A Comparison of Numerical Approaches to the Solution of the Time-Dependent Schroedinger Equation in One Dimension

HEMAN GHARIBNEJAD, BARRY SCHNEIDER, National Institute of Standards and Technology, MARK LEADINGHAM, Department of Mathematical Sciences - University of Delaware, HENRY SCHMALE, Conklin Media — We present a simple, one-dimensional model of an atom exposed to a time-dependent intense, short-pulse EM field with the objective of teaching undergraduates how to apply various numerical methods to study the behavior of this system as it evolves in time using several time propagation schemes. In this model, the exact coulomb potential is replaced by a soft-core interaction to avoid the singularity at the origin. While the model has some drawbacks, it has been shown to be a reasonable representation of what occurs in the fully three-dimensional hydrogen atom. A variety of approaches such as Crank-Nicholson, split-operator, Lanczos and Chebyshev are compared both for accuracy and efficiency. The model can be used as a tool to train undergraduate physics majors in the art of computation and software development.

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