Abstract Submitted
for the 4CF15 Meeting of
The American Physical Society

Understanding Integration Schemes in DFT[1] MATTHEW BURBIDGE, SPENCER HART, JEREMY JORGENSEN, GUS HART, Brigham Young University — The 1998 Nobel prize was given to Kohn and Pople for their development of Density Functional Theory. DFT allows one to do quantum-mechanical calculations for materials and has been developed into a powerful computational tool. Typical DFT calculations require a numerical integral over the electron occupied states in the material. Even though this integral is a small piece of the overall calculation, it is a primary source of error. Through the use of a simple toy problem, we will explain the fundamentals of the integration problem. We will introduce some of the attempts at resolving it and explore their effectiveness in current DFT codes. The resolution of this integration problem for metals will result in millions of CPU hours saved for a typical computational materials scientist.

[1]ONR (MURI N00014-13-1-0635)

Matthew Burbidge
Brigham Young University

Date submitted: 10 Sep 2015 Electronic form version 1.4