Spins as variables in electronic structure quantum Monte Carlo calculations[1] LUBOS MITAS, MINYI ZHU, SHI GUO, North Carolina State University — Current electronic structure quantum Monte Carlo (QMC) methods keep particle spins static in configurations that correspond to spin-space symmetries of calculated states. Here we present a generalization of the QMC approaches for treating fermionic spin degrees of freedom as variables. The developed method possesses two key properties that make it suitable for high accuracy calculations of real systems. First, the spinors entering the trial function are kept intact during the imaginary time evolution. Second, the approach has the zero variance property pointwise for arbitrary configurations of spatial and appropriately chosen spin coordinates. The spin coordinates are overcomplete and therefore can be smoothly evolved in the imaginary time propagation. The method is illustrated on molecules and atomic excitations of heavy elements with spin-orbit interactions and on 2D electron gas with the Rashba interaction. The performance of the method is similar to the commonly used static spin calculations in several aspects such as achieved accuracy and energy fluctuations. The corresponding wave functions have lower symmetries and therefore can exhibit potentially stronger multi-reference character as is observed in some cases.

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