

SPECIAL CHEMICAL PHYSICS AND PIZZA SEMINAR SERIES

***“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 renormalization procedure which markedly improves Hartree-Fock via melding with analytic large- D approximation for N -electron atoms ($N = 2 \rightarrow 290$), 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
Department of Physics**

(Pizza and soda to be served at 12:45 p.m. 256 JEB)