Boson Correlation Energies from Reduced Hamiltonian Interpolation

David A. Mazziotti †,‡ and Dudley R. Herschbach ‡

[†]Department of Chemistry, Duke University, Durham, NC 27708-0354 [‡]Department of Chemistry, 12 Oxford Street, Harvard University, Cambridge, MA 02138 (August 12, 1999)

Abstract

The ground state energies of interacting bosons are computed beyond the mean-field approximation through a new method which we call reduced Hamiltonian interpolation (RHI). Within RHI the N-particle Hamiltonian is represented through a sequence of p-particle expanded and reduced Hamiltonians which give upper and lower bounds on the true energy. Combining ideas from N-representability and dimensional interpolation, the RHI technique interpolates over the number p of quasi-particles (equivalent to spatial dimension) through sequential quadratic programming to calculate the N-particle energy as the mean of close upper and lower bounds. Application of the method to systems of spinless bosons with harmonic interactions yields more than ninety-nine percent of the correlation energy.