O.15 Are plane-waves basis packages able to predict the correct long range behavior of the local kinetic energy per particle?

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The Kinetic energy density $\tau(\mathbf{r})$ is an important quantity not only in density functional theory but also in wave-function methods used to compute the electronic structure of molecules and condensed matter systems. In particular, for finite systems it has been shown that $G = \tau(\mathbf{r})/n(\mathbf{r})$, which gives the local kinetic energy per particle, approaches asymptotically to the first ionization energy [1]. Such behavior is mostly due to the exponential decay of the multielectronic wave function as $r \to \infty$ [2]. It also represents an alternative to Koopmans' theorem for the calculation of the ionization energy in DFT [3]. In meta-GGA functionals τ is of prime importance since the XC energy depends explicitly on it. We propose to use this quantity as a quality indicator of the approximations and numerical implementations aiming to describe correctly the electronic properties of finite systems. In this work we have evaluated the asymptotic behavior of G in ABINIT for several rare gas atoms, Hydrogen and second raw elements using norm-conserving pseudopotentials and compare to Coupled Cluster and existing analytic solutions of the same problem. In the case of Hydrogen, the self-interaction error prevents an accurate DFT description. However, by using the Fermi-Amaldi correction and the bare coulomb potential of the proton, G approaches the exact value of the ionization energy in a systematic way. Our results show that for the case of finite systems, the common convergence studies of the total energy with respect to both plane-waves cut-off energy and unit cell size, is not enough to obtain the expected behavior of G in real space.

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