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ON SYMBOLIC-NUMERICAL REPRESENTATION OF EVOLUTION OPERATOR FOR FINITE-DIMENSIONAL QUANTUM SYSTEMS

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A symbolic algorithm to generate the multilayer operator-difference schemes for solving the evolution problem of time dependent Schrödinger equation is elaborated. An additional gauge transformation of operator-difference schemes to make a good use of the finite-element discretization is applied. The efficiency of the generated numerical schemes till the sixth order with respect to the time step and till the seventh order with respect to the spatial step is demonstrated by calculations of some finite-dimensional quantum systems in external fields.

Разработан символьный алгоритм, позволяющий генерировать многослойные неявные схемы решения эволюционной задачи для нестационарного уравнения Шредингера. Для более эффективного применения метода конечных элементов при построении операторно-разностных схем реализовано также дополнительное калибровочное преобразование. Эффективность сгенерированных схем до шестого порядка точности по шагу по временной переменной и до седьмого порядка точности по шагу по пространственной переменной демонстрируется расчетами некоторых конечномерных квантовых систем во внешних полях.

INTRODUCTION

The modern laser physics experiments have stimulated computer simulations announced in [1] for the time-dependent dynamics of few-body Coulomb systems in a train of laser pulses and the time-dependent Schrödinger equation (TSDE) for the control problems of quantum systems [2]. For any numerical method, a pair of requirements is always made: one is stability, and the other is accuracy. From the viewpoint of these requirements, the unitary splitting methods have a big advantage: the unitarity of the evolution operators applied in the methods preserves the norm of the wave functions, so that the conservation of probability density and robustness of methods are guaranteed.

In this paper, a new computational method is proposed to solve the TDSE, in which the unitary splitting algorithm with uniform time grids [3] is combined with an application of the finite-element method (FEM) and an interpolation method in nonuniform spatial grids [4]. The efficiency and the accuracy of the developed numerical algorithms are confirmed in certain integrable atomic models in external fields.

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1. GENERAL FORMULATION AND CALCULATION SCHEMES

Let us consider the Cauchy problem of the TDSE on the time interval $t \in [t_0, T]$

$$\begin{gathered} i\partial_t \psi(x,t) = H(x,t)\psi(x,t), \quad ||\psi||^2 = \int |\psi(x,t)|^2 dx = 1, \\ \psi(x,t_0) = \psi_0(x), \quad \psi(x,t) \in \mathbf{H}^1(\mathbf{R}^n \otimes [t_0,T]), \quad \psi_0(x) \in \mathbf{H}^1(\mathbf{R}^n), \end{gathered} \tag{1}$$

with initial state $\psi_0(x)$, which describes an atomic model in an external (electromagnetic) field[1]. We rewrite (1) for an unitary operator $U(t,t_0,\lambda)$ with a complementary parameter[2] carrying the initial state $\psi(x,t_0)$ to the solution $\psi(x,t)$ in the form

$$i\partial_t U(t,t_0,\lambda) = \lambda H(x,t) U(t,t_0,\lambda), \quad U(t_0,t_0,\lambda) = 1,$$

which we consider in the uniform grid, with time step τ, in the time interval $[0,T]$: $\Omega_\tau[t_0,T] = \{t_0, t_{k+1} = t_k + \tau, (k = 0,1,\ldots,K), t_K = T\}$. We express the unitary operator $U(t_{k+1},t_k,\lambda)$ carrying the solution $\psi(t_k) \equiv \psi(x,t_k)$ at $t = t_k$ to the one $\psi(t_{k+1})$ at $t = t_{k+1}$ in the form [3]

$$\begin{gathered} \psi(t_{k+1}) = U(t_{k+1},t_k,\lambda)\psi(t_k), \\ U(t_{k+1},t_k,\lambda) = \exp\left\{-\imath\tau A_k^{(M)}(t,\lambda)\right\} + O(\tau^{2M+1}). \end{gathered} \tag{2}$$

We start with the power-series expansion of $A_k^{(M)}(t,\lambda)$ in terms of the formal parameter λ, $A_k^{(M)}(t,\lambda) = \dfrac{1}{\tau}\displaystyle\sum_{j=1}^{2M} \lambda^j A_{(j)k}(t)$, where the coefficients $A_{(j)}(t) \equiv A_{(j)k}(t)$ are evaluated from the operator-identity [5]

$$-\imath\lambda H(t) = \sum_{n=1;q=0;l_1,\ldots,l_q=1}^{n+\Sigma_{i=1}^q l_i \leqslant 2M} \frac{\lambda^{n+\Sigma_{i=1}^q l_i}}{(q+1)!} \left(adA_{(l_1)}(t)\right) \cdots \left(adA_{(l_q)}(t)\right) \dot{A}_{(n)}\ (t). \tag{3}$$

Here linear operator (adA): $\mathcal{L}(X) \to \mathcal{L}(X)$ is defined for operators $A, B \in \mathcal{L}(X)$ in the form $(adA)B = [A,B] \equiv AB - BA$ and has the following properties: $(adA)^0 B = B$, $(adA)^j B = (adA)^{j-1}(adA)B$. Note that the dot over the operator $A_{(n)}(t)$ means the partial derivation, $\dot{A}_{(n)}\ (t) = \partial_t A_{(n)}(t)$, in t. Equating the coefficients at the same powers of λ in both sides of (3), we obtain a set of the first-order differential equations [1]. Solving sequentially the set of equations obtained, we are led to the effective Hamiltonians $A_{(k)}(t)$ connected with the original one $H(t)$ via the Magnus expansion written in terms of repeated integrals [5]. We wish to express the truncation $A_k^{(M)}$ given in terms of $H(t)$, its partial derivative in time and the higher ones. Putting the Taylor expansion of $H(t)$ in a vicinity of $t = t_k + \tau/2$ as $H(t) = \displaystyle\sum_{j=0}^{2M} \frac{(t-t_c)^j}{j!} \partial_t^j H(t_c)$ into the integrals, one can find an analytical

[1]The atomic units are applied throughout this paper.

[2]The complementary formal parameter λ will be replaced to be $\lambda = 1$ later.

(meaning non-numerical) expression of operators, $A_k^{(1)}, A_k^{(2)}, \ldots, A_k^{(M)}$, in principle: for $A_k^{(1)}$, we have only to calculate the coefficient of λ^0, and then obtain $A_k^{(1)} = \int\limits_0^1 d\xi_0 H(t_k + \xi_0\tau) = H(t_k + \tau/2) + O(\tau^2)$, without any difficulties. However, in the case of $A_k^{(M)}$ with large M, rather cumbersome calculations are required to fix all the coefficients of the power of λ in $A_k^{(M)}$ «by hand». Our algorithm GATEO (Generation of Approximations of the Time-Evolution Operator) is thereby motivated by the difficulty of calculation pointed out above, that provides the set of generators $A_k^{(M)}(t_{k+1})$ required in the operator-difference scheme derived in (7).

In the case of the expansion of the Hamiltonian $H(t)$ in a vicinity of $t = t_c \equiv t_k + \tau/2$, we will also find operators $A_k^{(M)}(t_{k+1})$ in the form of the series, $A_k^{(M)}(t_{k+1}) = \sum\limits_{j=0}^{2M} \frac{\tau^j}{2^j j!} A_{(j)k}$, with unknown coefficients $A_{(j)k}$. Recalling that the evolution operator $U(t_k, t_{k+1}, \lambda)$ is inverse to operator $U(t_{k+1}, t_k, \lambda)$, we have $A_{k+1}(t_k) = A_k(t_{k+1})$. It means that the above series of $A_k^{(M)}(t_{k+1})$ contains only even degrees of τ because expression of $A_{k+1}^{(M)}(t_k)$ will be obtained from $A_k^{(M)}(t_{k+1})$, by formal substitution $\tau \to -\tau$. Then the unknown coefficients $A_{(j)k}$ are calculated explicitly from a set of recurrence equations [6]

$$(j+1)A_{(j+1)}(t_c) = -\imath\frac{1+(-1)^j}{2^{j+1}j!}\partial_t^j H(t_c) + \sum_{n=0}^{j}\sum_{q=0}^{j-n}\sum_{l_1,\ldots,l_q\geqslant 1}^{n+\Sigma_{i=1}^q l_i = j} \frac{B^n_{l_1,\ldots,l_q}}{n!},$$

$$B^n_{l_1,\ldots,l_q} = \big(adA_{(l_1)}(t_c)\big)\cdots\big(adA_{(l_q)}(t_c)\big)\,Q_{qn};$$

$$Q_{qn} = -\imath\frac{(-1)^n}{2^{n+1}n!}\partial_t^n H(t_c) - \frac{q+1}{n+1}A_{(n+1)}(t_c).$$

To show the complexity of calculations, we present the first three approximations of the exponential (2) for the final effective Hamiltonians $A_k^{(M)}$ in the form $A_k^{(M)} = \hat{A}_k^{(M)} + \imath\breve{A}_k^{(M)}$:

$$\hat{A}_k^{(1)} = H, \quad \breve{A}_k^{(1)} = 0,$$

$$\hat{A}_k^{(2)} = \hat{A}_k^{(1)} + \frac{\tau^2}{24}\,\ddot{H}, \quad \breve{A}_k^{(2)} = \breve{A}_k^{(1)} + \frac{\tau^2}{12}(adH)\,\dot{H},$$

$$\hat{A}_k^{(3)} = \hat{A}_k^{(2)} + \frac{\tau^4}{1920}\,\dddot{H} - \frac{\tau^4}{720}(adH)^2\,\ddot{H} - \frac{\tau^4}{240}(ad\,\dot{H})^2 H, \tag{4}$$

$$\breve{A}_k^{(3)} = \breve{A}_k^{(2)} - \frac{\tau^4}{480}(ad\,\dddot{H})H + \frac{\tau^4}{480}(ad\,\ddot{H})\,\dot{H} + \frac{\tau^4}{720}(adH)^3\,\dot{H}.$$

where $H \equiv H(t_{k+1/2})$, $\dot{H} \equiv \partial_t H(x,t)|_{t=t_{k+1/2}}$, $\ddot{H} \equiv \partial_t^2 H(x,t)\big|_{t=t_{k+1/2}}$, $\ldots$ We wish to make further approximation of the unitary scheme of Eq. (2).

Application to the exponential operator (2) of the generalized $[M/M]$ Padé approximation yields

$$\begin{aligned} \exp\left(-i\tau A_k^{(M)}\right) &= \prod_{\zeta=1}^{M} T_{\zeta k} + O(\tau^{2M+1}), \\ T_{\zeta k} &= \left(I + \frac{\tau\overline{\alpha}_\zeta^{(M)} A_k^{(M)}}{2M}\right)^{-1} \left(I + \frac{\tau\alpha_\zeta^{(M)} A_k^{(M)}}{2M}\right), \end{aligned} \tag{5}$$

where the overline indicates the complex conjugate operation. The coefficients, $\alpha_\zeta^{(M)}$ ($\zeta = 1, \ldots, M$, $M \geqslant 1$), stand for the roots of the polynomial equation, ${}_1F_1(-M, -2M, 2Mi/\alpha) = 0$, where ${}_1F_1$ is the confluent hypergeometric function. The coefficients $\alpha_\zeta^{(M)}$ have the following properties: $\Im\alpha_\zeta^{(M)} < 0$ and $0.6 < |\alpha_\zeta^{(M)}| < \mu^{-1}$, where $\mu \approx 0.28$ is the root of equation $\mu \exp(\mu + 1) = 1$. Note that the condition $\tau < 2M\mu \left\| A_k^{(M)} \right\|^{-1}$ guarantees the validity of the approximation (5) for any bounded operator $A_k^{(M)}$.

We are now in a position to obtain the transition from $\psi(t_k)$ to $\psi(t_{k+1})$, by using the approximation (5) of the evolution operator in (2). To make it, we rewrite the transition in terms of the auxiliary functions defined by $\psi_k^{\zeta/M} = T_{\zeta k}\psi_k^{(\zeta-1)/M}$, $\zeta = 1, \ldots, M$. The fact that $\Im\alpha_\zeta^{(M)} < 0$ yields the operators, $T_{\zeta k}$, to be isometric, so that all the $\left\|\psi_k^{\zeta/M}\right\|$ have an equal norm, $\|\psi_k^0\| = \left\|\psi_k^{1/M}\right\| = \ldots = \|\psi_k^1\|$. To generate the schemes with extraction symmetric part $\tilde{A}_{t_c}^{(M)}$ of the operator $A_{t_c}^{(M)} = \hat{A}_{t_c}^{(M)} + \imath\breve{A}_{t_c}^{(M)}$, we apply a gauge transformation $\tilde{\psi} = \exp\left(\imath S_{t_c}^{(M)}\right)\psi$, that leads to a new operator $\tilde{A}_{t_c}^{(M)} = \exp\left(\imath S_{t_c}^{(M)}\right) A_{t_c}^{(M)} \exp\left(-\imath S_{t_c}^{(M)}\right)$. We will find $S_{t_c}^{(M)}$ in the form of a series by powers of τ: $S_{t_c}^{(M)} = \sum_{j=0}^{2M} \tau^j S_j$, where unknown coefficients $S^{(M)}$ are calculated from an additional condition: $\overset{\asymp}{A}{}_{t_c}^{(M)} \tilde{\psi} = O(\tau^{2M})$. Here $\overset{\asymp}{A}{}_{t_c}^{(M)} = \exp\left(\imath S_{t_c}^{(M)}\right) \breve{A}_{t_c}^{(M)} \exp\left(-\imath S_{t_c}^{(M)}\right)$ are evaluated in accordance with Hausdorff's formulae, $\exp(A)B\exp(-A) = \sum_{j=0} \frac{1}{j!}(adA)^j B$. Substituting the expansion of $S_{t_c}^{(M)}$ to the condition and equating at the same powers of τ, we obtain a set of algebraic (or operator) recurrence relations for evaluating unknown coefficients S_j with the initial condition $S_0 = 0$. Taking into account the above procedures at each kth time step of the grid Ω_τ ($k = 0, 1, \ldots, K-1$), we are led to the operator-difference scheme with a partial splitting of the evolution operator,

$$\begin{aligned} \tilde{\psi}_k^0 &= \exp(iS^{(M)})\psi(t_k), \\ \left(I + \frac{\tau}{2M}\overline{\alpha}_\zeta^{(M)}\tilde{A}_k^{(M)}\right)\tilde{\psi}_k^{\zeta/M} &= \left(I + \frac{\tau}{2M}\alpha_\zeta^{(M)}\tilde{A}_k^{(M)}\right)\tilde{\psi}_k^{(\zeta-1)/M},\ \zeta = 1, 2, \ldots, M, \\ \psi(t_{k+1}) &= \exp(-iS^{(M)})\tilde{\psi}_k^1. \end{aligned} \tag{6}$$

Hence, the auxiliary functions $\tilde{\psi}_k^{\zeta/M}$ ($\zeta = 1, \ldots, M-1$) in Eq. (6) can be treated as a kind of approximate solutions on a set of the fractional time steps $t_{k+\zeta/M} = t_k + \tau\zeta/M$, $\zeta =$

$1, \ldots, M-1$ in the time interval $[t_k, t_{k+1}]$. The scheme (6) is an implicit one of order $2M$ preserving the norm of the difference solution, so that this scheme is stable. Further, the scheme (6) provides an approximation of the order $O(\tau^{2M})$ in the sense of [7], while any individual equation in (6) provides only an approximation of degree not higher than $O(\tau^2)$. Note that in the case $M = 1$, i.e. $[1/1]$ Padé approximation of exponential operator (5), the scheme (6) reduces to the well-known Crank–Nicholson scheme [7].

2. APPLICATION OF THE FEM PARTIAL SPLITTING SCHEMES

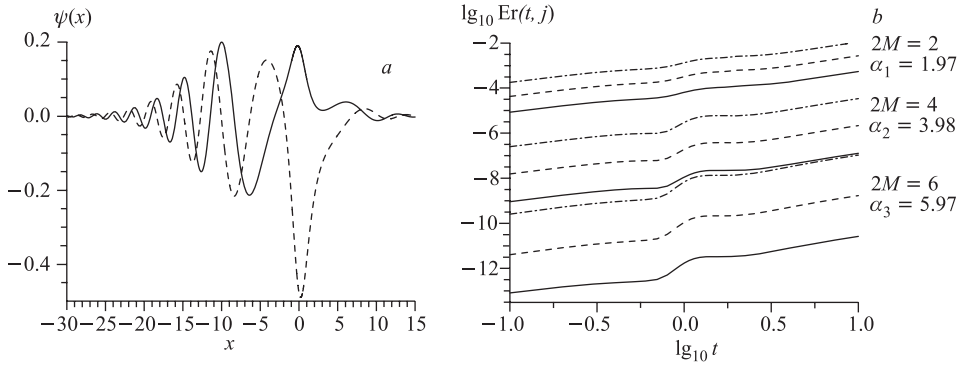
The Cauchy problem of the TDSE in the interval for an atom in an external field reads as

$$\imath \frac{\partial}{\partial t}\psi(x,\, t) = H(x,t)\psi(x,\, t), \quad H(x,t) = H(x) + q(x,t), \quad H(x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x),$$
$$\psi(-\infty, t) = \psi(\infty, t) = 0, \quad \psi(x, t_0) = \psi_0(x) \quad (x,t) \in \mathbf{R} \times [t_0, T], \tag{7}$$

and the normalization condition is claimed at any $t \geqslant t_0$: $||\psi||^2 = \int\limits_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$.

For the operators $q(x,t)$ and $H(x)$ and the wave function $\psi(x)$, we make the following assumptions: the $q(x,t)$ describes the dipole-approximation of the interaction between the atom and the external field $f(t)$, which is written in the form $q(x,t) = f(t)x$.

To illustrate how the above approach allows an efficient solution of the TDSE problem (7), we consider a Pöschl–Teller atom (PTA) in a laser pulse electric field. For the PT model the potential function $V(x) = -\cosh^{-2} x$ supports only one bound state $\psi_0(x) = 1/\sqrt{2}\cosh x$, with the eigenvalue $E_0 = -0.5$ a.u., and a continuum of the known scattering states with $E > 0$. The laser pulse $f(t)$ is given by $f(t) = \left\{ f_0 \sin^2\left(\frac{\pi t}{2t_0}\right), 0 < t < 2t_0; 0, |t - t_0| \geqslant t_0, \right\}$ where $f_0 = t_0 = 1$. We choose the corresponding ground state $\psi_0(x)$ as an initial state. To approximate the solution $\psi_i(x,t)$, $i = 1, 2, 3, 4$ we use 1600 finite elements



a) Real and imaginary parts of solution $\phi(x,t)$ (solid and dashed curves) for PTA atom at $t = T = 10$ and *b*) logarithm of discrepancy $Er(t;i), i = 1, 2, 3$ (dash-dotted, dashed and solid curves) for schemes with $M = 1, 2, 3$ calculated in Fortran by quadruple precision (33 significant digits)

of the sixth order and the finite element grid $\Omega = \{-1500(200) - 300(200) - 20(200) - 1(400)1(200)20(200)300(200)1500\}$, where the numbers in brackets denote the number of finite elements in the intervals. We calculated the above solution over the enclosed time grids $\Omega_\tau[t_0 = 0, T = 10]$ with four different time steps $\tau = 0.01, 0.005, 0.0025, 0.00125$. The figure displays the wave function calculated at time $T = 10$ and examines the behavior of discrepancy functions $Er(t;i), i = 1,2,3$, evaluated by formulae $Er^2(t;i) = \int\limits_{x_{\min}}^{x_{\max}} [\psi_4(x,t) - \psi_i(x,t)]^*[\psi_4(x,t) - \psi_i(x,t)]dx$, where the index $i = 1,2,3,4$ labels the numerical solutions, obtained for different values of the time step τ. Having these three values of $Er(t;i)$, we can calculate the Runge ratio $\alpha_M(t) = \ln(|Er(t;1) - Er(t,2)|/|Er(t;2) - Er(t,3)|)/\ln 2$. The figure shows the plots of $Er(t;i), i = 1,2,3$ for these schemes (upper three curves correspond to the second-order scheme, middle three curves to the fourth-order scheme and lower three ones to the sixth-order scheme) and the mean value of α_M over all values $\alpha_M(t_k)$ of the grid $\Omega_\tau[0,10]$. Hence, we obtain the numerical estimates of $\alpha_M(t)$ and their mean value, α_M, that strongly corresponds to the theoretical ones $\alpha_M(t) \approx 2M$.

CONCLUSIONS

We have presented a new computational approach to solve the TDSE, in which partial (unitary) splitting of evolution operator and the FEM are combined together effectively. Especially to realize our approach in an explicit form, we have derived the second-, fourth-, and sixth-order approximations with respect to time step. Several numerical results have been also given which turn out to agree with the theoretical ones to a good extent.

As our future program, we wish to mention an extension of our proposed approach to the nonlinear TDSE with the use of the Lie symmetry formalism [8], which some of the authors have a plausible reason to think of. If it is possible, «Lie-admissible» TDSEs could be thought of, from which we could find exact solutions [9]. Our approach would be worth being applied to the quantum control problem, some pre-experimental calculations in the atomic dynamics in traps and/or external-pulse fields, and other quantum calculations [2].

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