Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Understanding the correlation function of the inhomogeneous hard-sphere fluid JEFF SCHULTE, PATRICK KREITZBERG, CHRIS HAGLUND, DAVID ROUNDY, Oregon State University — We present a new functional for the correlation $g(r)$ at contact for an inhomogeneous distribution of hard spheres. This term is a key input into classical density functional theories developed using Statistical Associating Fluid Theory, a widely used approach for handling complex liquids in which hydrogen bonding plays an important role. We use a thermodynamic approach to derive an exact formula for the correlation expressed as a derivative of the free energy functional. We evaluate this approach using the approximate free energy of the "White Bear" version of Fundamental Measure Theory, and test our approach (and two previously published approximations) against correlation values found from Monte Carlo simulations.

Jeff Schulte
Oregon State University

Date submitted: 11 Dec 2012 Electronic form version 1.4