Development of Kinetic Energy Density Functional Using Response Function Defined on the Energy Coordinate

Hideaki Takahashi[1]

[1]Tohoku University

March 15, 2022

Abstract

A kinetic energy functional Ee was developed within the framework of the density-functional theory (DFT) based on the energy electron density for the purpose of realizing the orbital-free DFT. The functional includes the nonlocal term described with the linear-response function (LRF) of a reference system. As a notable feature of the present approach, the LRF is represented on the energy coordinate ε defined for each system of interest. In addition, an atomic system is taken as a reference system for the construction of the LRF, which shows a clear difference from the conventional approach based on the homogeneous electron gas. The explicit form of the functional Ee was formulated by means of the coupling-parameter integration scheme. The functional Ee was applied to the calculations of the kinetic energies of the pseudo atoms that mimics H, He, Ne, and Ar. Explicitly, the kinetic energy of each atom was computed using the functional Ee with respect to the variation of the valence charge Zv of each atom. In these calculations, the electron density n optimized by the Kohn-Sham DFT was adopted as an argument of the functional. It was found that the results are in excellent agreements with those given by the Kohn-Sham DFT. We also devised a method to perform the self-consistent field calculation utilizing the functional Ee The method was applied to the computation of the radial distribution functions of the electrons in the pseudo Ne and Ar atoms. It was demonstrated that the results reasonably agree with those yielded by the Kohn-Sham DFT.

Hosted file

`IJQC_H_Takahashi.pdf` available at https://authorea.com/users/465417/articles/560057-development-of-kinetic-energy-density-functional-using-response-function-defined-on-the-energy-coordinate