Application of a Coulomb energy density functional for atomic nuclei: Case studies of local density approximation and generalized gradient approximation†

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The exchange (x) and correlation (c) energy density functionals $E_{\rm x}[\rho]$ and $E_{\rm c}[\rho]$ formulated for electron systems are tested in the context of atomic nuclei, respectively. Both the local density approximation (LDA) and generalized gradient approximation (GGA) functionals are investigated. For quantitative calculations, we employed the experimental charge-density distributions $\rho_{\rm ch}$[1] of the selected nuclei as inputs of ground-state density distributions.

When it is assumed that the energy density ε_i depends only on the density at $\boldsymbol{r}$ locally as

$$E_i[\rho] = \int \varepsilon_i(\rho(\boldsymbol{r}))\,\rho(\boldsymbol{r})\,d\boldsymbol{r} \qquad (i = \mathrm{x},\,\mathrm{c}), \tag{1}$$

this approximation is called the LDA. In the GGA, the energy density depends not only on the density distribution ρ but also on its gradient $|\nabla\rho|$ at $\boldsymbol{r}$ locally as

$$E_i[\rho] = \int \varepsilon_i(\rho(\boldsymbol{r}), |\nabla\rho(\boldsymbol{r})|)\,\rho(\boldsymbol{r})\,d\boldsymbol{r} \qquad (i = \mathrm{x},\,\mathrm{c}). \tag{2}$$

The GGA exchange energy density weighted with $\rho_{\rm ch}(r)$ for ^{208}Pb is shown in Fig. 1. The LDA result is shown with the long-dashed line, and those given by the GGA functionals B88,[2] PW91,[3] PBE,[4] and PBEsol[5] are shown with the short-dashed, dot-dashed, solid, and dot-dot-dashed lines, respectively. The surface is defined as the region that has a density between 90% and 10% of the maximum density.

For the exchange Coulomb energies, it is found that the deviation between the LDA and GGA,

$$\Delta E_{\rm x} = \frac{E_{\rm x}^{\rm GGA} - E_{\rm x}^{\rm LDA}}{E_{\rm x}^{\rm GGA}}, \tag{3}$$

ranges from around 11% in ^{4}He to around 2.2% in ^{208}Pb, by taking the PBE functional as an example of the GGA. From light to heavy nuclei, it is seen that $\Delta E_{\rm x}$ shown in Fig. 2 behaves in a very similar way as the deviation between the Hartree-Fock-Slater approximation and the exact Hartree-Fock given by Le Bloas *et al.*[6] In this sense, the GGA exchange functionals of electron systems can be applied in a straightforward manner with practical accuracy to atomic nuclei. Furthermore, the numerical cost of GGA is $O(N^3)$, whereas that cost of exact Hartree-Fock is $O(N^4)$ for

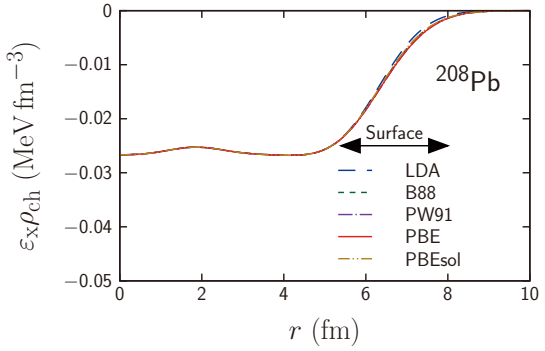

Fig. 1. GGA exchange energy densities weighted with $\rho_{\rm ch}$ for ^{208}Pb as a function of r.

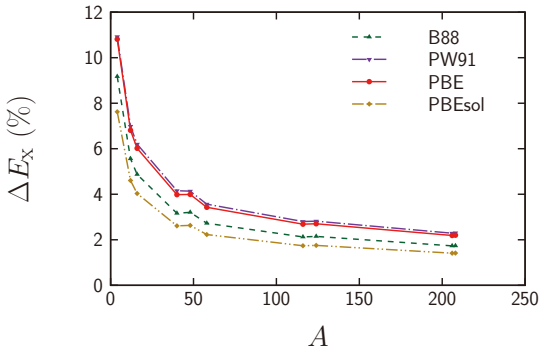

Fig. 2. Deviation between the LDA and GGA in $E_{\rm x}$ defined as Eq. (3) as a function of A.

self-consistent calculations. In contrast, the correlation Coulomb energy density functionals of electron systems are not applicable for atomic nuclei, because these functionals are not separable and the nuclear interaction determines the properties of atomic nuclei.

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