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An Exchange Energy Functional with a Derivative Discontinuity

RICKARD ARMIENTO, Linkoping University, STEPHAN KUEMMEL, Universitat Bayreuth — We explore a way to impose a derivative discontinuity onto a semi-local energy functional in density functional theory, rather than a model potential. The derivative discontinuity is a property of exact exchange that states that the exchange potential may have a uniform discontinuous shift as the particle number passes through an integer. The lack of this property is a known major deficiency of current approximate semi-local exchange functionals. We obtain a closed form expression with a number of attractive properties that can be related to an improved description of charge transfer, overdelocalized orbital states, and band gaps, i.e., deficiencies that are commonly seen in applied use of DFT. Various tests of the construction are presented that clarify the relationship between these issues and the derivative discontinuity.

Rickard Armiento
Linkoping University

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