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Generalization of the Hohenberg-Kohn theorem to the case of the presence of a magnetic field[1] VIRAHT SAHNI, Brooklyn College, CUNY, XIAOYIN PAN, Ningbo University — We generalize the HK theorem for the nondegenerate ground state of electrons in an external electrostatic field $\mathbf{E}(\mathbf{r}) = -\boldsymbol{\nabla} v(\mathbf{r})$ to the presence of an additional external magnetostatic field $\mathbf{B}(\mathbf{r}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r})$. We prove that the nondegenerate ground state wave function Ψ is a functional of the ground state density $\rho(\mathbf{r})$, the physical current density $\mathbf{j}(\mathbf{r})$, and a gauge function $\alpha(\mathbf{R})$, with $\mathbf{R} = \{\mathbf{r}\}$. In other words, the basic variables, viz. those that uniquely determine the external potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$, are $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. As the choice of $\alpha(\mathbf{R})$ is arbitrary, it is possible to construct a $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ functional theory, as well as the corresponding Kohn-Sham and quantal density functional theories.

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