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Bounds on the correlation energy of Coulomb interacting systems: How negative does E_c get, and what does this imply for approximate density functionals?[1]

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The indirect part of the Coulomb interaction energy of a three-dimensional many-fermion system has a lower bound in terms of a power of the particle density, known as the Lieb-Oxford bound. This bound can be reformulated as a bound on the correlation energy, and in this reformulated version is an ingredient in the construction of many modern density functionals. In this talk, I describe several recent investigations and refinements of this bound: (i) an empirical analysis strongly suggesting that the bound can be tightened without loosing its universality [collaboration: Mariana Odashima], (ii) the construction of a particle-number dependent version of the bound and an exploration of its consequences for PBE GGA [collaboration: Mariana Odashima and Sam Trickey], (iii) a simplified scaling derivation of the power law in the bound, and its application to construct similar bounds also for one- and two-dimensional systems [collaborators: César Proetto, Esa Räsänen and Stefano Pittalis], and (iv) a connection between the Lieb-Oxford bound and common hybrid functionals, providing an alternative rationale for why these functionals work, as well as a possible route for the construction of improved beyond-GGA functionals [collaborator: Mariana Odashima].

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