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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)

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