“Generic D-dependence and renormalization of large-D limit by combination with Hartree-Fock results”

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Abstract
We will examine prototypical D-dependence for simple atoms and molecules. Special attention will be given to the application of a simple renomalization procedure which markedly improves Hartree-Fock via melding with analytic large-D approximation for N-electron atoms (N = 2 → 290), thus improving the global Thomas-Fermi result. Potential applications include enhancement of density functional theory.

Wednesday, October 7, 2009
11:30 a.m. Room 256
Jack E. Brown
(Chemical Engineering Building)

Texas A&M University
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(Pizza and soda to be served at 12:45 p.m. 256 JEB)