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Pseudospectral Calculation of Helium Wave Functions, Expectation Values, and Oscillator Strength[1] PAUL GRABOWSKI, Los Alamos National Laboratory, DAVID CHERNOFF, Cornell University — We extend the pseudospectral method from the solution of Schrödinger's equation for two-electron atom S states to arbitrary angular momentum states. We evaluate the oscillator strength for the helium $1^1S \rightarrow 2^1P$ transition. The result, 0.27616499(27), compares favorably to the best determination in the literature. The length, velocity, and acceleration expressions all have roughly the same accuracy in a pseudospectral treatment. We evaluate leading order finite-nuclear-mass and relativistic corrections for the helium ground state. The pseudospectral method achieves near state-of-the-art accuracy without requiring the implementation of any special-purpose numerical treatments. All the relevant quantities tested converge exponentially with increasing resolution and at roughly the same rate. Quantum mechanical matrix elements are directly and reliably calculable with pseudospectral methods. A general prescription is given for choosing coordinates and subdomains to achieve exponential convergence when two-particle Coulomb singularities are present.

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