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Development of correlation energy functional based on the transcorrelated density functional theory

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概　要

We propose a new formulation of the correlation energy functional derived from the transcorrelated method in use in density functional theory (TC-DFT). An effective Hamiltonian, H_{TC}, is introduced by a similarity transformation of a many-body Hamiltonian, H, with respect to a complex function F: $H_{TC} = 1/F\ H\ F$. It is proved that an expectation value of H_{TC} for a normalized single Slater determinant, D^n, corresponds to the total energy:$E[n]=\langle\Psi^n|H|\Psi^n\rangle/\langle\Psi^n|\Psi^n\rangle=\langle D^n|H_{TC}|D^n\rangle$ under the two assumptions: (1) The electron density $n(\mathbf{r})$ associated with a trial wave function $\Psi^n = D^nF$ is v-representable and (2) Ψ^n and D^n give rise to the same electron density n ($\mathbf{r}$). This formulation, therefore, provides an alternative expression of the total energy that is useful for the development of novel correlation energy functionals. By substituting a specific function for F, we successfully derived a model correlation energy functional, which resembles the functional form of the screened exchange method. The proposed functional, named the extended screened exchange (ESX) functional, is described within two-body integrals and is parametrized for a numerically exact correlation energy of the homogeneous electron gas. The ESX functional does not contain any ingredients of (semi-) local functionals and thus is totally free from self-interactions. The computational cost for solving the self-consistent-field equation is comparable to that of the Hartree-Fock method. We apply the ESX functional to electronic structure calculations for a solid silicon, H ion, and small atoms. The results demonstrate that the TC-DFT formulation is promising for the systematic improvement of the correlation energy functional.

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