

Insights into analytical relations between pair density and first-order density matrix from model atom wave functions in different spin states

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Abstract

Exact analytical wave functions can be obtained for some model atoms with few electrons. The most tractable of these is the so-called Moshinsky atom model (MAM). This is therefore the starting point of this article, in which the focus will be the gaining of insight into correlated density matrix-theory and its connection with DFT.

Therefore, for MAM the relation between the ground-state density $\rho(\mathbf{r})$ and the corresponding first-order density matrix $\gamma(\mathbf{r}, \mathbf{r}')$ [1DM] is briefly summarized. Very recent work of Akbari, March and Rubio is next discussed, and the relation between the pair density $n_2(\mathbf{r}_1, \mathbf{r}_2)$ and the above 1DM γ exhibited. This then allows the Euler-Lagrange equation for the 1DM γ to be set up.

The next example concerns what is essentially a generalization of MAM to treat 4 electrons. For the case when the four spins are parallel, and for attractive harmonic interparticle interactions but after switching off the confinement potential, the wave function for this spin state is available from early work of Bruch. Ali et al have used this to obtain the corresponding second-order density matrix Γ . Their result relating Γ to γ is discussed in the present context. Finally the N-representability problem is referred to, in the context of variationally valid density matrices.