Non-Local Potentials in Density Functional Theory VASILY SHAGINYAN, Petersburg Nuclear Physics Institute, Russia, M.YA. AMUSIA, Hebrew University, Israel, A.Z. MSEZANE, Clark Atlanta University, USA — There has been many unsuccessful efforts to accommodate the Hartree- Fock (HF) method into the Kohn-Sham (KS) scheme of the density functional theory. A great number of HF numerical calculations based on the KS method with local potentials demonstrated the impossibility of the accommodation but have not proven it. We have proven that the HF method cannot be reproduced within the framework of KS theory because the single-particle densities of finite systems obtained in HF calculations are not v-representable, i.e., do not correspond to any ground state of a non-interacting electron system in a local external potential [1]. As a result, while the kinetic energy of a finite electron system evaluated in the HF method is larger than that calculated in the KS scheme, the corresponding exchange energy is lower. However, the HF ground state energy is obviously the lowest. The problem with the HF method is the non-local nature of the HF potential, while the KS theory deals with local potentials and v-representable densities. For all other atoms, except the He atom, the HF potentials are non-local, so that the HF and the KS methods yield different results.

[1] M.Ya. Amusia, et al., Phys. Lett. A **330**, 10 (2004).

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