Abstract Submitted
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Bond Breaking of Simple Molecules in Auxiliary-Field Quantum Monte Carlo with GVB Wave Functions[1] WIRAWAN PURWANTO, HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary, WISSAM AL-SAIDI, Cornell University — Accurate potential energy curves are an essential ingredient in understanding chemical reactions. This problem spans a wide range of correlations, with correlation effects being the most important in the bond-breaking regime. We report potential energy curves of simple molecules, including water and the carbon dimer, within the framework of the auxiliary-field quantum Monte Carlo (AFQMC) method. AFQMC projects the many-body ground-state from a trial wave function, which is also used to control the sign/phase problem. A previous calculation[2] showed that AFQMC could provide a fairly uniform description of the bond stretching of a water molecule, even with a simple unrestricted Hartree-Fock (UHF) trial wave function. We investigate the use of Generalized Valence Bond (GVB). GVB gives a better description of the molecule than UHF; so it is a simple yet efficient alternative to using a single Slater determinant trial wave function. We will compare AFQMC results with other correlated methods and the exact configuration interaction calculations.

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[2]Al-Saidi, Zhang, Krakauer, J. Chem. Phys. **124**, 224101 (2006)

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