Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

New Perspectives on the Fundamental Theorem of Density Functional Theory[1] VIRAHT SAHNI, The Graduate School, CUNY, XIAO-YIN PAN, Ningbo University — The fundamental theorem of time-dependent/time-independent DFT due to Runge-Gross(RG)/Hohenberg-Kohn(HK) proves the bijectivity between the density $\rho(\mathbf{r}t)/\rho(\mathbf{r})$ and the Hamiltonian $\hat{H}(t)/\hat{H}$ to within a function $C(t)$/constant C, and wave function $\Psi(t)/\Psi$. (Implicit in the RG theorem is that the initial condition $\Psi(t_0)$ is fixed.) As such in DFT the wave function is considered solely a functional of the density. Since the density is gauge invariant, the wave function as a functional of the density is also gauge invariant. However, it is well known that the Hamiltonian and wave function are gauge variant. There is, therefore, an inherent inconsistency in the RG/HK theorem. We resolve this inconsistency of the theorem via a unitary or equivalently a gauge transformation. As a consequence we generalize the theorem to external potentials that include the momentum operator and a curl-free vector potential operator. The RG/HK theorems each then constitute a special case of this generalization.

[1]Supported in part by RF CUNY.

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Date submitted: 25 Nov 2007 Electronic form version 1.4