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Scaling properties of the kinetic energy density of atoms – towards an orbital-free meta-GGA. ANTONIO CANCIO, JEREMY REDD, Ball State University — The scaling properties of atoms, combining periodicity with gradual increase in density, make a fruitful probe of relationships in density functional theory, and have driven advances in understanding the exchange and correlation energy. Although focus is normally upon the properties of integrated energies, insights can be generated from studying energy density functions as well. We visualize the behavior of the positive-definite kinetic energy density (KED) in closed-shell atoms, in comparison to invariant quantities based upon the gradient and Laplacian of the density. The latter are potential variables for constructing orbital-free functionals for the KE and can be used for analyzing the electronic structure of atoms and molecules. We notice a striking fit of the KED within the core of any atom to a gradient expansion model using both the gradient and the Laplacian, but one different from that derived from first principles for a slowly-varying electron gas. Correlated with this feature, we notice unexpected structure to the KED near the nucleus that cannot be explained simply by the von Weizsacker model, as is often presumed. These unexpected features provide potential insights for developing better orbital-free meta-GGA models for the kinetic energy.

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