REAL ANALYTICITY AWAY FROM THE NUCLEI OF PSEUDORELATIVISTIC HARTREE-FOCK ORBITALS

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We prove that the Hartree–Fock orbitals of pseudorelativistic molecules, that is, molecules where the kinetic energy of the electrons is given by the pseudorelativistic operator $\sqrt{-\Delta + 1} - 1$, are real analytic away from the positions of the nuclei. As a consequence, the quantum mechanical ground state of such molecules is never a Hartree-Fock state. The proof is inspired by the classical proof of analyticity by nested balls of Morrey and Nirenberg. However, the technique has to be adapted to take care of the non-local pseudodifferential operator, the singularity of the potential at the positions of the nuclei, and the non-linear terms in the equation.

Keywords: Hartree–Fock, pseudorelativistic atoms and molecules, elliptic regularity, analyticity.

[1] Analysis & PDE, to appear (2012); `arXiv:1103.5026v2`.