Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

On the Hohenberg-Kohn and Levy-Lieb Constrained Search Proofs of Density Functional Theory VIRAHT SAHNI, Brooklyn College CUNY, XIAO-YIN PAN, Ningbo University — In HK, a 1-1 relationship between the density $\rho(\mathbf{r})$ and the potential $v(\mathbf{r})$ is established. (The relationship between $v(\mathbf{r})$ and the ground state Ψ is 1-1.) The proof, valid for v-representable densities, shows $\rho(\mathbf{r})$ to be a basic variable. The LL proof is independent of $v(\mathbf{r})$, and is valid for N-representable densities. In,[1] we have proved that in an external magnetic field $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$, there is a 1-1 relationship between $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, with $\mathbf{j}(\mathbf{r})$ the physical current density, and the potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$. (The relationship between $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and Ψ is *many-to-one*.) This proves that $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ are the basic variables. The LL proof independent of $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ follows readily. However, such a proof also follows if $\{\rho(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$, with $\mathbf{j}_p(\mathbf{r})$ the paramagnetic current density, are considered the basic variables. As such knowledge of the basic variables as determined via HK is a pre-requisite to any LL type proof.

[1]Pan and Sahni, IJQC 110, 2833 (2010)

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Date submitted: 15 Nov 2011

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