Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

**Bond breaking in auxiliary-field quantum Monte Carlo**[1] WISSAM A. AL-SAIDI[2], HENRY KRAKAUER, SHIWEI ZHANG, College of William and Mary — Bond stretching mimics different levels of electron correlations in the system and provides a challenging testbed for all approximate many-body computational methods. Using the recently developed phaseless auxiliary-field quantum Monte Carlo (AF QMC) method, we study the potential-energy curves of several well-known molecules — BH, $N_2$, and $F_2$ — and of the $H_{50}$ chain. To control the sign/phase problem, the phaseless AF QMC method constrains the random walks with an approximate phase condition that depends on a trial wave function. With single-determinant unrestricted Hartree-Fock trial wave functions, the phaseless AF QMC method generally gives better overall accuracy and a more uniform behavior than the coupled cluster CCSD(T) method in mapping the potential-energy curve. In the molecules, the use of multiple-determinant trial wave functions from multi-configuration self-consistent-field calculations is also explored. The increase in computational cost versus the gains in statistical and systematic accuracy are examined. With such trial wave functions, excellent results are obtained across the entire region between equilibrium and the dissociation limit.

[1]Work was supported by ONR, NSF,DOE CMSN, and ARO.
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Date submitted: 27 Nov 2006 Electronic form version 1.4