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Asymptotic Neutrality of Large Ions

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Abstract. It is proved that a nucleus of charge Z can bind at most $Z + O(Z^a)$ electrons, with a = 47/56.

Consider the Hamiltonian for a nucleus of charge Z and N quantized electrons,

$$H_{Z,N} = \sum_{i=1}^{N} \left[(-\Delta_{x_i}) - \frac{Z}{|x_i|} \right] + \frac{1}{2} \sum_{i \neq j} \frac{1}{|x_i - x_j|} = -\Delta + V_{\text{Coulomb}}.$$

The ground state energy is then

$$E(Z) = \inf_{N} E(Z, N) = \inf_{\substack{N \\ \|\psi\|_{2} = 1}} \inf_{\substack{\psi \in \mathscr{H} \\ \|\psi\|_{2} = 1}} \langle H_{Z,N}\psi, \psi \rangle,$$

where $\mathscr{H} = \bigwedge_{i=1}^{N} (L^2(\mathbf{R}^3) \otimes \mathbf{C}^q)$ is the space of antisymmetric wave functions with q spins. Throughout this paper we will simply refer to them as "antisymmetric" wave functions.

For each Z, call N(Z) the smallest number for which E(Z) = E(Z, N). It is an interesting problem to obtain sharp estimates for N(Z). The sharpest known result appears in [8], where the reader will find a discussion of the history of the problem. In particular, $N(Z)/Z \rightarrow 1$ as $Z \rightarrow \infty$, although there were no estimates for the rate of convergence. Our main result is the following:

Theorem.

$$N(Z) = Z + O(Z^{\alpha}) \quad \text{for} \quad \alpha = \frac{47}{56}.$$

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