Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Frozen core method in auxiliary-field quantum Monte Carlo[1] WIRAWAN PURWANTO, SHIWEI ZHANG, HENRY KRAKAUER, Department of Physics, College of William and Mary, Williamsburg, VA — We present the implementation of the frozen-core approach in the phaseless auxiliary-field quantum Monte Carlo method (AFQMC). Since AFQMC random walks take place in a many-electron Hilbert space spanned by a chosen one-particle basis, this approach can be achieved without introducing additional approximations, such as pseudopotentials. In parallel to many-body quantum chemistry methods, tightly-bound inner electrons occupy frozen canonical orbitals, which are determined from a lower level of theory, e.g. Hartree-Fock or CASSCF. This provides significant computational savings over fully correlated all-electron treatments, while retaining excellent transferability and accuracy. Results for several systems will be presented. This includes the notoriously difficult Cr_2 molecule, where comparisons can be made with near-exact results in small basis sets, as well as an initial implementation in periodic systems.

[1]Supported by DOE, ONR, and NSF. Calculations were performed at OLCF Jaguar and CPD.

Wirawan Purwanto
Department of Physics, College of William and Mary, Williamsburg, VA

Date submitted: 11 Nov 2011 Electronic form version 1.4