



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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1. Introduction

Solutions of the time-dependent Schrödinger equation (TSDE) with a required accuracy are needed for the control problems of the finite-dimensional quantum systems [1] and molecular processes [2], the decay problem in nuclear physics [3], the ionization problems of atomic and molecular physics in pulse fields [4, 5, 6, 7, 8], impact electron-atom and electron-molecule ionization [9, 10] and others. For solving the TDSE in a finite-dimensional spatial domain [11, 12], it is common to seek a wave-packet solution expanded over an appropriate angular basis and then apply a certain discrete numerical scheme to the resulting system of the ordinary second-order differential hyperradial equations [13, 14] (e.g., finite-difference [15, 16, 17, 18], spline [19, 20] or finite-element [21, 22] method).

There are two main requirements for numerical methods that are used in practice for numerical solution of the Cauchy problem for multidimensional time-independent Schrödinger equation. More specifically, such methods should be stable and guarantee a high accuracy of discretization in the time-dependent and spacial variables. In that respect, splitting methods have important advantages, namely, unitarity of the evolution operator preserves the norm of a wave packet and guarantees preservation of probability and unconditional stability of the method [23]. This approach has been used in Refs. [24, 25, 26] to construct nonsymmetric evolutionary schemes on the basis of the Magnus expansion of unitary evolution operator using the unitary $[M/M]$ Padé approximation up to the sixth-order of accuracy in the time-dependent variable. This method has been successfully applied to one-dimensional and three-dimensional time-independent Schrödinger equation, for example [3, 6, 16]. Nevertheless, this scheme when used for numerical solution of time-independent Schrödinger equation leads to systems of algebraic equations with nonsymmetric complex matrices of large dimensions which complicates achievement of a given accuracy of the required approximate solution.

Hence the construction of more economical and stable symmetric schemes is an important and challenging problem [27, 28, 29, 30]. For its solution one could use an approximation of a wave packet in angular variables by the Kantorovich method and finite element method (FEM) in the radial variable [31, 32]. Efficiency of such combination for the described class of problems has been proven in [21, 22, 33, 34, 35].

In paper [13], a more efficient approach has been developed for construction of operator-difference schemes with symmetric operators on a basis of the explicit Magnus expansion, i.e., expansion of logarithm of evolution operator into Taylor series over a step of time-dependent variable on a uniform mesh [36, 37]. In this approach, coefficients of evolution operator expansion are calculated in explicit form from a system of recurrence relations. Using partial splitting of evolution operator with the help of gauge transformation dependent on the operators, multi-layer operator-difference schemes with symmetric operators up to the fourth-order of accuracy in step of time-dependent variable have been constructed for Hamiltonian of a general type, as well as scheme up to the sixth-order of accuracy under the

condition of equality to zero of a commutator of the first and second partial derivatives of the Hamiltonian in time-dependent variable. This circumstance allows us to use this approach for solving a wide range of evolutionary boundary problems with a required accuracy.

The main advantage of the Magnus proposal is that very often the truncated series still share important qualitative properties with the exact solution at variance with other conventional methods of perturbation theory. For instance, in classical mechanics the symplectic character of the time evolution is preserved at every order of approximation. Similarly, the unitary character of the time evolution operator in quantum mechanics is also preserved [38].

Another advantage of the symmetric operator-difference schemes considered is that the number of exponential operators is considerably less than in similar conventional symmetric split-operator schemes (without commuting operators and with commuting operators) with the same accuracy [39, 40, 41, 42, 43, 44, 45, 46]. For example, the sixth-order symmetric split-operator scheme [44, 45, 46] with a minimal number of exponential operators has fifteen exponential operators including eight exponential operators with Laplacian, while the scheme considered has only three exponential operators. In the framework of the unitary $[M/M]$ Padé approximation, the sixth-order scheme considered contains only five layers, but the symmetric split-operator scheme has 24 layers! Therefore for the high-order symmetric split-operator schemes one usually uses the fast Fourier transform techniques for the exponential of the Laplacian on only uniform mesh in the spatial variable.

However, there are sets of evolutionary boundary problems in complex domains and effective potentials with practical applications for solving of which one can use the nonuniform mesh too, e.g., [47]. From this point of view the FEM and variational methods will play a fundamental role in elucidating dynamical aspects of both basic quantum mechanics and quantum devices. The FEM is especially useful in this respect due to its adaptability and flexibility in using the nonuniform meshes [48]. The application of the FEM in designing and modeling a new generation of quantum devices will define the field of quantum wave function engineering [49].

The main purpose of this paper is to present the algorithm for solving one-dimensional TDSE using the second-, fourth- and sixth-order approximations in the time-dependent variable and achieving the desired level of accuracy for a sufficiently smooth solution in spatial variable approximated on a nonuniform finite interval by means of the high-order FEM. This work presents the next step in creating a set of programs for numerical solutions of the initial-boundary problem for multi-dimensional equations of the Schrödinger type with a required accuracy started in [24, 25]. It is based on our set of programs which implement both the Kantorovich method and FEM [21, 22, 34, 35]. In this paper we present the algorithm implemented as the FORTRAN 77 program TIME6T for calculating an approximate solution of the TDSE with controllable high accuracy and analysis of its efficacy in comparison with conventional calculation schemes based on symmetric splitting exponential operator techniques using the Padé approximations and

fast Fourier transform method.

The paper is organized as follows. In Section 2 we give a brief overview of the problem. In section 3 the general formulation and the high-order operator-difference multi-layer calculation schemes in time variable are presented. An efficiency of computational schemes and comparison with conventional ones are presented in Section 4. Test deck is discussed in Section 5.

2. Statement of the problem

Consider the Cauchy problem for the time-dependent Schrödinger equation on time interval $t \in [t_0, T]$

$$\begin{aligned} i \frac{\partial \psi(x, t)}{\partial t} &= H(x, t) \psi(x, t), \quad \psi(x, t_0) = \psi_0(x), \\ H(x, t) &= -\frac{1}{2} \frac{\partial^2}{\partial x^2} + f(x, t). \end{aligned} \quad (1)$$

We require the solution $\psi(x, t)$ to be continuous, have the general first derivatives that are square integrable and belonging to the Sobolev space $\mathbf{W}_2^1([x_{\min}, x_{\max}] \otimes [t_0, T])$. Also we suppose that function $f(x, t)$ is of sufficiently high smoothness in spatial variable x , which has continuous partial derivatives up to the $2M$ -order ($M = 1, 2, 3$ is the order of approximation) in time variable t .

The first and second type boundary conditions and normalization condition in spatial variable x on finite interval $[x_{\min}, x_{\max}]$ have the form

$$\left. \frac{\partial \psi(x, t)}{\partial x} \right|_{x=x_{\min}} = 0, \quad \text{or} \quad \psi(x_{\min}, t) = 0, \quad (2)$$

$$\left. \frac{\partial \psi(x, t)}{\partial x} \right|_{x=x_{\max}} = 0, \quad \text{or} \quad \psi(x_{\max}, t) = 0, \quad (3)$$

$$\|\psi(x, t)\|^2 = \int_{x_{\min}}^{x_{\max}} |\psi(x, t)|^2 dx = 1, \quad t \in [t_0, T]. \quad (4)$$

3. High-order operator-difference multi-layer calculation schemes in time variable

Eq. (1) can be rewritten in terms of unitary evolution operator $U(t, t_0)$ carrying the initial state $\psi_0(x)$ to the solution $\psi(x, t)$:

$$i \frac{\partial U(t, t_0)}{\partial t} = H(x, t) U(t, t_0), \quad U(t, t) = 1, \quad (5)$$

which is considered on the uniform grid $\Omega_\tau[t_0, T] = \{t_0, t_{k+1} = t_k + \tau, t_K = T\}$ with time step τ on the time interval $[t_0, T]$. Unitary operator $U(t_{k+1}, t_k)$ carrying the

solution $\psi(x, t_k)$ at $t = t_k$ ($k = 0, \dots, K - 1$) to the $\psi(x, t_{k+1})$ at $t = t_{k+1}$ can be expressed in the form [13, 24, 25]

$$\psi(x, t_{k+1}) = U(t_{k+1}, t_k)\psi(x, t_k), \quad U(t_{k+1}, t_k) = \exp(-i\tau A_k), \quad (6)$$

Here the effective time-independent Hamiltonian is related to the original one $H(x, t)$ by the Magnus expansion [36, 37],

$$A_k = \frac{1}{\tau} \int_{t_k}^{t_{k+1}} dt_1 H(x, t_1) + \frac{i}{2\tau} \int_{t_k}^{t_{k+1}} dt_1 \int_{t_k}^{t_1} dt_2 [H(x, t_2), H(x, t_1)] + \dots, \quad (7)$$

where $[,]$ is the operator commutator.

To solve the Cauchy problem (1)–(4) numerically at each step by transforming $\psi(x, t_k)$ into $\psi(x, t_{k+1})$, we use the explicit truncated Magnus expansion (7) of the evolution operator $U(t_{k+1}, t_k)$ up to order $O(\tau^{2M+1})$

$$U(t_{k+1}, t_k) = \exp\left(-i\tau A_k^{(M)}\right) + O(\tau^{2M+1}). \quad (8)$$

Now, we would like to express the truncation $A_k^{(M)}$ in terms of $H(x, t)$ and its time partial derivatives. Substituting the Taylor expansion of $H(x, t)$ in the vicinity of $t_c = t_k + \tau/2$

$$H(x, t) = \sum_{j=0}^{2M-1} \frac{(t - t_c)^j}{j!} \partial_t^j H(x, t_c) + O(\tau^{2M}) \quad (9)$$

into the integrals, one can derive an analytical expression of the operators $A_k^{(1)}$, $A_k^{(2)}, \dots, A_k^{(M)}$ by means of the symbolic algorithm GATEO (Generation of Approximations of the Time-Evolution Operator) [28]. To show the complexity of calculations, we present the first three approximations of the exponential (8) for the final effective Hamiltonians $A_k^{(M)}$ in the form $A_k^{(M)} = \hat{A}_k^{(M)} + \check{A}_k^{(M)}$

$$\begin{aligned} \hat{A}_k^{(1)} &= H, \\ \check{A}_k^{(1)} &= 0, \\ \hat{A}_k^{(2)} &= \hat{A}_k^{(1)} + \frac{\tau^2}{24} \ddot{H}, \\ \check{A}_k^{(2)} &= \check{A}_k^{(1)} + \frac{\tau^2}{12} [H, \dot{H}], \\ \hat{A}_k^{(3)} &= \hat{A}_k^{(2)} + \frac{\tau^4}{1920} \ddot{\ddot{H}} - \frac{\tau^4}{720} [H, [H, \ddot{H}]] - \frac{\tau^4}{240} [\dot{H}, [\dot{H}, H]], \\ \check{A}_k^{(3)} &= \check{A}_k^{(2)} - \frac{\tau^4}{480} [\ddot{\ddot{H}}, H] + \frac{\tau^4}{480} [\ddot{\ddot{H}}, \dot{H}] + \frac{\tau^4}{720} [H, [H, [\dot{H}, \dot{H}]]], \end{aligned} \quad (10)$$

where $H \equiv H(x, t_c)$, $\dot{H} \equiv \partial_t H(x, t)|_{t=t_c}, \dots$

Table 1: The real and imaginary parts of the coefficients $\alpha_\zeta^{(M)}$, $\zeta = 1, \dots, M$, $M = 1, 2, 3$.

M	ζ	$\text{Re } \alpha_\zeta^{(M)}$	$\text{Im } \alpha_\zeta^{(M)}$
1	1	+0	-1
2	1	$-1/\sqrt{3} \approx -0.577350269189625$	-1
2	2	$+1/\sqrt{3} \approx +0.577350269189625$	-1
3	1	-0.814799554248922	-0.854056730651663
3	2	+0.0	-1.291886538696673
3	3	+0.814799554248922	-0.854056730651663

After the application of the known generalized $[M/M]$ Padé approximation [50] to the exponential operator (8), the scheme (6) yields to the following implicit operator-difference [13, 24, 25]

$$\begin{aligned} \psi_k^0 &= \psi(x, t_k), \\ \left(I + \frac{\tau \overline{\alpha}_\zeta^{(M)} A_k^{(M)}}{2M} \right) \psi_k^{\zeta/M} &= \left(I + \frac{\tau \alpha_\zeta^{(M)} A_k^{(M)}}{2M} \right) \psi_k^{(\zeta-1)/M}, \quad \zeta = 1, \dots, M, \quad (11) \\ \psi(x, t_{k+1}) &= \psi_k^1, \end{aligned}$$

where I is the unit operator. The coefficients, $\alpha_\zeta^{(M)}$ ($\zeta = 1, \dots, M$), stand for the roots of the polynomial equation ${}_1F_1(-M, -2M, 2M\iota/\alpha) = 0$, where ${}_1F_1(a, b, x)$ is the confluent hypergeometric function and the overline indicates the complex conjugate. Table 1 lists the values of the coefficients $\alpha_\zeta^{(M)}$ for $M = 1, 2, 3$.

Note, that this approach preserves the unitarity of the approximate evolution operator, since the truncated $A_k^{(M)}$ is always self-adjoint. $\text{Im} \alpha_\zeta^{(M)} \neq 0$ yields that all the functions $\psi_k^{\zeta/M}$ have an equal norm, $\|\psi_k^0\| = \|\psi_k^{1/M}\| = \dots = \|\psi_k^1\|$.

The scheme (11) has two disadvantages. Firstly, this scheme contains the non-symmetric operator $\check{A}_k^{(M)}$ at $M \geq 2$. Secondly, this scheme contains the third-order differential operator by the spatial variable for implementation at $M = 3$, and requires more difficult and long calculations.

To generate the schemes with a symmetric operator $\tilde{A}_k^{(M)}$ (also free of the differential operator by the spatial variable with third-order at $M = 3$), we apply a gauge transformation $\tilde{\psi} = \exp(\iota S_k^{(M)}) \psi$, that yields a new operator

$$\tilde{A}_k^{(M)} = \exp(\iota S_k^{(M)}) A_k^{(M)} \exp(-\iota S_k^{(M)}). \quad (12)$$

The unknown symmetric operator $S_k^{(M)}$ is found from the additional condition [13]:

$$\exp(\iota S_k^{(M)}) \check{A}_k^{(M)} \exp(-\iota S_k^{(M)}) = O(\tau^{2M}), \quad (13)$$

in accordance with the well-known formula

$$\exp(A)B \exp(-A) = \sum_{j=0}^{\infty} \frac{1}{j!} \{A^j, B\}, \quad (14)$$

with $\{A^0, B\} = B$ and $\{A^{j+1}, B\} = [A, \{A^j, B\}]$. We seek for $S_k^{(M)}$ in the form of a power series with respect to τ

$$S_k^{(M)} = \sum_{j=0}^{2M-1} \tau^j S_{(j)}. \quad (15)$$

Substituting the expansion of $S_k^{(M)}$ into condition (13) and equating the terms with the same powers of τ in (14), we obtain a set of algebraic (or operator) recurrence relations for evaluating the unknown operator coefficients $S_{(j)}$ with the initial condition $S_{(0)} = 0$. The first three approximations of the operators (12) and (15) have the form

$$\begin{aligned} \tilde{A}_k^{(M)} &= -\frac{\partial}{\partial x} f_1^{(M)}(x, t_c) \frac{\partial}{\partial x} + f_2^{(M)}(x, t_c), \\ S_k^{(M)} &= -\frac{\partial}{\partial x} g_1^{(M)}(x, t_c) \frac{\partial}{\partial x} + g_2^{(M)}(x, t_c). \end{aligned} \quad (16)$$

The functions $f_1^{(M)}(x, t_c)$, $f_2^{(M)}(x, t_c)$ and $g_1^{(M)}(x, t_c)$, $g_2^{(M)}(x, t_c)$ are defined as follows

$$\begin{aligned} f_1^{(1)}(x, t_c) &= f_1^{(2)}(x, t_c) = \frac{1}{2}, & f_1^{(3)}(x, t_c) &= \frac{1}{2} + \frac{\tau^4}{720} \frac{\partial^2 \ddot{f}}{\partial x^2}, \\ f_2^{(1)}(x, t_c) &= f(x, t_c), & f_2^{(2)}(x, t_c) &= f(x, t_c) + \frac{\tau^2}{24} \ddot{f}, \\ f_2^{(3)}(x, t_c) &= f(x, t_c) + \frac{\tau^2}{24} \ddot{f} + \frac{\tau^4}{1920} \dots \ddot{f} + \frac{\tau^4}{1440} \left(\frac{\partial \dot{f}}{\partial x} \right)^2 \\ &\quad - \frac{\tau^4}{720} \frac{\partial \dot{f}}{\partial x} \frac{\partial f}{\partial x} - \frac{\tau^4}{2880} \frac{\partial^4 \ddot{f}}{\partial x^4}, \\ g_1^{(1)}(x, t_c) &= g_1^{(2)}(x, t_c) = 0, & g_1^{(3)}(x, t_c) &= -\frac{\tau^4}{720} \frac{\partial^2 \dot{f}}{\partial x^2}, \\ g_2^{(1)}(x, t_c) &= 0, & g_2^{(2)}(x, t_c) &= \frac{\tau^2}{12} \dot{f}, \\ g_2^{(3)}(x, t_c) &= \frac{\tau^2}{12} \dot{f} + \frac{\tau^4}{480} \ddot{f} + \frac{\tau^4}{720} \frac{\partial \dot{f}}{\partial x} \frac{\partial f}{\partial x} + \frac{\tau^4}{2880} \frac{\partial^4 \dot{f}}{\partial x^4}, \end{aligned} \quad (17)$$

where $f \equiv f(x, t_c)$, $\dot{f} \equiv \partial_t f(x, t)|_{t=t_c}$, \dots and $t_c = t_k + \tau/2$.

As the result, we obtain the following symmetric implicit operator-difference scheme:

$$\begin{aligned}\tilde{\psi}_k^0 &= \exp\left(\iota S_k^{(M)}\right) \psi(x, t_k), \\ \left(I + \frac{\tau \bar{\alpha}_\zeta^{(M)} \tilde{A}_k^{(M)}}{2M}\right) \tilde{\psi}_k^{\zeta/M} &= \left(I + \frac{\tau \alpha_\zeta^{(M)} \tilde{A}_k^{(M)}}{2M}\right) \tilde{\psi}_k^{(\zeta-1)/M}, \quad \zeta = 1, \dots, M, \quad (18) \\ \psi(x, t_{k+1}) &= \exp\left(-\iota S_k^{(M)}\right) \tilde{\psi}_k^1.\end{aligned}$$

Note that, in the case of $M = 1$, this scheme corresponds to well-known Crank-Nicolson scheme [51]. One can see, that for $M = 3$, operator $S_k^{(M)}$ in a general case contains the second-order differential operator $\partial^2/\partial x^2$. Hence in this case we use again the generalized $[L/L]$ Padé approximations for $\exp(\pm \iota S_k^{(M)})$. This approximation has the order of $O(\tau^{4L+2})$, while $4L+2 \geq 2M$, so that we can choose $L = 1$ at $M = 3$. In this case we lead to the following implicit operator-difference scheme [13]:

$$\begin{aligned}\psi_k^0 &= \psi(x, t_k), \\ \left(I - \frac{\bar{\alpha}_\eta^{(1)} S_k^{(3)}}{2}\right) \psi_k^1 &= \left(I - \frac{\alpha_1^{(1)} S_k^{(3)}}{2}\right) \psi_k^0, \\ \tilde{\psi}_k^0 &= \psi_k^1, \\ \left(I + \frac{\tau \bar{\alpha}_\zeta^{(M)} A_k^{(M)}}{2M}\right) \tilde{\psi}_k^{\zeta/M} &= \left(I + \frac{\tau \alpha_\zeta^{(M)} A_k^{(M)}}{2M}\right) \tilde{\psi}_k^{(\zeta-1)/M}, \quad \zeta = 1, \dots, M, \quad (19) \\ \psi_k^0 &= \tilde{\psi}_k^1, \\ \left(I + \frac{\bar{\alpha}_1^{(1)} S_k^{(3)}}{2}\right) \psi_k^1 &= \left(I + \frac{\alpha_1^{(1)} S_k^{(3)}}{2}\right) \psi_k^0, \\ \psi(x, t_{k+1}) &= \psi_k^1.\end{aligned}$$

Let us present operator $H(t) \equiv H(x, t)$ as

$$H(t) = H_0 + g(t), \quad (20)$$

where H_0 is positively defined linear self-adjoint operator that is time-independent and satisfying condition $\|\psi\| \leq \|H_0\psi\|$, and $g(t)$ is a function with bounded derivatives in time-dependent variable up to the order $2M$:

$$\left\| \frac{\partial^m}{\partial t^m} g(t) \right\| \leq c_1, \quad 0 \leq m \leq 2M. \quad (21)$$

Suppose further that on each time-dependent interval $t_i \in [t_k, t_{k+1}]$, $i = 1, \dots, s+1 \leq 2M$ the following estimates are valid at $0 \leq m \leq 2M$:

$$\left\| (adH(t_{s+1})) \cdots (adH(t_2)) \frac{\partial^m g(t_1)}{\partial t^m} \psi \right\| \leq c_2 \|H_0^{s/2} \psi\|, \quad (22)$$

$$\tau \|H_0^{1/2}\| < c_3, \quad \tau < 2M\mu \|A_k^{(M)}(t)\|^{-1}. \quad (23)$$

Here ψ belongs to Sobolev space $\mathbf{W}_2^s([x_{\min}, x_{\max}] \otimes [t_0, T])$; constants c_1, c_2, c_3 do not depend on time-dependent step τ , and $\mu \approx 0.28$ is a root of transcendental equation $\mu \exp(\mu + 1) = 1$.

Theorem. [13] Suppose that $\tau A_k^{(M)}$, the explicit Magnus expansion of linear self-adjoint operator $H(t) = H_0 + g(t)$ of order $O(\tau^{2M+1})$, $M = 1, 2, 3$, at the moment of time $t_c = t_k + \tau/2$ on uniform grid $\Omega_\tau[t_0, T] = \{t_0, t_{k+1} = t_k + \tau, t_K = T\}$, satisfies conditions (21), (22), (23) at fixed time-dependent step τ . Then errors of numerical solutions $\psi(t_{k+1}) \equiv \psi(x, t_{k+1})$ at the moment of time $t = t_{k+1}$ for symmetric operator-difference multi-layer schemes (18) and (19) are bounded with estimate

$$\epsilon_M = \|\psi_{ext}(t_{k+1}) - \psi(t_{k+1})\| \leq C\tau^{2M}(t_{k+1} - t_0)\|H_0^{2M+1}\psi_0\|, \quad (24)$$

where $\psi_{ext}(t_{k+1})$ is the exact solution of evolutionary equation and C is some constant independent on τ and M .

Proof is straightforward following the schemes of proof in accordance with [26, 52].

From estimate (24) it follows that the symmetric operator-difference multi-layer schemes with step $\tau = \tau_M < 1$ at $M = 1, 2, 3$ have almost the same errors ϵ_M , if the following conditions are fulfilled

$$\tau_1 = \tau_3^3, \quad \tau_2 = \sqrt{\tau_3^3}. \quad (25)$$

In each transition from $\psi(t_k)$ to $\psi(t_{k+1})$ we get the 1, 2, 5-layered schemes at $M = 1, 2, 3$, i.e., at $M = 2, 3$ calculation times on the same grids are about 2 and 5 times longer than at $M = 1$, respectively. Nevertheless, according to (25) in order to reach the same accuracy when selecting time-dependent steps for a scheme with $M = 1, 2$ the total computation time is $1/(5\tau_3^2)$ and $2/(5\sqrt{\tau_3})$ times longer than at $M = 3$, respectively. For example, if $\tau_3 = 0.01$, then the total computation time using schemes $M = 1$ and $M = 2$ is 2000 and 4 times longer than using scheme with $M = 3$, respectively. This result following from the theorem is confirmed by numerical experiments performed in [3, 13] and in the test calculations of Section 5 of the present paper.

4. Efficiency of the computational schemes and comparison with conventional ones

Let us consider the TDSE (1)–(4) on the finite time interval $t \in [t_0, T]$ for the two-center problem with Pöschl-Teller potentials [8] similar to an ionization problem [7]. We choose a special case of a resting well, $A_0 < 0$, and a barrier, $A_1 > 0$ (or a well $A_1 < 0$), that moved with velocity v with respect to the resting well:

$$\begin{aligned} i\frac{\partial\psi(x, t)}{\partial t} &= H(x, t)\psi(x, t), \\ H(x, t) &= -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{A_0}{\cosh^2(x)} + \frac{A_1}{\cosh^2(x - x_0(t))}, \end{aligned} \quad (26)$$

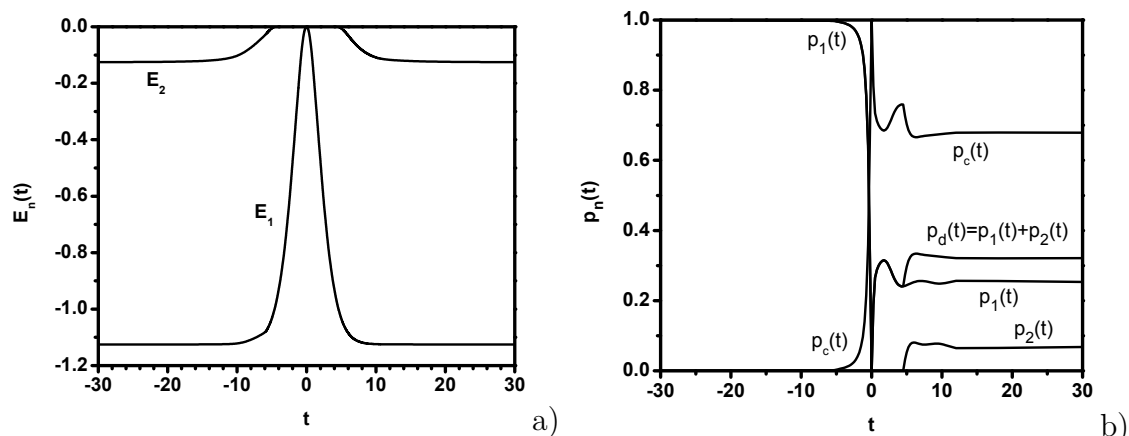


Figure 1: a) Eigenenergies $E_n(t)$ of the instant Hamiltonian in dependence of the time as a parameter t . b) The bound state probabilities $p_1(t)$, $p_2(t)$ and the ionization probability $p_c(t)$ vs the time t . Here $v = 1/2$, $x_0(t_0) = vt_0 = -15$, $t_0 = -30$.

where $H(x, t)$ is an instant Hamiltonian and $x_0(t) = vt$ is an position of the center of moving barrier. For numerical calculation with required accuracy the initial boundary problem in a spatial axis is reduced to a sufficiently large finite interval $x \in (x_{\min}, x_{\max})$, with boundary and normalization conditions

$$\psi(x_{\min}, t) = 0, \quad \psi(x_{\max}, t) = 0, \quad \|\psi(x, t)\|^2 = \int_{x_{\min}}^{x_{\max}} |\psi(x, t)|^2 dx = 1. \quad (27)$$

We consider an example of the evolution of the wave packet in the time-interval $t \in [t_0, T]$, induced by the moving barrier ($A_1 = 15/8$) with velocity v , with respect to the resting well ($A_0 = -15/8$) supporting two bound states $n_0 = 2$ with energies $E_1(t = t_0) \cong E_1^W = -9/8 = -1.125$ and $E_2(t = t_0) \cong E_2^W = -1/8 = -0.125$. At $v > 0$ we choose the initial time t_0 and the final time T from the following values of initial $x_0(t_0) = vt_0 = -15$ and final $x_0(T) = vT = 15$ positions of the center of moving barrier to preserve with required accuracy the discrete spectrum states supported by the resting well in both the initial time t_0 and the final time T . So, we start from the initial state that corresponds with required accuracy to the ground state supported by the resting well

$$\psi(x, t_0) \cong \psi_1^W(x) = N_1(\cosh x)^{-(\sqrt{1-8A_0}-1)/2}. \quad (28)$$

Note that in the case $A_1 + A_0 = 0$ at $t = 0$ the potential of the problem (26) is equal to zero on the whole axis and the instant Hamiltonian $H(x, t)$ at $t = 0$ has pure continuous spectrum that provide full ionization of the considered quantum system and capture to the discrete spectrum states during further evolution.

Calculations were performed on the spatial variable interval $x \in (-512, 512)$ that is sufficient to avoid reflection from its boundaries on considered time interval $t \in [t_0, T]$. The wave functions $\psi_n(x; t)$ of discrete spectrum $E_n < 0$, and $\psi_E^<(x; t) \equiv \psi_E^<(x; t)$ of continuous spectrum $E \geq 0$ of the instant Hamiltonian $H(x, t)$ from (26)

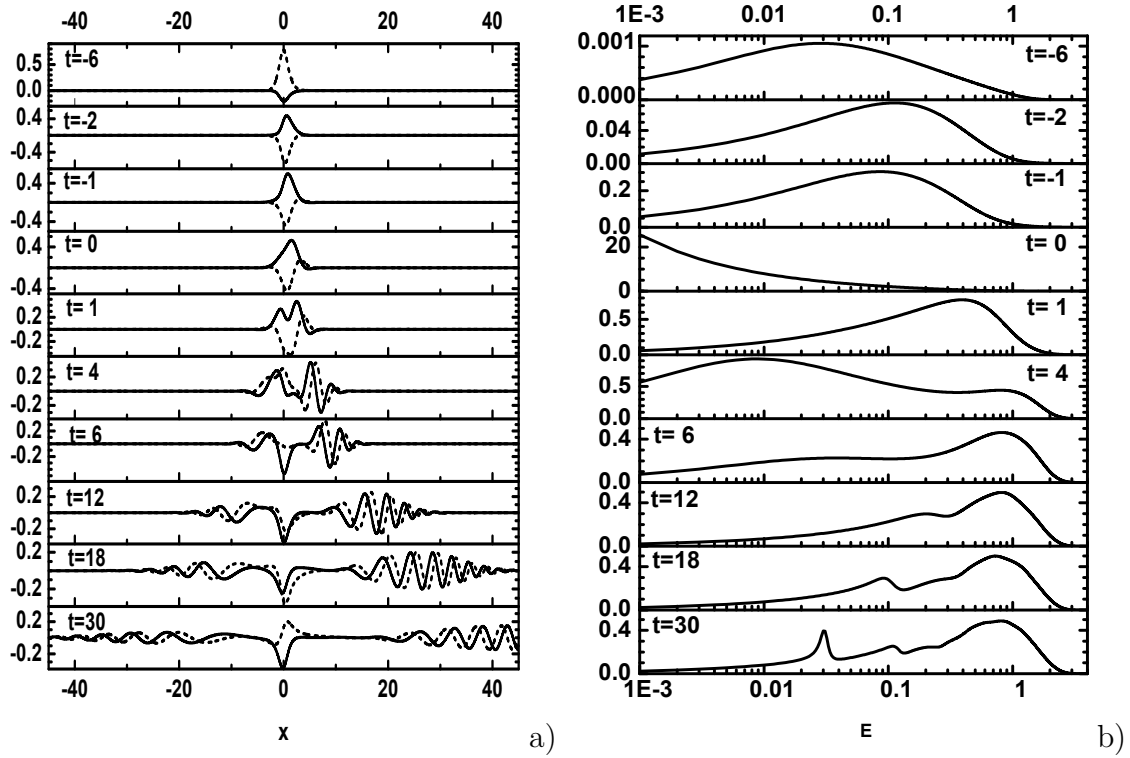


Figure 2: a) Real (solid line), image (dashed line) parts of the wave function and b) the distribution of ionization probability $p_E(t)$ vs the time t for fixed value of velocity $v = 1/2$ and initial position of the moving barrier $x_0(t_0) = vt_0 = -15$, $t_0 = -30$.

dependent on t as a parameter are calculated in spatial interval $x \in (x_{\min}, x_{\max})$ with the corresponding homogeneous third-type boundary conditions by modified [33] version of KANTBP program [34] using appropriate asymptotes of solutions. The subscript ν equals to \rightarrow or \leftarrow that corresponds to the positive or negative directions of the final momentum $q = \pm\sqrt{2E}$, respectively. After attaching the asymptotes on whole axis $x \in (-\infty, +\infty)$ these functions satisfy the conventional orthogonality and completeness relations

$$\int_{-\infty}^{+\infty} dx (\psi_E^{\nu'}(x; t))^* \psi_{E'}^{\nu}(x; t) = (2\pi) \delta(E - E') \delta_{\nu\nu'}, \quad (29)$$

$$\int_{-\infty}^{+\infty} dx (\psi_E^{\nu}(x; t))^* \psi_n(x; t) = 0, \quad (30)$$

$$\sum_{n=1}^{n_0} \psi_n(x; t) \psi_n(x'; t) + \sum_{\nu=\leftarrow}^{\rightarrow} \int_0^{+\infty} dE (\psi_E^{\nu}(x; t))^* \psi_E^{\nu}(x'; t) = \delta(x - x'). \quad (31)$$

Dependence of eigenenergies $E_n < 0$ of the instant Hamiltonian on time parameter t is shown in Fig. 1a. One can see that in a vicinity of time value $t = 0$ the Hamiltonian has only one eigenvalue $E_1 < 0$ and at time $t = 0$ it has only continuous spectrum.

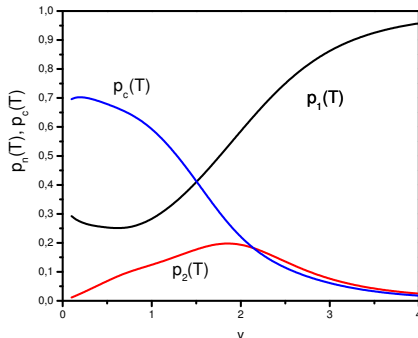


Figure 3: The probabilities $p_1(T)$, $p_2(T)$ of ground and first excited states, and ionization probability $p_c(T)$ vs velocity v for time $T = 15/v$ and initial time $t_0 = -15/v$ when the position of the center of barrier is equal $x_0(T) = 15$ and $x_0(t_0) = -15$, correspondingly.

The probabilities $p_n(t)$ and $p_c(t)$ of transition to the bound and continuum states and its distribution $p_E(t)$ vs energy $E \geq 0$ of continuum spectrum in the above capture and ionization processes are calculated by formulas

$$p_n(t) = |t_{n0}(t)|^2, \quad t_n(t) = \int_{x_{\min}}^{x_{\max}} dx (\psi_n(x, t))^* \psi(x, t) \quad (32)$$

$$p_E(t) = \frac{|t_E^{\rightarrow}(t)|^2 + |t_E^{\leftarrow}(t)|^2}{2\pi}, \quad t_E^{\leftarrow}(t) = \int_{x_{\min}}^{x_{\max}} dx (\psi_E^{\leftarrow}(x, t))^* \psi(x, t), \quad (33)$$

and as follows from (31), at $E_{\max} \gg 1$ they satisfy, with required accuracy, the condition

$$\sum_{n=1}^{n_0} p_n(t) + p_c(t) = 1, \quad p_c(t) = \int_0^{E_{\max}} p_E(t) dE. \quad (34)$$

As it is mentioned above, at time moment $t = 0$ the effective potential is equal zero, and eigenfunctions of the instant Hamiltonian correspond to continuous spectrum wave functions. After that the effective potential becomes again nonzero and processes of captures to the excited and ground states may occur which is shown by evolution of probabilities $p_E(t)$ and $p_c(t)$ in Figs. 1b and 2. In Fig. 2 it is shown that at $t \geq 1$ the maxima of energy distribution $p_{E \sim 1} \sim 0.5$ correspond to the forward and backward ionization waves with similar frequencies moved to left and right. The maxima of $p_c(t)$ at $t \sim 4$ on Fig. 1b correspond to the maxima of $p_{E \sim 0.01} \sim 1$ at frame $t = 4$ on Fig. 2b and coincide with ionization and capture processes. With increasing velocity the probability densities of the excited states at large velocity tend to zero (see Fig. 3). The wave function and the distribution of ionization probability $p_E(t)$ for some values of velocity are shown in Fig. 4. As it is seen from Fig. 4 with increasing v the forward ionization waves dominate and their energy increase.

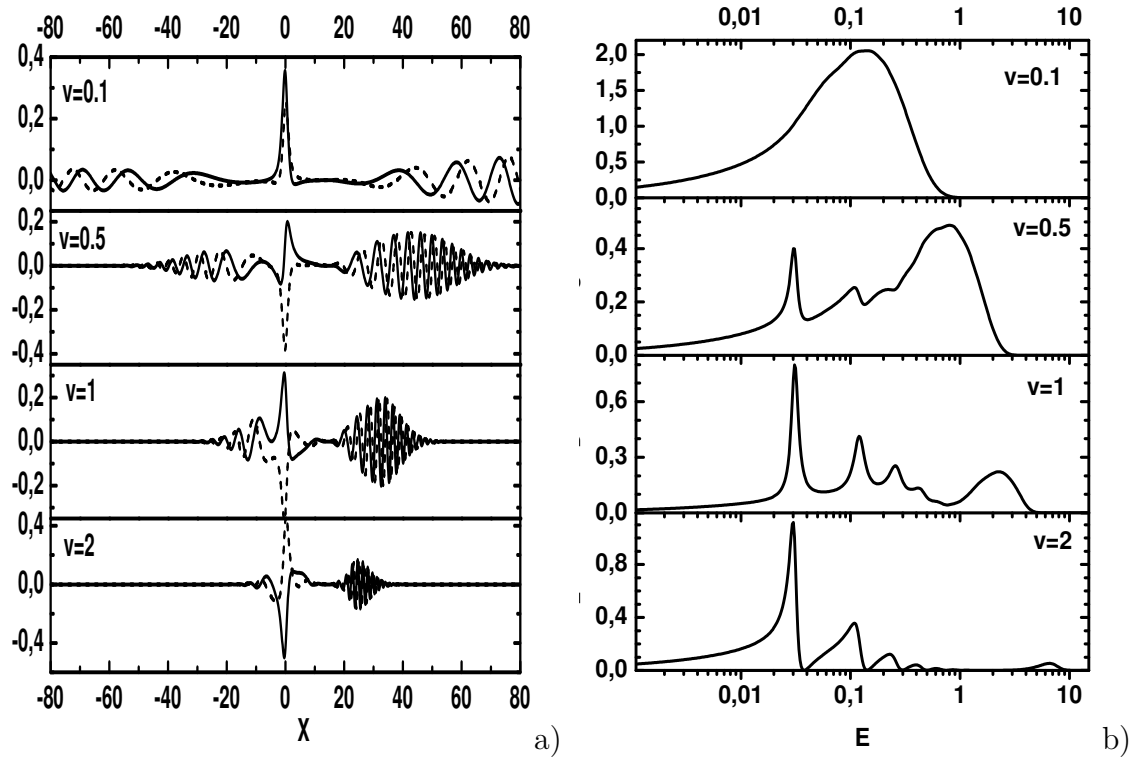


Figure 4: a) Real (solid line), image (dashed line) parts of the wave function and b) the distribution of ionization probability $p_E(T)$ by energy E for fixed values of velocity $v = 0.1, 0.5, 1, 2$ for values of parameters given in Fig. 3.

The reason why we have chosen this problem is related to the fact that it has suitable properties to demonstrate the efficiency of different computational unitary schemes mentioned in introduction during an evolution of initial state in strongly reformed effective barrier potential that leads to excitation, ionization of the states and capture to the states considered above.

In framework for the symmetric split-step exponential methods we have used the following approximations of the unitary evolution operator [46]:

$$U(t_{k+1}, t_k) \equiv U(t_k + \tau, t_k) = S_{2M+1}(t_{k+1}, t_k) + O(\tau^{2M+1}), \quad (35)$$

where $M = 1, 2, 3$ and the symmetric unitary operators S_3 , S_5 and S_7 have the forms

$$S_3(t_{k+1}, t_k) = \exp\left(i \frac{t_{k+1} - t_k}{2} \frac{1}{2} \frac{\partial^2}{\partial x^2}\right) \exp\left(-i \int_{t_k}^{t_{k+1}} f(x, s) ds\right) \times \exp\left(i \frac{t_{k+1} - t_k}{2} \frac{1}{2} \frac{\partial^2}{\partial x^2}\right), \quad (36)$$

$$S_5(t_{k+1}, t_k) = \prod_{j=1}^3 S_3(a_j, a_{j+1}), \quad S_7(t_{k+1}, t_k) = \prod_{j=1}^7 S_3(b_j, b_{j+1}),$$

Table 2: Comparison of the discrepancy functions $Er(t = 20, 1)$ for the approximations of the order $O(\tau^3)$, $O(\tau^5)$ and $O(\tau^7)$ with the time step $\tau = \tau_3^3$, $\tau = \sqrt{\tau_3^3}$ and $\tau = \tau_3 = 0.0625$, respectively.

	$O(\tau^3)$		$O(\tau^5)$		$O(\tau^7)$	
	$Er(t, 1)$	CPU,s	$Er(t, 1)$	CPU,s	$Er(t, 1)$	CPU,s
Magnus	0.2521(-6)	3841	0.2296(-7)	105	0.1262(-8)	69
SSOS+Padé	0.6765(-7)	4355	0.3210(-6)	327	0.2246(-6)	208
SSOS+FFT	0.2776(-3)	1475	0.3104(-6)	62	0.2225(-6)	33

depending on the set of parameters

$$\begin{aligned}
a_1 &= t_k, & a_2 &= a_1 + \omega\tau, & a_3 &= a_2 + (1 - 2\omega)\tau, & a_4 &= t_{k+1}, \\
b_1 &= t_k, & b_2 &= b_1 + \omega_3\tau, & b_3 &= b_2 + \omega_2\tau, & b_4 &= b_3 + \omega_1\tau, \\
b_5 &= b_4 + \omega_0\tau, & b_6 &= b_5 + \omega_1\tau, & b_7 &= b_6 + \omega_2\tau, & b_8 &= t_{k+1}, \\
\omega_0 &= 1 - 2(\omega_1 + \omega_2 + \omega_3),
\end{aligned} \tag{37}$$

with the following numerical values given with the double precision accuracy:

$$\begin{aligned}
\omega &= \frac{1}{2-\sqrt[3]{2}}, & \omega_1 &= -1.177679984178871, \\
\omega_2 &= 0.235573213359358, & \omega_3 &= 0.784513610477557.
\end{aligned} \tag{38}$$

The unitary operator S_3 has three exponential operators including two exponential operators with Laplacian, S_5 has seven exponential operators including four exponential operators with Laplacian, S_7 has fifteen exponential operators including eight exponential operators with Laplacian. According to [44, 45], the unitary operators S_3 , S_5 and S_7 have a minimal number of exponential operators for the indicated leading errors. We have considered two different expansions of the exponential of the Laplacian.

For the first one, we have used generalized $[M/M]$ Padé approximation [50] (denoted here by SSOT+Padé). In this case the second-order scheme has two layers, the fourth-order scheme has eight layers, and the sixth-order scheme has 24 layers. For the second one, we have used the straightforward and inverse fast Fourier transform (FFT) techniques for the exponential of the Laplacian, using a uniform mesh (the number of grids is a power of 2) for the spatial variable (denoted here by SSOT+FFT).

Calculation by all three schemes were performed on the spatial variable interval $x \in (-512, 512)$ that was sufficient to avoid reflection from its boundaries on considered time interval $t \in [-20, 20]$. For the schemes with the Padè approximation, we have used the nonuniform finite-element grid $\hat{\Omega}_x[x_{\min}, x_{\max}] = \{x_{\min} = -512, (256), -128, (512), -32, (512), 32, (512), 128, (256), x_{\max} = 512\}$, where the

Table 3: The same results Table 2, but only for Magnus schemes with the time step $\tau = \tau_3 = 0.125$.

	$O(\tau^3)$		$O(\tau^5)$		$O(\tau^7)$	
	$Er(t, 1)$	CPU,s	$Er(t, 1)$	CPU,s	$Er(t, 1)$	CPU,s
Magnus	0.1613(-4)	456	0.1450(-5)	37	0.3635(-6)	34

number in the brackets denotes the number of finite-element in the intervals. Between each two nodes we have applied the Lagrange interpolation polynomials up to the order $p = 8$. For FFT, the uniform spatial grid $\hat{\Omega}_x[x_{\min}, x_{\max}] = \{x_{\min} = -512, (2048), x_{\max} = 512\}$ is used.

In Table 2 we present the discrepancy functions of the numerical wave packet as a function of the computation time in CPU seconds for various orders of accuracy in the time increments. The Table shows that the fourth- and sixth-order SSOS+Padé and SSOS+FFT schemes give similar errors, nevertheless the SSOS+Padé schemes requires much more CPU time. The fourth- and sixth-order Magnus schemes give the best results, but require about twice CPU time than SSOT+FFT. We observed that error of the second-order SSOS+Padé scheme is smaller than of the second-order Magnus scheme. Also the second-order SSOS+FFT scheme gives the low accuracy, because a norm of the wave packet at the moment $t = 20$ equals 0.999 (i.e., correct only up to 3 digits after the decimal point). *Note that both calculation schemes with Padé approximations saved the norm of the wave packet during calculation process with the accuracy that is not less than 10^{-13} .*

In Table 3 we show the same results for Magnus schemes with doubled time step. In this case the discrepancy function of the sixth-order Magnus scheme has the same order as SSOS+Padé and SSOS+FFT schemes, and calculation CPU times are similar to the SSOS+FFT's ones. Analysis of these results show that Magnus's scheme with optimal choice of nonuniform mesh has the efficiency comparable with SSOT+FFT, and much more efficient than SSOT+Padé. Presented results clearly show that calculation CPU times needed to obtain a solution with the same accuracy are essentially lower for all sixth-order schemes than for the corresponding lower-order schemes.

5. Test calculations

The TDSE from (1)–(4) for a one-dimensional harmonic oscillator with an explicit time-dependent frequency $\omega(t)$ on the finite time interval $t \in [0, T]$ has the form [1]

$$i \frac{\partial \psi(x, t)}{\partial t} = \left(-\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{\omega^2(t)x^2}{2} \right) \psi(x, t). \quad (39)$$

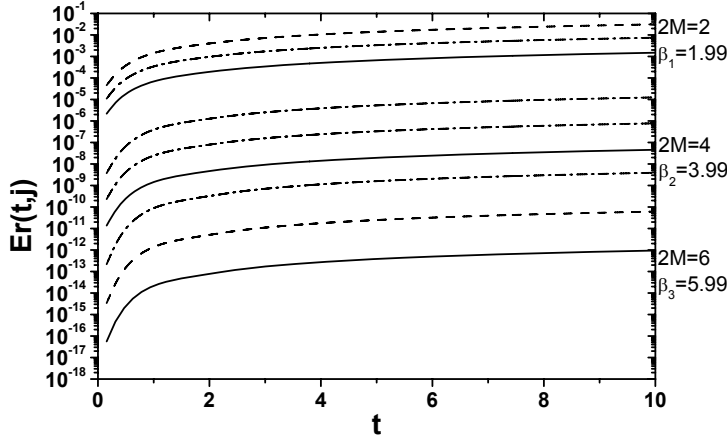


Figure 5: The test results of the discrepancy functions $Er(t, j)$, $j = 1, 2, 3$ (dash-dotted, dashed and solid curves) for the approximations of order $2M = 2, 4, 6$ with the time step $\tau = 0.009765625$.

Time-dependent frequency $\omega(t)$ and initial wave packet $\psi_0(x)$ are chosen following [13, 24]

$$\omega^2(t) = 4 - 3 \exp(-t), \quad \psi_0(x) = \sqrt[4]{\frac{1}{\pi}} \exp\left(-\frac{1}{2}(x - \sqrt{2})^2\right). \quad (40)$$

For $M = 3$, functions $f_1^{(M)}(x, t)$, $f_2^{(M)}(x, t)$ and $g_1^{(M)}(x, t)$, $g_2^{(M)}(x, t)$ are defined as follows

$$\begin{aligned} f_1^{(3)}(x, t) &= \frac{1}{2} - \frac{\tau^4}{240} \exp(-t), \\ f_2^{(3)}(x, t) &= \frac{4 - 3 \exp(-t)}{2} x^2 - \frac{\tau^2}{16} \exp(-t) x^2 \\ &\quad - \frac{\tau^4}{3840} \exp(-t) (24 \exp(-t) - 61) x^2, \\ g_1^{(3)}(x, t) &= -\frac{\tau^4}{240} \exp(-t), \\ g_2^{(3)}(x, t) &= \frac{\tau^2}{8} \exp(-t) x^2 - \frac{\tau^4}{960} \exp(-t) (12 \exp(-t) - 19) x^2. \end{aligned} \quad (41)$$

For $M = 1$ terms with orders τ^2 and τ^4 should be neglected while at $M = 2$ only terms of order τ^4 .

To analyze the convergence on a sequence of three doubly-condenced time grids, we define the auxiliary time dependent discrepancy functions

$$Er^2(t, j) = \int_{x_{\min}}^{x_{\max}} |\psi(x, t_k) - \psi^{\tau^j}(x, t_k)|^2 dx, \quad j = 1, 2, 3, \quad (42)$$

and the Runge coefficient

$$\beta(t) = \log_2 \left| \frac{Er(t, 1) - Er(t, 2)}{Er(t, 2) - Er(t, 3)} \right|, \quad (43)$$

where $\psi^{\tau_j}(x, t)$ are the numerical solutions with the time step $\tau_j = \tau/2^{j-1}$. For the function $\psi(x, t)$ one can use the numerical solution with the time step $\tau_4 = \tau/8$. Hence, we obtain the numerical estimates for the convergence order of the numerical scheme (19), that strongly correspond to theoretical ones $\beta(t) \equiv \beta_M(t) \approx 2M$.

For performing an accuracy control over the numerical solution in step τ , the Runge coefficient (43) is calculated on four doubly condensed grids using the additional subroutine RUNGE.

To approximate the solution $\psi(x, t)$ in the variable x , we make use of the finite-element grid $\hat{\Omega}_x[x_{\min}, x_{\max}] = \{x_{\min} = -11, (220), x_{\max} = 11\}$ and the time step $\tau = 0.009765625$, where the number in the brackets denotes the number of finite elements for the intervals. Between each two nodes we apply the Lagrange interpolation polynomials up to the order of $p = 8$. Fig. 5 displays the behavior of discrepancy functions $Er(t; j)$, $j = 1, 2, 3$ (dash-dotted, dashed and solid curves, respectively) and convergence rate $\beta_M(t)$ for the approximations of the order $2M = 2, 4, 6$ with the time step $\tau = 0.009765625$. To demonstrate high efficiency of sixth-order scheme, we have used the quadruple precision version of TIME6T fortran code.

The double precision version of TIME6T fortran code with the above test calculations as well as with benchmark calculations [14] of the Cauchy problem for the multidimensional time-dependent Schrödinger equation is available for user in JINRLIB [53].

The considered examples clearly demonstrate the advantages of the new method and its efficiency. The proposed technique and software will be asked-for and will find applications in solving wave-packed problems in physics of atomic, molecular and quantum-dimensional systems as well as in quantum calculations.

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