Basis-set correction based on density-functional theory: Rigorous framework for a one-dimensional model

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Recently, we proposed a method for accelerating the convergence of wave-function calculations with respect to the size of the basis B

$$E_0^{\mathcal{B}} = \langle \Psi^{\mathcal{B}} | \hat{\mathcal{H}} | \Psi^{\mathcal{B}} \rangle + \bar{\mathcal{E}}^{\mathcal{B}} [\rho_{\Psi^{\mathcal{B}}}]$$

► Here, we rexamine this method more closely for a one-dimensional model Hamiltonian with delta-potential interactions

We give a new formulation of the method and we develop an adapted local-density approximation (LDA) for the basis-set correction functional *Ē*^B[ρ] for any basis B using a finite uniform electron gas