Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Semiclassical approach to the exchange energy from potential functional theory

ATTILA CANGI, PETER ELLIOTT, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Germany), STEFANO PITTLALIS, CNR-NANO S3, Via Campi 213A, I-41125 Modena, Italy, E.K.U. GROSS, Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Germany), KIERON BURKE, Department of Chemistry, University of California, Irvine, CA 92697 — Although Kohn-Sham (KS) density functional theory is being successfully and ever increasingly applied for computing the electronic structure of matter, there is a lack of a systematic procedure for deriving reliable approximations for its main ingredient – the exchange-correlation (XC) energy functional. Potential functional theory\cite{1,2,3} is an alternative approach that may provide a solution to this long-standing problem. In our line of research we had only considered potential functional approximations to the KS kinetic energy\cite{4,5} so far. In this work, we (i) propose approximating the XC energy straight as a functional of the KS potential and (ii) derive a highly accurate potential functional approximation to the exchange energy for the simplest relevant model system using semiclassical techniques\cite{6}.

\begin{thebibliography}{9}
\end{thebibliography}

Attila Cangi
Max Planck Institute of Microstructure Physics,
Weinberg 2, 06120 Halle (Germany)

Date submitted: 14 Nov 2013

Electronic form version 1.4