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Algorithm for computing a wave packet evolution of the time-dependent Schrödinger equation

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Abstract. The algorithm implemented as FORTRAN 77 program TIME6T which calculates, with controlled accuracy, the wave-packet evolution of the one-dimensional time-dependent Schrödinger equation on a finite time interval is presented. Symmetric implicit operator-difference multi-layer schemes based on decomposition of the evolution operator up to the sixth-order of accuracy with respect to the time step are utilized. This decomposition is obtained via the explicit truncated Magnus expansion and Padé approximations. The additional gauge transformations which provide the symmetry properties needed for discretization, within the framework of the high-order finite-element method, of the evolutionary boundary problem on a finite spatial interval with the first and/or second type boundary conditions are applied. Solution of time-dependent Schrödinger equation for the Pöschl-Teller two-center problem is used to illustrate an efficiency of the proposed schemes by comparing the computational error and execution time with those obtained by conventional symmetric splitting exponential operator techniques using the Padé approximations and fast Fourier transform method. The program is applied to the benchmark calculations of the exactly solvable model of a one-dimensional time-dependent oscillator.

Keywords: time-dependent Schrödinger equation, finite-element method, partial differential equations, high-order accuracy approximations

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