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Electron Wavefunctions and Densities for Atoms

Maria Hoffmann-Ostenhof, Thomas Hoffmann-Ostenhof,
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Abstract. With a special ‘Ansatz’ we analyse the regularity properties of atomic electron wavefunctions and electron densities. In particular we prove an a priori estimate, $\sup_{y \in B(x, R)} |\nabla \psi(y)| \leq C(R) \sup_{y \in B(x, 2R)} |\psi(y)|$ and obtain for the spherically averaged electron density, $\bar{\rho}(r)$, that $\bar{\rho}'(0)$ exists and is non-negative.