# SPECIAL CHEMICAL PHYSICS AND PIZZZA SEMINAR SERIES

## "D-scaling as a means to tame dynamical correlations among strongly interacting particles"

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#### Abstract

Basic method will be outlined with illustrations to include electron correlation in atoms, shapes of random walks, and equation of state for hard-sphere fluids. Key aspect to be emphasized is that many-body effects, when normalized to one- or few-body problems, tend to have only a mild dependence on dimensionality.

> Wednesday, September 2, 2009 10:30 a.m. Room 501 Engineering /Physics Building

> > Texas A&M University Department of Physics

(Pizza and soda to be served at 12:00 p.m. suite 301 Doherty)

#### **Dimensional Scaling in Chemical Physics**

Dudley Herschbach

This fall, I'll offer a series of talks and discussion meetings designed to approximate an informal seminar course. The intent is to complement the graduate course given last spring by Dr. Goong Chen, Math 689, with the same title. He is leading a project to produce a book that will include both tutorial material and research contributions from several members of the TAMU Institute for Quantum Studies. I plan to give three seminars, which will be held on Wednesdays, correlated with discussion meetings, held on adjacent Tuesdays and/or Thursdays. Everyone is invited to the Wednesday meetings, which will be largely heuristic in style; a chief aim is to exhibit aspects likely to find wider application. The pre- or post-sessions will be limited to students and postdocs (in response to the evaluation comments elicited by my course on molecular collisions last year). There students & postdocs will be invited to present solutions to homework problems and go over details of derivations, etc. Dates, locations, and main topics for the Wednesday talks are as follows.

**2 September (ENPH 501, 10:30 am – 11:30 am):** *D-scaling as a means to tame dynamical correlations among strongly interacting particles*. Outlines basic method; illustrations include electron correlation in atoms; shapes of random walks; equation of state for hard-sphere fluids. Key aspect: many-body effects, when normalized to one- or few-body problems, tend to have only mild dependence on dimensionality.

7 October (CHEN 256, 11:30 am – 12:30 pm): Generic D-dependence and renormalization of large-D limit by combination with Hartree-Fock results. Examines prototypical D-dependence for simple atoms and molecules; applies simple renomalization procedure to markedly improve Hartree-Fock via melding with analytic large-D approximation for N-electron atoms (N =  $2 \rightarrow 290$ ), thereby improves global Thomas-Fermi results with potential application to enhance density functional theory.

9 December (CHEN 256, 11:30 am – 12:30 pm): *Further ways, indicated or anticipated, to extend utility and scope of D-scaling.* Examines relation to uncertainty principle, how D-scaling permits computing quantum tunneling by purely classical means, how it reveals hidden symmetries and phase transitions involved in electronic structure. Considers prospects for joining with other unconventional methods.

Dates, times, and locations for the Tuesday/Thursday meetings to be announced later. Also, during intermediate weeks, Prof. Chen and others at TAMU working on D-scaling may offer some additional talks or discussion meetings.