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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 PITTALIS, 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[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[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[6]. [1] W. Yang, P. W. Ayers, and Q. Wu, Phys. Rev. Lett. 92, 146404 (2004). [2] A. Cangi, D. Lee, P. Elliott, K. Burke, and E.K.U. Gross, Phys. Rev. Lett. 106, 236404 (2011). [3] A. Cangi, E.K.U. Gross, K. Burke, Phys. Rev. A (2013), accepted. [4] P. Elliott, D. Lee, A. Cangi, and K. Burke, Phys. Rev. Lett. 100, 256406 (2008). [5] A. Cangi, D. Lee, P. Elliott, and K. Burke, Phys. Rev. B 81, 235128 (2010). [6] A. Cangi, P. Elliott, S. Pittalis, E.K.U. Gross, K. Burke, submitted.

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