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Chapter 1

Concept of covariant density functional theory

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The concept of density functional theory is introduced. The history of nuclear density functional theory is briefly reviewed. The complexity and specialty of the density functional theories in nuclear system in connection with the degrees of freedom, covariance and pairing correlations are discussed in contrast to Coulombic systems. The existing problems and limits of the nuclear density functional theory are discussed. Perspective on the way to derive *ab initio* functionals is given.

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1. Kohn–Sham density functional theory

Density Functional Theory (DFT) is one of the most popular and successful *ab initio* approaches to many quantum many-body systems (atoms, molecules, solids). The basic idea is that the ground-state energy of a stationary many-body system can be represented in terms of the ground-state density alone. Since the density is only a function with three spatial coordinates, rather than the N -body wave function with $3N$ coordinates,