

How to Improve Functionals in Density Functional Theory?

Thursday, 23 August 2018 16:40 (15 minutes)

The density functional theory (DFT) is one of the most successful approaches to calculate the ground-state properties of atoms, molecules, and solids [1, 2]. The DFT is also applicable to nuclear systems [3, 4]. In principle, the DFT gives the exact ground-state density ρ_0 and energy $E_0 = T_0[\rho_0] + \int v_{\text{ext}}(\mathbf{r}) \rho_0(\mathbf{r}) \, d\mathbf{r} + E_{\text{H}}[\rho_0] + E_{\text{xc}}[\rho_0]$, where T_0 is the kinetic energy, v_{ext} is the external field, and $E_{\text{H}}[\rho_0]$ and $E_{\text{xc}}[\rho_0]$ is the Hartree and exchange-correlation energy density functional (EDF), respectively. However, in practice, $E_{\text{xc}}[\rho]$ is unknown, and thus the accuracy of the DFT calculation depends on the accuracy of the exchange-correlation EDF. Improvement of EDFs is one of the important topics both in electron systems and in nuclear systems.

As one way to tackle the improvement of EDFs, the inverse approach of the DFT, so-called the inverse Kohn-Sham method (IKS), was proposed [5]. In the IKS, the Kohn-Sham potential, $v_{\text{xc}}(\mathbf{r}) = \delta E_{\text{xc}}[\rho] / \delta \rho(\mathbf{r})$, is calculated from the input ground-state density $\rho_0(\mathbf{r})$. The information obtained from the IKS, for example, the single-particle energies ε_i , is helpful for checking the accuracy of EDFs [6]. However, the way to improve EDFs directly has not been proposed yet.

We proposed the way to improve EDFs based on the density functional perturbation theory (DFPT) [7] and the IKS [8]. Improvement of EDFs is performed under the assumption for $E_{\text{xc}}^{(1)}[\rho]$, which is added to conventional EDFs. As a benchmark, we check the reproducibility of the exchange [9] and correlation functionals [10] in the local density approximation (LDA). The assumed form of $E_{\text{xc}}^{(1)}[\rho]$ is $A \int \rho^\alpha(\mathbf{r}) \, d\mathbf{r}$, and input ground-state densities are pair of two ground-state density of noble gases. For the LDA exchange functional, it is found that A and α are obtained within 7.2% and 1.0% from the pair of He and Ne, and within 2.3% and 0.1% from the pair of Xe and Rn. Although the LDA correlation functional is not a power functional of ρ , it is found that it is reproduced reasonably well especially in the low-density region from the pair of He and Ne, and in the high-density region from the pair of Xe and Rn.

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Session Classification: YSS