

Abstract Submitted  
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**Modeling of the exact exchange derivative discontinuity in semi-local potentials** ALEXANDER LINDMAA, RICKARD ARMIENTO, Linkping University — The derivative discontinuity (DD), i.e., the abrupt constant shift of the exchange-correlation potential at integer particle numbers plays a crucial role in Kohn-Sham density-functional theory (KS DFT). It is needed to determine the fundamental gap of a system, and is, e.g. related to obtaining an adequate description of charge transfer. While usual semi-local approximations give good results for properties related to the total energy, they do not in general possess a DD. A recently proposed semi-local exchange functional, AK13 [1], mimics features related to the DD by a discontinuous change of its asymptote upon adding a fraction of an electron through an integer. This is because its potential depends asymptotically on the highest occupied KS eigenvalue. In this work we investigate the behavior of the DD in exact exchange (EXX) within the optimized effective potential (OEP) method for simple systems such as spherically symmetric atoms. We compare with the general behavior that results from the AK13 construction, and other alternatives. We discuss some challenges related to describing the EXX DD correctly in future development of semi-local functionals based on the AK13 construction. [1] Phys. Rev. Lett. 111, 036402 (2013)

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