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Spin-orbit interaction in quantum Monte Carlo LUBOS MITAS, North Carolina State University, RENE DERIAN, Institute of Physics, Slovak Academy of Sciences, SHI GUO, North Carolina State University — For spinless Hamiltonians (ie, no explicit spin operators), real space quantum Monte Carlo (QMC) methods such as variational and fixed-node diffusion Monte Carlo are well established. In these cases the electron spins and their components commute with the Hamiltonian and therefore are conserved quantities. This implies that spins can be fixed as given by the symmetry of a considered state and one solves only for the spatial part of the corresponding wave function. Indeed, this is a common practice in electronic structure QMC and also in most quantum chemical calculations. However, many systems require treating spins as quantum dynamical variables. We will present progress of our studies in this direction both in variational and diffusion Monte Carlo for heavy atoms with spin-orbit operators. One possibility is to use possibilities offered by various formulations of Hubbard-Stratonovitch transformation as realized in QMC for nuclear systems. We explore also other options both in variational and diffusion Monte Carlo framework. In particular, we define new representation for spinors which enable to formulate the diffusion Monte Carlo along the lines of fixed-phase approximation. We compare the results for the considered approaches also from the point of computational efficiency.

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