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A Lower Bound with the best Possible Constant for Coulomb Hamiltonians*

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The reason for stability of matter with Coulomb interactions has become more transparent once it was recognized that the no-binding Theorem of Thomas–Fermi (TF) theory is the key to the problem. In fact, in [1] it was conjectured that TF-theory always gives a lower bound to the ground state energies of Coulomb systems. Unfortunately one inequality on which this conjecture is based has resisted all attempts of proof or disproof. On the other hand one knows that for large nuclear charges Z TF-theory becomes exact and one could hope that at least for large Z the TF-energy is a lower bound. More precisely the question is the following. Suppose we have a neutral system, M nuclei with charges Z, $N = MZ$ electrons. For the ground state energy $E(M, Z)$ one knows [4]

$$\lim_{Z \to \infty} E(M, Z)/Z^{7/3} = -M\varepsilon_{\mathrm{TF}}$$

where

$$\varepsilon_{\mathrm{TF}} = 0.77\, me^{4}/\hbar^{2} = 0.385 \text{ in our units with } 2m = e = \hbar = 1.$$

For stability of matter one considers the other limit $M \to \infty$, $Z =$ fixed. In ref. [1]

$$E(M, Z) \geqq -(4\pi)^{2/3} M\varepsilon_{\mathrm{TF}} Z^{7/3}\,(1 + O(Z^{-2/3}))$$

was proved. (The value $(4\pi)^{2/3}$ was subsequently improved to $(4\pi)^{2/3}/1.5$ [2].) In this note we shall produce a family of inequalities which among other things imply

$$E(M, Z) \geqq -M\varepsilon_{\mathrm{TF}} Z^{7/3}(1 + O(Z^{-2/33})).$$

Thus the constant in front is the best possible, the correction $O(Z^{-2/33})$ is probably not.

Our general strategy is to split the Coulomb potential into a regularized long-range part v_r and a short-range singular part v_s

$$\frac{1}{r} = v_r(r) + v_s(r), \quad v_r = g^2 * \frac{1}{r} * g^2, \quad g^2(x) = e^{-\mu r}\frac{\mu^3}{8\pi} \tag{1}$$

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