

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Analytic Treatment of the Pair Density in Kohn-Sham Density Functional Theory¹ MARKUS DAENE, Oak Ridge National Laboratory, ANTONIOS GONIS, Lawrence Livermore National Laboratory, DON M. NICHOLSON, G. MALCOLM STOCKS, Oak Ridge National Laboratory — We have developed a new treatment of the LDA functional in Kohn-Sham density functional theory which is expressed in terms of the pair density of a non-interacting system of particles, thus avoiding from the outset self-interaction effects. The pair density is expressed explicitly in terms of the density using a orthonormal and complete basis expressed as a functional of the density. This allows its functional differentiation with respect to the density by analytic means. The method is illustrated with numerical results for the potential in the case of one and three dimensional systems and is compared to the potentials obtained from the Hartree term.

¹This material is based upon work supported as part of the Center for Defect Physics, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

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Date submitted: 19 Nov 2010

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