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Gedanken Densities and Lower Bounds in Density Functional Theory[1]

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A gedanken density is not a real one but one imagined in the construction of density functional approximations. The uniform electron gas is the original gedanken density, but we will be concerned here with two others: (1) the ground-state density of one electron in the presence of a nonuniform periodic potential , in which the reduced density gradient $s = |\nabla n| / [2(3\pi^2)^{1/3} n^{4/3}$diverges almost everywhere as the volume tends to infinity. This density was used in the construction [1] of a generalized gradient approximation (GGA): To satisfy the general Lieb-Oxford lower bound [2] on the exchange-correlation energy for all possible densities, the exchange enhancement factor $F_x \equiv \varepsilon_x^{approx} / \varepsilon_x^{unif}$ in the large-s limit for a spin-unpolarized density must be less than or equal to 1.804. (2) a two-electron spherical ground-state density in which s takes the same arbitrary positive value wherever the density is non-zero [3]. This density can be used to show that, to satisfy the tight Lieb-Oxford bound on the exchange energy of a two-electron density for every possible such density, F_x for such a density (and probably for every density) must be less than 1.174. The local spin density approximation (LSDA) for exchange ($F_x = 1$) satisfies this tight bound, but standard GGA's and meta-GGA's do not. A talk by Jianwei Sun will present what may be the first beyond-LSDA approximation to satisfy this strong new constraint.

[1] J.P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. *77,* 3815 (1996).
[2] E.H. Lieb and S. Oxford, Int. J. Quantum Chem. *19*, 427 (1981).
[3] J.P. Perdew, J. Sun, A. Ruzsinszky, and K. Burke, in preparation.

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