An Improved Pressure Estimator for quantum Monte Carlo[1]
JEREMY MCMINIS, JEONGNIM KIM, DAVID CEPERLEY, Department of Physics, University of Illinois, CARLO PIERLEONI, Department of Physics, University of L'Aquila — Assaraf and Caffarel have developed a systematic method for deriving reduced variance estimators for observables for quantum Monte Carlo calculations and have applied to forces[1], the one body density and the spherical and system averaged pair density. It has yet to be applied to a thermodynamic observable. In this work we derive an expression for an improved pressure estimator for use in variational Monte Carlo and diffusion Monte Carlo calculations. We show that because the dependence of the trial wave function on the density is known, for the homogeneous electron gas this new estimator is accurate and efficient to implement. We discuss its application to many-body Hydrogen at high pressure. [1] Roland Assaraf and Michel Caffarel, J. Chem. Phys. 113, 4028 (2000)

Jeremy McMinis
University of Illinois, Department of Physics

Date submitted: 27 Nov 2007   Electronic form version 1.4