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Basic Variables of Quantum Mechanics for Electrons in Electrostatic and Magnetostatic Fields XIAO-YIN PAN, Ningbo University, VIRAHT SAHNI, The Graduate Center, CUNY — We consider a system of N electrons in an external electrostatic $\boldsymbol{\mathcal{E}} = - \boldsymbol{\nabla} v(\mathbf{r})$ and magnetostatic $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ fields, and the Hamiltonian to include the interaction of the latter with both the orbital and spin angular momentum. We prove the one-to-one relationship $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\} \leftrightarrow \{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, where $\rho(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$ are the nondegenerate ground state density and physical current density. The proof accounts for the many-to-one relationship between the $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and the ground state Ψ. In parallel with the Hohenberg-Kohn theorem proof in which the wave function Ψ of the different physical systems considered is constrained[1] to a fixed electron number N, the corresponding Ψ in our proof is constrained to having the same total orbital $\mathbf{L}$ and spin $\mathbf{S}$ angular momentum. Thus, $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ constitute the basic variables in the rigorous HK sense.

[1]X.-Y. Pan and V. Sahni, J. Chem. Phys. **132**, 164116 (2010)

Viraht Sahni
The Graduate Center, CUNY

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