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Quantal density functional theory (QDFT) in the presence of a magnetic field[1] XIAOYIN PAN, TAO YANG, Ningbo University, VIRAHT SAHNI, Brooklyn College, CUNY — We present the QDFT of electrons in an external electrostatic $\mathbf{E}(\mathbf{r}) = -\boldsymbol{\nabla} v(\mathbf{r})$ and magnetostatic $\mathbf{B}(\mathbf{r}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r})$ field. This is the mapping from the interacting system of electrons to one of noninteracting fermions with the same density $\rho(\mathbf{r})$ and physical current density $\mathbf{j}(\mathbf{r})$. The mapping, based on the 'quantal Newtonian' first law, is in terms of 'classical' fields and quantal sources, the fields being separately representative of electron correlations due to the Pauli exclusion principle and Coulomb repulsion, and correlation-kinetic and correlation-magnetic effects. The theory is valid for ground and excited states. It is explicated by application to a ground state of the exactly solvable Hooke's atom in the presence of a magnetic field.

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