Abstract Submitted
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Basic Variables in the Presence of a Magnetostatic Field[1] VIRAHT SAHNI, Brooklyn College, CUNY, XIAO-YIN PAN, Ningbo University — We present our recent understanding of the issue of what properties constitute the basic variables in quantum mechanics for electrons in the presence of external electrostatic $\mathcal{E}(\mathbf{r}) = -\boldsymbol{\nabla} v(\mathbf{r})$ and magnetostatic $\mathbf{B}(\mathbf{r}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r})$ fields. In this case, the relationship between the potentials $\{v, \mathbf{A}\}$ and the ground state wave function Ψ can be many-to-one. We discuss our prior work[2] in which we claimed that the basic variables are the ground state density $\rho(\mathbf{r})$ and physical current density $\mathbf{j}(\mathbf{r})$. We prove here more fully this to be the case for the nondegenerate ground state for which Ψ is real. The proof explicitly accounts for the many-to-one relationship between $\{v, \mathbf{A}\}$ and Ψ. We also draw parallels between our work on the density and physical current density functional theory and those of the Hohenberg-Kohn and Percus-Levy-Lieb definitions of density functional theory.

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[2]Pan and Sahni, Int. J. Quantum Chem. 110, 2833 (2010); J. Phys. Chem. Solids. 73, 630 (2012).

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