

Abstract Submitted
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The discontinuous nature of the exchange-correlation functional – critical for strongly correlated systems PAULA MORI-SANCHEZ, ARON COHEN, WEITAO YANG, Duke University — Standard approximations for the exchange-correlation functional have been found to give big errors for the linearity condition of fractional charges, leading to delocalization error, and the constancy condition of fractional spins, leading to static correlation error. These two conditions are now unified for states with both fractional charge and fractional spin: the exact energy functional is a plane, linear along the fractional charge coordinate and constant along the fractional spin coordinate with a line of discontinuity at the integer. This sheds light on the nature of the derivative discontinuity and calls for explicitly discontinuous functionals of the density or orbitals that go beyond currently used smooth approximations. This is key to understand the physics of strongly correlated systems within DFT, for example the band-gap of Mott insulators. [arXiv:0809.5108]

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