A proposal of the kinetic energy functional for the pair density functional theory

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The diagonal element of the second-order reduced density matrix, which is called the pair density (PD), has much information about the electron correlation. Therefore, the density functional scheme to calculate the PD is expected to be effective for describing the electron correlation of various solids such as heavy fermion systems, magnetic materials and etc. We have recently developed the computational PD functional theory.[1,2] In order to perform the actual calculations on the basis of the computational PD functional theory, the approximate form of the kinetic energy functional is indispensable.
In this paper, we propose a new kind of approximate forms of the kinetic energy functional. Approximate forms are developed by using as restrictive conditions two exact relations that should be satisfied with the kinetic energy functional. In order to check their abilities, we perform the test calculations for the neutral neon atom. It is shown that the root-mean-square error of the external potential and electron-electron interaction energies is much reduced as compared to the previous one.[2] This means that correlation effects are reasonably incorporated into the resultant PDs.

[1]M. Higuchi and K. Higuchi, Phys. Rev. B **78**, 125101 (2008).
[2]K. Higuchi and M. Higuchi, Phys. Rev. B **82**, 155135 (2010).