Coulomb exchange functional with generalized gradient approximation for self-consistent Skyrme Hartree-Fock calculations†

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Recently, it was shown that the Coulomb energy density functionals of the generalized gradient approximation (GGA) give almost the same accuracy as that of the exact-Fock energy[1] by using the experimental charge density distribution as inputs of the functional. As a step further, we carry out the corresponding self-consistent Skyrme Hartree-Fock calculation by using the Perdew-Burke-Ernzerhof GGA (PBE-GGA) Coulomb exchange functional[2] instead of the exact-Fock. The GGA Coulomb exchange functionals have been proposed as

$$E_{\mathrm{Cx}}\left[\rho_{\mathrm{ch}}\right]=-\frac{3e^2}{16\pi\varepsilon_0}\left(\frac{3}{\pi}\right)^{1/3}\int\left[\rho_{\mathrm{ch}}\left(\boldsymbol{r}\right)\right]^{4/3}F\left(s\left(\boldsymbol{r}\right)\right)\,d\boldsymbol{r}, \tag{1}$$

where F is the enhancement factor due to the density gradient, $F\equiv 1$ is the hold for the local density approximation (LDA), and ρ_{ch} is the charge distribution. Here, s denotes the dimensionless density gradient

$$s=\frac{|\boldsymbol{\nabla}\rho_{\mathrm{ch}}|}{2k_{\mathrm{F}}\rho_{\mathrm{ch}}},\qquad k_{\mathrm{F}}=\left(3\pi^2\rho_{\mathrm{ch}}\right)^{1/3}. \tag{2}$$

In particular, the enhancement factor F in the PBE-GGA Coulomb exchange functional is assumed to be[2]

$$F\left(s\right)=1+\kappa-\frac{\kappa}{1+\mu s^2/\kappa}, \tag{3}$$

in order to satisfy some physical conditions.[3] Accordingly, the parameter $\kappa=0.804$ is determined for any value of μ by the Hölder inequality. In contrast, two different values of μ have been widely used in the studies of atoms[2] and solids.[4] For the PBE-GGA functional, $\mu=0.21951$ is determined by the random phase approximation of the homogeneous electron gas. Since this μ can be a different value for nuclear systems, the free parameter of the PBE-GGA Coulomb exchange functional, μ, is multiplied by a factor λ. For the nuclear part, the SAMi functional[5] is used in the self-consistent calculation. For comparison, the exact-Fock energies are also calculated, where the exact-Fock calculation is carried out using the first-order perturbation theory.[6]

The deviation of the Coulomb exchange energy E_{Cx} in the PBE-GGA from that in the LDA, $\Delta E_{\mathrm{Cx}}^{\mathrm{LDA}}$, and the deviation from that in the exact-Fock $\Delta E_{\mathrm{Cx}}^{\mathrm{exact}}$,

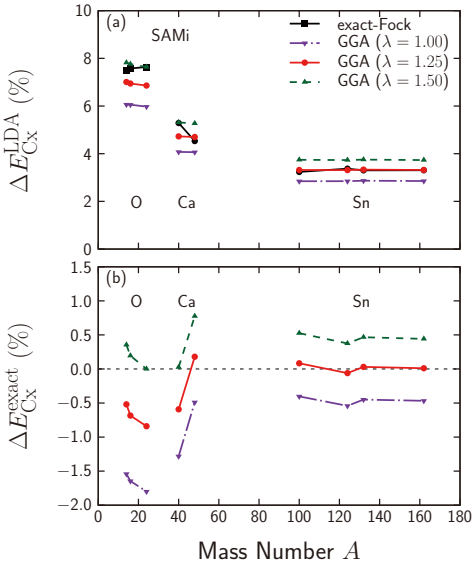

Fig. 1. Deviation between the PBE-GGA and the LDA, $\Delta E_{\mathrm{Cx}}^{\mathrm{LDA}}$, and the deviation between the PBE-GGA and the exact-Fock $\Delta E_{\mathrm{Cx}}^{\mathrm{exact}}$, defined as Eq. (4).

$$\Delta E_{\mathrm{Cx}}^{\mathrm{LDA}}=\frac{E_{\mathrm{Cx}}-E_{\mathrm{Cx}}^{\mathrm{LDA}}}{E_{\mathrm{Cx}}},\quad \Delta E_{\mathrm{Cx}}^{\mathrm{exact}}=\frac{E_{\mathrm{Cx}}-E_{\mathrm{Cx}}^{\mathrm{exact}}}{E_{\mathrm{Cx}}}, \tag{4}$$

are shown as functions of mass number A in Figs. 1(a) and (b), respectively.

In conclusion, λ does not have an obvious isospin dependence, and $\lambda=1.25$ reproduces the exact-Fock calculation well in general. Here, note that the PBE-GGA Coulomb potential is the local potential and hence the numerical cost of the self-consistent calculation is $O\left(N^3\right)$, while the exact-Fock Coulomb potential is the non-local potential and hence the numerical cost is $O\left(N^4\right)$. This scheme helps to achieve a better description and understanding of the observables in which the Coulomb interaction plays important roles, such as the mass difference of the mirror nuclei and the energy of the isobaric analog state.

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