Trial Functions for the Two-Particle Density Functional Variational Method

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The N-particle quantum mechanical system in an external field is considered on the basis of two-particle density functions. The main point of the presented work is to reveal the advantages of the two-particle density formalism as compared to the common one-particle density formalism applied to a simple example. The two-particle density formalism permits us to take into account the exact two-particle interaction without additional models. The exchange and correlation effects can be considered by a proper choice of the trial function. By using the presented formalism we calculate the density of the electron gas on different metal surfaces. A simple trial function allowing for correlations gives us a more correct fit to the experimental data on the metal dipol barriers than corresponding calculations with the one-particle density formalism. It is also shown that a pertubation of the external potential can be effectively taken into account by a pertubation calculation for the trial function.

Key words: Quantum Theory; Two-particle Density; Density Functional; Metallic Surface.

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