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Particle Number and Probability Density Functional Theory, and A-representability[1] VIRAHT SAHNI, Brooklyn College, CUNY, XIAOYIN PAN, Ningbo University, China — In Hohenberg-Kohn (HK) density functional theory (DFT), the functional $F_{HK}[\rho]$ of the density $\rho(\mathbf{r})$ representing the expectation of the electron-interaction and kinetic energy operators is universal. Knowledge of $F_{HK}[\rho]$ by itself is insufficient to obtain the energy: the electron number N is primary. By emphasizing this primacy of N, we rewrite the energy E as a nonuniversal functional of N and probability density $p(\mathbf{r}) : E = E[N, p]$, with $p(\mathbf{r})$ satisfying the constraints of normalization to unity and positivity. A particle number N and probability density $p(\mathbf{r})$ functional theory is constructed, and examples of exact functionals provided. The concept of A-representability is introduced as the set of functions ψ_p that lead to quantum mechanical $p(\mathbf{r})$ as the expectation of the probability density operator. We show via the Harriman and Gilbert constructions that the A- and N-representable probability density $p(\mathbf{r})$ sets are equivalent, with the latter defined as $p(\mathbf{r}) = \rho(\mathbf{r})/N$.

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