Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Basic Variables in Density Functional Theory in the Presence of a Magnetic Field[1] VIRAHT SAHNI, The Graduate Center CUNY, XIAOYIN PAN, Ningbo University — We have shown[†] via a unitary or equivalently a gauge transformation that for a system of N electrons in an external field $\vec{\mathcal{F}}^{ext} = -\vec{\nabla} v(\vec{r})$, the wave function Ψ is in general a functional of the ground state density $\rho(\vec{r})$ and a gauge function $\alpha(\vec{R})$; $\vec{R} = \vec{r}_1, \ldots, \vec{r}_N$, i.e. $\Psi = \Psi[\rho, \alpha]$. The functions $\alpha(\vec{R})$ are arbitrary, the choice $\alpha(\vec{R}) = 0$ being equally valid. It is the presence of $\alpha(\vec{R})$ that ensures the wave function functional is gauge variant. Similarly, in the presence of a magnetic field $\vec{B}(\vec{r}) = \vec{\nabla} \times \vec{A}(\vec{r})$, we show that in general the wave function is a functional of the density $\rho(\vec{r})$, the physical current density $\vec{j}_{\vec{A}}(\vec{r})$, and a gauge function $\alpha(\vec{R}) : \Psi = \Psi[\rho, \vec{j}_{\vec{A}}, \alpha]$. Again, the $\alpha(\vec{R})$ are arbitrary, the choice $\alpha(\vec{R}) = 0$ being valid. Hence, it is possible to construct a theory in which the basic variables are $\rho(\vec{r})$ and $\vec{j}_{\vec{A}}(\vec{r})$. The generalized Hohenberg-Kohn theorems, as well as the equations for the noninteracting fermion Kohn-Sham system that reproduces the $\rho(\vec{r})$ and $\vec{j}_{\vec{A}}(\vec{r})$ of the interacting system of electrons, are derived.
[†]X.-Y. Pan and V. Sahni, Int. J. Quantum Chem. **108**, 2756 (2008).

[1]X.Pan: National Natural Science Foundation, China. Grant 10805029

Viraht Sahni
The Graduate Center CUNY

Date submitted: 21 Nov 2008 | Electronic form version 1.4