The performance of the parameterized TFDW kinetic functional on molecules

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We assess the performance of parameterized orbital-free (OF) functionals on atoms and molecules self-consistently with all-electron values obtained with projector augmented-wave method[1] (PAW).

Specifically we investigate Thomas-Fermi-Weizsäcker model for kinetic functional where fractions of Thomas-Fermi and Weizsäcker are parameterized as (γ, λ), respectively, in atoms [2]. Our interest lies in total energy and Euler equation eigenvalue. The optimum (γ, λ) with respect to Kohn-Sham values is however different for each property and atom investigated. Recently these results have been combined to investigate the transferrability of these parameters from atoms to molecules [3]. We also look at the optimum parameters with respect to other properties, like bond length, in molecules HF, HCl, CO, and H_2O

We also present some findings on how the parameterized kinetic functional describes charged systems. Banguria and Lieb have shown that certain orbital-free model $(\gamma = 1, \lambda = 0.37)$ does not have negative ions[4] and our numerics indicate that this seems to be the case also for some other (γ, λ) models.

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