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The problems in the density functional theory with the total spin and space symmetry and the invariant properties of the electron density. I.G. KAPLAN, Instituto de Investigaciones en Materiales, UNAM, Apdo. Postal 70-360, 04510 México D.F. México — The problems in the density functional theory (DFT) arising when it is applied to the spin and space multiplets are discussed. It is rigorously proved that the electron density of an arbitrary N-electron system does not depend upon the value of the total spin S of the state and preserves the same analytical form for all states with the definite S. It is also proved that the diagonal element of the full density matrix is invariant respecting all operation of the group symmetry of the state, i.e, it is a group invariant. From these results follows that the problems in DFT with the total spin and degenerated states cannot be solved within the framework of density matrix formalism.

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