Pauli Potential in the Density and Pair Density Functional Theories

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A link between density and pair density functional [1] theories is presented. Density and pair density scaling [2,3] are used to derive the Euler equation in both theories. Density scaling provides a constructive way of obtaining approximations for the Pauli potential [4]. The Pauli potential (energy) of the density functional theory is expressed as the difference of the scaled and original exchange-correlation potentials (energies). A relationship between the effective potentials of the Euler equation of the density functional theory and the Pauli potential of the pair density functional theory is also presented [5].

References

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