Non-Uniqueness of Local Effective Potential Energy in Density Functional Theory

VIRAHT SAHNI, XIAO-YIN PAN, The Graduate School, CUNY, MARLINA SLAMET, Sacred Heart University — As a consequence of the first Hohenberg-Kohn (HK) theorem, in the mapping from a ground state of an interacting system to an S system of noninteracting fermions with equivalent density, the effective potential energy of the latter is unique. But it is so only if these fermions are in their ground state. It can be shown via Quantal Density Functional Theory,\(^1\) that the ground state density of an interacting system can also be reproduced by S systems that are in an excited state. Hence, in principle, there are an infinite number of functions that can reproduce a ground state density. Similarly, in the mapping from an excited state of the interacting system to an S system with equivalent density, the state of the latter is arbitrary. Hence, there are an infinite number of functions that can reproduce the excited state density. The latter proves the lack of a first HK theorem for excited states. The difference between the potential energy functions in either case is due solely to Correlation-Kinetic effects.

\(^1\)Quantal Density Functional Theory, V. Sahni (Springer-Verlag, 2004)