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КОМПЬЮТЕРНЫЕ ТЕХНОЛОГИИ В ФИЗИКЕ

MULTILAYER EVOLUTION SCHEMES FOR THE FINITE-DIMENSIONAL QUANTUM SYSTEMS IN EXTERNAL FIELDS

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The operator-difference multilayer (ODML) schemes for solving the time-dependent Schrödinger equation (TDSE) till six order accuracy by a time step are presented. The reduced schemes for solving a set of the coupled TDSEs are devised by using a set of appropriate basis angular functions and a finite element method with respect to a hyperradial variable. Convergence by a number of the basis functions and efficiency of the numerical schemes are demonstrated in the case of an exactly solvable model of the two-dimensional oscillator in time-dependent electric fields.

Представлены операторно-разностные многослойные схемы для решения нестационарного уравнения Шредингера до шестого порядка точности по временной переменной. Выведены редуцированные схемы для решения набора связанных нестационарных уравнений Шредингера с помощью набора соответствующих угловых базисных функций и метода конечных элементов относительно гиперрадиальной переменной. Сходимость по числу базисных функций и эффективность численных схем демонстрируются в случае точно решаемой модели двухмерного осциллятора во внешних переменных электрических полях.

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INTRODUCTION

Solving the TDSE with a required accuracy is needed for the control problems of quantum systems [1], the decay problem in nuclear physics [2], the ionization problems of atomic and molecular physics in pulse fields or impact collisions beyond a dipole approximation [3]. For solving the TDSE in a finite-dimensional region with respect to spacial variables one conventionally seeks a required wave-packet solution in a form of expansion over appropriate angular basis functions and further discretization of hyperradial equations, for example, the finite-difference [4], finite-element [5], spline [6] methods, etc.

Usually a rate convergence by a number of angular basis functions is controlled by solving corresponded stationary Schrödinger equation [7]. However, in some special cases of long-range effective potentials acting in asymptotic regions, like confinement potentials, a key problem consists in additional study [8]. So, using exact solvable models of the TDSE, one can have an additional experience in the field.

In this paper, a new computational method is applied to solve the TDSE, in which the unitary splitting algorithm with uniform time grids [9] is combined with an application of the Kantorovich or Galerkin reductions to a set of the TDSE by a hyperradial variable [5] and the finite-element method (FEM) [10] and an interpolation method in nonuniform spatial grids [5]. The efficiency, convergence and accuracy of the elaborated numerical schemes are confirmed by benchmark calculations of an exactly solvable model of the two-dimensional oscillator in time-dependent external fields [1].

1. ODML EVOLUTION SCHEME

Let us consider the d-dimensional TDSE with a self-adjoint Hamiltonian $H(\mathbf{r},t)$ and a governing function $f(\mathbf{r},t)$ on the time interval $t \in [t_0, T]$:

$$\imath \frac{\partial \Psi(\mathbf{r},t)}{\partial t} = H(\mathbf{r},t)\Psi(\mathbf{r},t), \quad \Psi(\mathbf{r},t_0) = \Psi_0(\mathbf{r}), \quad \|\Psi\|^2 = \int |\Psi(\mathbf{r},t)|^2 d\mathbf{r} = 1, \tag{1}$$

$$H(\mathbf{r},t) = H_0(\mathbf{r}) + f(\mathbf{r},t), \quad H_0(\mathbf{r}) = -\frac{1}{2}\nabla^2_{\mathbf{r}} + U(\mathbf{r}), \quad f(\mathbf{r},t_0) \equiv 0. \tag{2}$$

We also require continuity of derivatives of the control function $f(\mathbf{r},t)$ and continuity of solutions $\Psi(\mathbf{r},t) \in \mathbf{W}^1_2(\mathbf{R}^d \otimes [t_0,T])$ and $\Psi_0(\mathbf{r}) \in \mathbf{W}^1_2(\mathbf{R}^d)$. We solve the above Cauchy problem (1), (2) in the uniform grid $\Omega_\tau[t_0,T] = \{t_0, t_{k+1} = t_k + \tau, t_K = T\}$ with time step, τ, in the time interval $[t_0,T]$ by means of the ODML calculation scheme [9] rewritten after factorization of a gauge transformation, with operator S, in the following symmetric form:

$$\begin{aligned}
&\psi_k^0 = \Psi(t_k),\\
&\left(I - \frac{\overline{\alpha}_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{\eta/L} = \left(I - \frac{\alpha_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{(\eta-1)/L}, \quad \eta = 1,\ldots,L,\\
&\tilde{\psi}_k^0 = \psi_k^1,\\
&\left(I + \frac{\tau\overline{\alpha}_\zeta^{(M)} \tilde{A}_k^{(M)}}{2M}\right)\tilde{\psi}_k^{\xi/M} = \left(I + \frac{\tau\alpha_\zeta^{(M)} \tilde{A}_k^{(M)}}{2M}\right)\tilde{\psi}_k^{(\xi-1)/M}, \quad \zeta = 1,\ldots,M,\\
&\psi_k^0 = \tilde{\psi}_k^1,\\
&\left(I + \frac{\overline{\alpha}_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{\eta/L} = \left(I + \frac{\alpha_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{(\eta-1)/L}, \quad \eta = 1,\ldots,L,\\
&\Psi(t_{k+1}) = \psi_k^1.
\end{aligned} \tag{3}$$

The coefficients, $\alpha_\zeta^{(M)}$ ($\zeta = 1,\ldots,M,\ M \geqslant 1$), stand for the roots of the polynomial equation, ${}_1F_1(-M,-2M,2M\imath/\alpha) = 0$, where ${}_1F_1$ is the confluent hypergeometric function. This scheme has the accuracy of order $O(\tau^{2M})$ with respect to time step τ, if we choose $L = [M/2]$. Below we consider the scheme with $M \leqslant 3$, that is sufficient for a practical utilization. For the Hamiltonian given in (2) the operators $\tilde{A}_k^{(M)}$ and $S_k^{(M)}$ read as

$$\begin{aligned}
&\tilde{A}_k^{(1)} = H, \quad S_k^{(1)} = 0,\\
&\tilde{A}_k^{(2)} = \tilde{A}_k^{(1)} + G^{(2)}, \quad S_k^{(2)} = S_k^{(1)} + Z^{(2)}, \qquad (4)\\
&\tilde{A}_k^{(3)} = \tilde{A}_k^{(2)} + G^{(3)} - \frac{\tau^4}{720}\nabla_{\mathbf{r}}\left(\nabla_{\mathbf{r}}^2 \ddot{f}\right)\nabla_{\mathbf{r}}, \quad S_k^{(3)} = S_k^{(2)} + Z^{(3)} + \frac{\tau^4}{720}\nabla_{\mathbf{r}}\left(\nabla_{\mathbf{r}}^2 \dot{f}\right)\nabla_{\mathbf{r}},\\
&G^{(2)} = \frac{\tau^2}{24}\ddot{f}, \quad Z^{(2)} = \frac{\tau^2}{12}\dot{f},\\
&G^{(3)} = \frac{\tau^4}{1920}\ddddot{f} + \frac{\tau^4}{1440}\left(\nabla_{\mathbf{r}}\dot{f}\right)^2 - \frac{\tau^4}{720}\left(\nabla_{\mathbf{r}}\ddot{f}\right)\left(\nabla_{\mathbf{r}}(U+f)\right) - \frac{\tau^4}{2880}\left(\nabla_{\mathbf{r}}^4\ddot{f}\right), \qquad (5)\\
&Z^{(3)} = \frac{\tau^4}{480}\dddot{f} + \frac{\tau^4}{720}\left(\nabla_{\mathbf{r}}\dot{f}\right)\left(\nabla_{\mathbf{r}}(U+f)\right) + \frac{\tau^4}{2880}\left(\nabla_{\mathbf{r}}^4\dot{f}\right),
\end{aligned}$$

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

2. REDUCED ODML SCHEME

In the framework of a coupled-channel hyperspherical adiabatic approach [5], known in mathematics as the Kantorovich method [4], the partial wave function $\Psi(\mathbf{r}, t)$ is expanded over the one-parametric basis functions $\{B_j(\Omega; r)\}_{j=1}^N$

$$\Psi(\mathbf{r}, t) = \sum_{j=1}^{N} B_j(\Omega; r)\chi_j(r, t). \qquad (6)$$

In Eq. (6), the vector-function $\boldsymbol{\chi}(r, t) = (\chi_1(r, t), \ldots, \chi_N(r, t))^T$ is unknown, and the surface function $\mathbf{B}(\Omega; r) = (B_1(\Omega; r), \ldots, B_N(\Omega; r))^T$ is an orthonormal basis with respect to the set of angular coordinates Ω for each value of hyperradius r which is treated here as a given parameter. The functions $B_j(\Omega; r)$ are determined as solutions of the following parametric eigenvalue problem [7, 11]:

$$\left(-\frac{1}{2r^2}\hat{\mathbf{\Lambda}}_{\Omega}^2 + U(\mathbf{r})\right) B_j(\Omega; r) = E_j(r) B_j(\Omega; r), \qquad (7)$$

where the generalized self-adjoint angular momentum operator $\hat{\mathbf{\Lambda}}_{\Omega}^2$ corresponds to the d-dimensional Laplace operator $\nabla_{\mathbf{r}}^2$. The eigenfunctions of this problem satisfy the same boundary conditions in angular variable Ω for $\Psi(\mathbf{r}, t)$ and are normalized as follows:

$$\left\langle B_i(\Omega; r) \middle| B_j(\Omega; r)\right\rangle_{\Omega} = \int \overline{B}_i(\Omega; r)\, B_j(\Omega; r)\, d\Omega = \delta_{ij}, \qquad (8)$$

where δ_{ij} is the Kronecker symbol.

After minimizing the Rayleigh–Ritz variational functional (see [11]), and using expansion (6), Eq. (1) is reduced to a finite set of N ordinary second-order differential equations

$$\imath \mathbf{I}\frac{\partial \boldsymbol{\chi}(r,t)}{\partial t} = \mathbf{H}(r,t)\boldsymbol{\chi}(r,t), \quad \boldsymbol{\chi}(r,t_0) = \boldsymbol{\chi}_0(r),$$
$$\mathbf{H}(r,t) = -\frac{1}{2r^{d-1}}\mathbf{I}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r} + \mathbf{V}(r,t) + \mathbf{Q}(r)\frac{\partial}{\partial r} + \frac{1}{r^{d-1}}\frac{\partial r^{d-1}\mathbf{Q}(r)}{\partial r}. \tag{9}$$

Here $\mathbf{V}(r,t)$, $\mathbf{I}$ and $\mathbf{Q}(r)$ are matrices of dimension $N \times N$, whose elements are given by the relation

$$V_{ij}(r,t) = \frac{E_i(r) + E_j(r)}{2}\delta_{ij} + \frac{1}{2}\left\langle \frac{\partial B_i(\Omega;r)}{\partial r}\middle|\frac{\partial B_j(\Omega;r)}{\partial r}\right\rangle_\Omega + \\ + \left\langle B_i(\Omega;r)\middle| f(\mathbf{r},t)\middle| B_j(\Omega;r)\right\rangle_\Omega,$$
$$I_{ij} = \delta_{ij}, \quad Q_{ij}(r) = -\frac{1}{2}\left\langle B_i(\Omega;r)\middle|\frac{\partial B_j(\Omega;r)}{\partial r}\right\rangle_\Omega. \tag{10}$$

The boundary conditions and normalization condition have the form

$$\boldsymbol{\chi}(0,t) = 0, \quad \text{if} \quad \min_{1\leqslant j\leqslant N}\lim_{r\to 0} r^{d-1}|V_{jj}(r,t)| = \infty,$$
$$\lim_{r\to 0} r^{d-1}\left(\mathbf{I}\frac{\partial}{\partial r} - \mathbf{Q}(r)\right)\boldsymbol{\chi}(r,t) = 0, \quad \text{if} \quad \min_{1\leqslant j\leqslant N}\lim_{r\to 0} r^{d-1}|V_{jj}(r,t)| < \infty, \tag{11}$$
$$\lim_{r\to\infty}\boldsymbol{\chi}(r,t) = 0,$$
$$\int_0^\infty \left(\bar{\boldsymbol{\chi}}(r,t)\right)^T \boldsymbol{\chi}(r,t) r^{d-1}\, dr = 1. \tag{12}$$

In this case we obtain the finite $N \times N$ matrix operator-difference scheme for unknown vector-functions $\boldsymbol{\chi}(r,t)$, analogous to (3)

$$I \mapsto \mathbf{I}, \quad \tilde{A}_k^{(M)} \mapsto \tilde{\mathbf{A}}_k^{(M)}, \quad S_k^{(M)} \mapsto \tilde{\mathbf{S}}_k^{(M)}, \tag{13}$$

where $\tilde{\mathbf{A}}_k^{(M)}$ and $\tilde{\mathbf{S}}_k^{(M)}$ are matrix operators of dimension $N \times N$ given by the relation

$$\begin{aligned} \tilde{\mathbf{A}}_k^{(1)} &= \mathbf{H}(r,t_c), & \tilde{\mathbf{S}}_k^{(1)} &= \mathbf{0}, \\ \tilde{\mathbf{A}}_k^{(2)} &= \tilde{\mathbf{A}}_k^{(1)} + \tilde{\mathbf{G}}^{(2)}, & \tilde{\mathbf{S}}_k^{(2)} &= \tilde{\mathbf{S}}_k^{(1)} + \tilde{\mathbf{Z}}^{(2)}, \\ \tilde{\mathbf{A}}_k^{(3)} &= \tilde{\mathbf{A}}_k^{(2)} + \tilde{\mathbf{G}}^{(3)} + \dot{\mathbf{C}}_k^{(3)}, & \tilde{\mathbf{S}}_k^{(3)} &= \tilde{\mathbf{S}}_k^{(2)} + \tilde{\mathbf{Z}}^{(3)} - \mathbf{C}_k^{(3)}, \\ \tilde{G}_{ij}^{(M)} &= \left\langle B_i(\Omega;r)\middle| G^{(M)}\middle| B_j(\Omega;r)\right\rangle_\Omega, \\ \tilde{Z}_{ij}^{(M)} &= \left\langle B_i(\Omega;r)\middle| Z^{(M)}\middle| B_j(\Omega;r)\right\rangle_\Omega. \end{aligned} \tag{14}$$

The operator $\mathbf{C}_k^{(3)}$ is equal to zero for $\left(\nabla^2_{\mathbf{r}} f\right) = 0$ and in other case has the form

$$\mathbf{C}_k^{(3)} = \frac{\tau^4}{720}\left(-\frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\tilde{\mathbf{D}}(r)\frac{\partial}{\partial r} + \tilde{\mathbf{V}}(r) - \tilde{\mathbf{Q}}^T(r)\frac{\partial}{\partial r} + \frac{1}{r^{d-1}}\frac{\partial r^{d-1}\tilde{\mathbf{Q}}(r)}{\partial r}\right), \quad (15)$$

where $\tilde{\mathbf{D}}(r)$, $\tilde{\mathbf{V}}(r)$ and $\tilde{\mathbf{Q}}(r)$ are matrices of dimension $N \times N$, whose elements are given by the relations

$$\begin{aligned}
\tilde{D}_{ij}(r) &= \left\langle B_i(\Omega;r)\middle|\left(\nabla^2_{\mathbf{r}}\,\dot{f}\right)\middle|B_j(\Omega;r)\right\rangle_\Omega,\\
\tilde{V}_{ij}(r) &= \left\langle \frac{\partial B_i(\Omega;r)}{\partial r}\middle|\left(\nabla^2_{\mathbf{r}}\,\dot{f}\right)\middle|\frac{\partial B_j(\Omega;r)}{\partial r}\right\rangle_\Omega +\\
&\qquad + \frac{1}{r^2}\left\langle \hat{\mathbf{\Lambda}}_\Omega B_i(\Omega;r)\middle|\left(\nabla^2_{\mathbf{r}}\,\dot{f}\right)\middle|\hat{\mathbf{\Lambda}}_\Omega B_j(\Omega;r)\right\rangle_\Omega, \quad (16)\\
\tilde{Q}_{ij}(r) &= -\left\langle B_i(\Omega;r)\middle|\left(\nabla^2_{\mathbf{r}}\,\dot{f}\right)\middle|\frac{\partial B_j(\Omega;r)}{\partial r}\right\rangle_\Omega.
\end{aligned}$$

3. THE EXACTLY SOLVABLE TWO-DIMENSIONAL MODEL

The TDSE for a two-dimensional oscillator (or a charged particle in a constant uniform magnetic field) in the external governing electric field with components $E_1(t)$ and $E_2(t)$ nonequal to zero in the finite time interval $t \in [0,T]$ in the dipole approximation and atomic units has the form [1]

$$\imath\frac{\partial}{\partial t}\phi(x_1,y_1,t) = -\frac{1}{2}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2}\right)\phi(x_1,y_1,t) + \frac{\imath\omega}{2}\left(x_1\frac{\partial}{\partial y_1} - y_1\frac{\partial}{\partial x_1}\right)\phi(x_1,y_1,t) + \\ + \frac{\omega^2}{8}(x_1^2+y_1^2)\phi(x_1,y_1,t) - (x_1E_1(t) + y_1E_2(t))\phi(x_1,y_1,t). \quad (17)$$

The transformation to a rotated coordinate system with frequency $\omega/2$, $x_1 = x\cos(\omega t/2) + y\sin(\omega t/2)$, $y_1 = y\cos(\omega t/2) - x\sin(\omega t/2)$, and polar coordinates $x = r\cos(\theta)$, $y = r\sin(\theta)$, leads to the following equation:

$$\imath\frac{\partial}{\partial t}\phi(r,\theta,t) = \left[-\frac{1}{2}\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} - \frac{1}{2}\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\omega^2 r^2}{8} + \right. \\ \left. + r(f_1(t)\cos(\theta) + f_2(t)\sin(\theta))\right]\phi(r,\theta,t), \quad (18)$$

where $f_1(t) = -E_1(t)\cos(\omega t/2) + E_2(t)\sin(\omega t/2)$, $f_2(t) = -E_1(t)\sin(\omega t/2) - E_2(t)\times$ $\times\cos(\omega t/2)$. Using the Galerkin projection of solutions by means of the angular basis

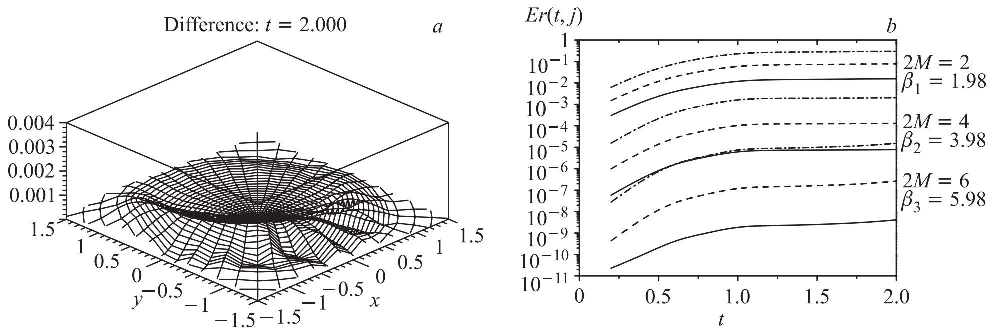

Fig. 1. The absolute values of the difference $|\phi_{\rm ext}(x,y,t)-\phi(x,y,t)|$ at $t=2$ (a) and the test results of the discrepancy functions $Er(t,j)$, $j=1,2,3$ (dash-dotted, dashed and solid curves) for the approximations of order $M=1,2,3$ with the time step $\tau=0.00625$ (b)

functions $B_j(\theta)$

$$\phi(r,\theta,t)=\sum_{j=1}^{N} B_j(\theta)\chi_j(r,t),\quad B_1(\theta)=\frac{1}{\sqrt{2\pi}},$$
$$B_{2j}(\theta)=\frac{\sin(j\theta)}{\sqrt{\pi}},\quad B_{2j+1}(\theta)=\frac{\cos(j\theta)}{\sqrt{\pi}}, \tag{19}$$

we arrive at the matrix equation (9) with $\mathbf{Q}(r)\equiv 0$ for unknown coefficients $\{\chi_j(r,t)\}_{j=1}^{N}$ in the interval $t\in[0,T]$. The initial functions $\chi_j(r,t)$ at $t=0$ are chosen in the form

$$\chi_1(r,0)=\sqrt{\omega}\,\exp\left(-\frac{1}{4}\omega r^2\right),\quad \chi_j(r,0)\equiv 0,\quad j\geqslant 2. \tag{20}$$

Note that Eq. (17) has an exact solution $\phi_{\rm ext}(x,y,t)$ for a partial choice of the field $E_j(t)=$ $=a_j\sin(\omega_j t)$ which provides a good test example to examine efficiency of numerical algorithms and a rate of convergence of the projection by a number N of radial equations and by time T. We choose $\omega=4\pi,\omega_1=3\pi,\omega_2=5\pi,a_1=24$ and $a_2=9$. For these parameters the absolute value of the solution $\phi(r,\theta,t)$ should be periodical with period $T=2$.

To approximate the solution $\chi_j(r,t)$ in the variable r, we used the finite-element grid $\hat{\Omega}_r[r_{\rm min},r_{\rm max}]=\{r_{\rm min}=0,(120),1.5,(60),r_{\rm max}=4\}$ and time step $\tau=0.0125$, where the number in the brackets denotes the number of finite-element in the intervals. Between each two nodes we apply the Lagrange interpolation polynomials to the $p=8$ order. To analyze the convergence on a sequence of three double-crowding time grids, we define the auxiliary time-dependent discrepancy functions $Er(t,j)$, $j=1,2,3$, and the Runge coefficient $\beta(t)$

$$Er^2(t,j)=\sum_{\nu=1}^{N}\int\limits_{0}^{r_{\rm max}}|\chi_\nu(r,t)-\chi_\nu^{\tau_j}(r,t)|^2 r\,dr,$$
$$\beta(t)=\log_2\left|\frac{Er(t,1)-Er(t,2)}{Er(t,2)-Er(t,3)}\right|, \tag{21}$$

where $\chi_\nu^{\tau_j}(r,t)$ are the numerical solutions with the time step $\tau_j = \tau/2^{j-1}$. For the function $\chi_\nu(r,t)$ 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 (13), that strongly correspond to theoretical ones $\beta(t) \equiv \beta_M(t) \approx 2M$. Figure 1 displays absolute values of the difference $|\phi_{\rm ext}(x,y,t) - \phi(x,y,t)|$ shown at $t = 2$ and behavior of the discrepancy functions $Er(t;j)$, $j = 1,2,3$, and the convergence rates $\beta_M(t)$, $M = 1,2,3$, at some time values t for $N = 30$, respectively. The figures show that one can solve a key problem: a control of needed number N of angular basis functions should be done by solving not only stationary Schrödinger equation [7], but also by solving the exact solvable TDSE. Such benchmark calculations give an opportunity to control distribution of moving region by space variables which are covered by time-dependent wave packet expanded by the angular basis.

CONCLUSION

The developed schemes provide a useful tool for calculations of threshold phenomena in the formation and ionization of (anti)hydrogen-like atoms and ions in magnetic traps [3], quantum dots in magnetic field [12], channelling processes [13, 14], potential scattering with confinement potentials [8] and control problems for finite-dimensional quantum systems [1].

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