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Quantal Density Functional Theory (QDFT) in the Presence of an Electromagnetic Field[1] XIAO-YIN PAN, Ningbo University, VIRAHT SAHNI, Brooklyn College, CUNY — We derive the QDFT equations of electrons in an external time-dependent field $\mathcal{E}(\mathbf{r}\sqcup) = -\boldsymbol{\nabla} v(\mathbf{r}t)$ and in the presence of an electromagnetic field characterized by the magnetic induction $\mathbf{B}(\mathbf{r}t) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r}t)$ and electric field $\mathbf{E}(\mathbf{r}t) = -\boldsymbol{\nabla} \Phi(\mathbf{r}t) - (1/c)\partial \mathbf{A}(\mathbf{r}t)/\partial t$. The QDFT is comprised of the mapping from this system to one of noninteracting fermions with the same density $\rho(\mathbf{r}t)$ and physical current density $\mathbf{j}(\mathbf{r}t)$. The mapping is in terms of 'classical' fields representative of the different electron correlations that must be accounted for. On deriving the 'quantal Newtonian' second law for the interacting and model systems, we obtain the local electron-interaction potential $v_{ee}(\mathbf{r}t)$ of the latter to be the work done in a conservative effective field $\mathcal{F}^{\text{eff}}(\mathbf{r}\sqcup)$. The components of $\mathcal{F}^{\text{eff}}(\mathbf{r}\sqcup)$ are representative of correlations due to the Pauli exclusion principle and Coulomb repulsion and the Correlation-(Kinetic, Current Density, Electric, and Magnetic) effects.

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