Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**The Hubbard Dimer: A Complete DFT Solution to a Many-Body Problem**[1] JUSTIN SMITH, Univ of California - Irvine, DIEGO CARRASCAL, JAIME FERRER, Universidad de Oviedo, KIERON BURKE, Univ of California - Irvine — In this work we explain the relationship between density functional theory and strongly correlated models using the simplest possible example, the two-site asymmetric Hubbard model. We discuss the connection between the lattice and real-space and how this is a simple model for stretched $H_2$. We can solve this elementary example analytically, and with that we can illuminate the underlying logic and aims of DFT. While the many-body solution is analytic, the density functional is given only implicitly. We overcome this difficulty by creating a highly accurate parameterization of the exact function. We use this parameterization to perform benchmark calculations of correlation kinetic energy, the adiabatic connection, etc. We also test Hartree-Fock and the Bethe Ansatz Local Density Approximation. We also discuss and illustrate the derivative discontinuity in the exchange-correlation energy and the infamous gap problem in DFT.

[1]DGE-1321846, DE-FG02-08ER46496

Justin Smith
Univ of California - Irvine

Date submitted: 14 Nov 2014 Electronic form version 1.4