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Auxiliary field quantum Monte Carlo with a localized basis—applications to atoms and molecules¹ WISSAM A. AL-SAIDI, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — We extended the recently introduced phaseless auxiliary field quantum Monte Carlo approach [1] to any single-particle basis, and applied it to study atoms and molecules using localized Gaussian basis. This method maps the interacting many-body problem into a linear combination of non-interacting problems using a complex Hubbard-Stratonovich transformation, and controls the phase/sign problem using a trial wave function. It employs a random walk approach in Slater determinant space to project the many-body ground state of the system. The computational cost scales as a low power of system size. In all of the presented results the trial wave function was from a Hartree-Fock calculation. The obtained total energies of the atoms and molecules agree to within a few milli Hartrees with the exact value from full configuration interaction or density matrix renormalization group. The results are comparable in accuracy to those of CCSD(T) for equilibrium geometries but are superior for bond breaking. [1] S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003).

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