Study of the large reduced density gradient limit for the exchange energy JOSE GAZQUEZ, JAVIER CARMONA-ESPINDOLA, Universidad Autonoma Metropolitana-Iztapalapa, ALBERTO VELA, Centro de Investigacin y de Estudios Avanzados, SAM TRICKEY, University of Florida — The generalized gradient approximation (GGA) for the Kohn-Sham exchange-correlation functional has become widely used in electronic structure calculations of small, medium and large systems, because it provides rather reasonable results with moderate computational effort. Usually the GGA for exchange (X) is expressed in terms of an analytical expression of the X enhancement function, Fx(s), where s is the reduced density gradient. When a non-empirical approach based on constraint satisfaction is followed, the analytical expression of Fx(s) is the result of interpolating between the small- and large-s limits. However, neither of those limits is uniquely defined. In both cases there are several possibilities. The present work is a study of the influence of the several large-s limit possibilities upon the calculation of properties that depend on energy differences, versus those that depend on response functions, and excitation energies.

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