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Space-Pseudo-Time Method: Application to the One-Dimensional Coulomb Potential and Density Funtional Theory[1]

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— A new and efficient way of evolving a solution to an ordinary differential equation is presented. A finite element method is used where we expand in a convenient local basis set of functions that enforce both function and first derivative continuity across the boundaries of each element. We also implement an adaptive step size choice for each element that is based on a Taylor series expansion. The method is applied to solve for the eigenpairs of the one-dimensional soft-coulomb potential and the hard-coulomb limit is studied. The method is then used to calculate a numerical solution of the Kohn–Sham differential equation within the local density approximation is presented and is applied to the helium atom.

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