Tightening the Lieb Oxford bound for atoms, molecules and solids

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Universal constraints, obeyed by all Coulomb interacting systems, are important ingredients in the construction of improved density functionals. Here we investigate one such universal property, the Lieb-Oxford lower bound on the exchange-correlation energy [1]. In a recent study [2,3] we showed, via case studies of atoms, ions, molecules, solids, and some model Hamiltonians, that the presently accepted value of this lower bound can be substantially reduced, leading to a tighter bound. In the present work we point out that different classes of systems can be classified with respect to class-specific (but not fully universal) similar bounds. Since a substantial change in this bound has consequences for the performance of modern exchange-correlation functionals, we explore a non-empirical tightening of the Lieb-Oxford bound for PBE in both universal and electron-number-dependent form [4].

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