the desired eigenstate. However, for heavy atoms the spin-orbit interaction becomes important and its influence on electronic structure becomes comparable to the electron exchange, correlations or other many-body effects. In such cases the simplest antisymmetric wave function based on one-particle states is a determinant of spinors, while the simplest pairing wave function is a pfaffian. We will present calculations using variational and diffusion Monte Carlo for heavy atoms systems with spin-orbit operators. We eliminate the atomic cores by effective core potentials (pseudopotentials) which are formulated so as to include also effective spin-orbit operators. We test both discrete spin sampling as well as continuous spin representation in the variational and diffusion Monte Carlo methods. Corresponding generalizations of the fixed-node/fixed-phase methods will be discussed as well.

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