C^2 Regularity of Electronic Eigenfunctions for Schrodinger Operators with Coulomb Potentials

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The Coulomb electrostatic potential for a collection of point charges has strong discontinuities at the nuclear charge positions, and the corresponding electronic eigenfunctions have cusps at those positions. This leads to only a finite degree of differentiability of those eigenfunctions with respect to changes in the nuclear positions in the usual Sobolev spaces: they are C^2 and not better. We outline the proof of C^2 smoothness of the matrix elements of the Hamiltonian, focusing on the parts of the proof where the analysis gets interesting. The account of smoothness does not fit into the Frechet theory in a single Sobolev space, but requires a scale of such spaces.

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