Is the Wave Function Solely a Functional of the Density?

Xiao-Yin Pan[1,2] and Viraht Sahni[2]

[1]*Department of Physics, Ningbo University, Ningbo 315211, China*
[2]*The Graduate School of the City University of New York, New York, New York 10016*

The fundamental theorem of time-dependent(TD)/time-independent(TI) density functional theory (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 $H(t)/H$ to within a function $C(t)$/constant C, and the wave function $\Psi(\mathbf{X}t)/\Psi(\mathbf{X})$. (The proof is for arbitrary external potential operators that are *scalars*. Also implicit in the RG theorem is that the initial condition on the wave function $\Psi(\mathbf{X}t_0)$ is fixed.) As such, in DFT, the wave function is considered as being *solely* a functional of the density: $\Psi[\rho(\mathbf{r}t)]/\Psi[\rho(\mathbf{r})]$. Since the density $\rho(\mathbf{r}t)/\rho(\mathbf{r})$ is gauge invariant, the wave function as a functional of the density $\Psi[\rho(\mathbf{r}t)]/\Psi[\rho(\mathbf{r})]$, is also gauge invariant. However, it is well known that the Hamiltonian $H(t)/H$ and the wave function $\Psi(t)/\Psi$ are gauge variant. There is, therefore, an inherent inconsistency in the RG/HK theorem.

In this paper we resolve this inconsistency in the RG/HK theorem via a unitary transformation or equivalently a gauge transformation. We thereby prove

(i) The wave function $\Psi(\mathbf{X}t)/\Psi(\mathbf{X})$ in addition to being a functional of the density $\rho(\mathbf{r}t)/\rho(\mathbf{r})$ is also simultaneously a functional of a gauge function $\alpha(\mathbf{R}t)/\alpha(\mathbf{R})$. This then makes the wave function functional gauge variant.
(ii) The unitary transformation generalizes the RG/HK theorem to Hamiltonians $H(t)/H$ that in addition to the *scalar* external potential include the momentum operator and a curl-free *vector* potential operator.
(iii) The transformation proves that the bijectivity is between the density $\rho(\mathbf{r}t)/\rho(\mathbf{r})$ of a physical system and the Hamiltonian representation of that system: the Hamiltonian $H(t)/H$ and the Hamiltonians $H(t) + C(t)/H + C$ *all* correspond to the *same physical system*. (Note that it is possible to construct [1, 2] an *infinite* number of Hamiltonians $H(t)/H$ that differ by $C(t)/C$ and correspond to *different physical systems*, but which all have the *same* density $\rho(\mathbf{r}t)/\rho(\mathbf{r})$.)
(iv) The original RG/HK theorems then each constitute a special case of the more general description of the Hamiltonian.

Other understandings achieved by the transformation will also be discussed.

1. X.-Y. Pan and V. Sahni, Int. J. Quantum Chem. **95**, 387 (2003).
2. V. Sahni, *Quantal Density Functional Theory*, Springer-Verlag, Berlin (2004).