Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

An energy density estimator for quantum Monte Carlo calculations JARON KROGEL, University of Illinois at Urbana-Champaign, JEONGNIM KIM, University of Illinois at Urbana-Champaign; Oak Ridge National Laboratory, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — We establish a physically meaningful representation of a quantum energy density for use in quantum Monte Carlo calculations. The energy density operator, defined in terms of Hamiltonian components and density operators, returns the correct Hamiltonian when integrated over a volume containing a cluster of particles. This property is demonstrated for a Helium-Neon "gas," showing that atomic energies obtained from the energy density correspond to eigenvalues of isolated systems. The formation energies of defects or interfaces are typically calculated as total energy differences. Using a model of delta doped Silicon (where dopant atoms form a thin plane) we show how interfacial energies can be calculated more efficiently with the energy density, since the region of interest is small. We also demonstrate how the energy density correctly transitions to the bulk limit away from the interface where the correct energy is obtainable from a separate total energy calculation.

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Date submitted: 11 Nov 2011 Electronic form version 1.4