

Title: Exchange-Correlation functionals inspired to the exact strong-coupling limit of density functional theory

P. Gori-Giorgi

Vrije Universiteit Amsterdam

De Boelelaan 1083

1081 HV Amsterdam

The Netherlands

email: p.gorigiorgi@vu.nl

ABSTRACT:

The exact strong-coupling limit of density functional theory (DFT) reveals a mathematical structure very different from the one of traditional approximations for the exchange-correlation functionals. Instead of the usual local density, local density gradients, Kohn-Sham orbitals, and related quantities, in this limit we observe the appearance of certain integrals of the density. I will illustrate some approximations that we have proposed inspired to this mathematical structure. These approximations retain some of the non-locality of the exact strong-coupling limit of DFT while being computationally affordable.