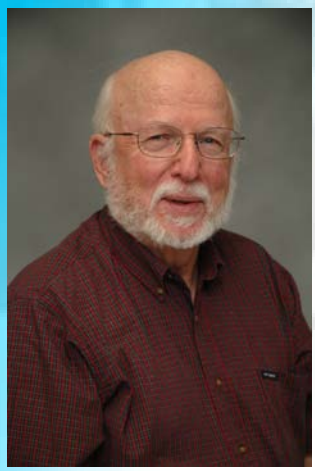
Physics Colloquium

Michigan Technological University

Thursday, October 13, 2011 at 4:00 pm
Room 139 Fisher Hall



Many-electron Quantum Statistical Mechanics without Orbitals

Sam B. Trickey
Quantum Theory Project
Dept. of Physics and Dept. of Chemistry
Univ. of Florida, Gainesville, FL

Abstract: Early in quantum mechanics, a seductive question arose: can many-electron systems be treated without many-electron wave functions? Provocatively, the over-simplification of Thomas-Fermi- Dirac theory does just that. Modern density functional theory gives, formally, an affirmative answer. But DFT almost always is implemented with the Kohn-Sham decomposition of the variational principle via one-electron wave functions (orbitals.)

Orbital-free DFT is immensely appealing both for its intellectual purity and its potential for speedier simulations. OF-DFT would give Born-Oppenheimer forces for first-principles molecular dynamics at a computational cost which scales as the relevant system volume, not some power of the electron count N_e.

The notorious barrier to OF-DFT is lack of an accurate, orbital-free approximation for the Kohn-Sham kinetic energy functional T_s. At non-zero temperature, the KS entropy functional S_s is an added barrier. Ironically, Perdew's exchange-correlation (XC) functional ladder raises another barrier: higher rungs depend explicitly on the KS orbitals.

After an orientation to DFT basics, I shall discuss recent work on the physics of constructing useful, constraint-based T_s, S_s, and E_{xc} approximations, with emphasis on T = 0 K. For T_s, I shall discuss single-point OF-functionals of the generalized gradient approximation (GGA) type, as well as physical limitations on the information-theory type of functional. I shall discuss improved GGA-type E_{xc} functionals, VMT and VT{84}, that come from tightening and refining the enforcement of important constraints. For free-energies, I shall discuss recent tests of published functionals via finite temperature Hartree-Fock simulations of several H atoms in a box. I shall conclude with a summary of the outlook for both zero-temperature and finite-temperature (free-energy) orbital-free density functionals.
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Biography: Professor Samuel B. Trickey obtained his Ph.D. from Texas A&M University in 1968. He is currently professor emeritus at the University of Florida. He was the director of the Quantum Theory project as well as the executive director of Information Technology and Services at the University of Florida. Prior to that, he was the Professor and department chair at Texas Tech University. He is a Fellow of American Physical Society. He has made number of seminal contributions towards the development of density functional theory including the publication of several DFT codes WIEN, PUPIL, GTOFF.

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