Quantum Chemistry by Random Walk

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The fixed-node diffusion quantum Monte Carlo (FN-DQMC) method is a random walk based approach to solving the Schrödinger equation. We developed a variant of the FN-DQMC based on the Ornstein-Uhlenbeck random walk and the floating spherical Gaussian orbitals and spherical Gaussian geminals (designated as the OUDQMC/FSGO-SGG). We present the basics, applications, and further directions of this approach. The calculated results for equilibrium atomization energy, equilibrium dipole moment, optimized geometry, harmonic frequency, potential energy surface, and electron affinity of first-row molecules are given and compare with the experimental values and calculated results from other sophisticated levels of theory. This comparison demonstrates the performance and systematic accuracy of the OUDQMC/FSGO-SGG method.