

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 $t \in [t_0, T]$:

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

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

We also require continuity of derivatives of the control function $f(\mathbf{r}, t)$ and continuity of solutions $\Psi(\mathbf{r}, t) \in \mathbf{W}_2^1(\mathbf{R}^d \otimes [t_0, T])$ and $\Psi_0(\mathbf{r}) \in \mathbf{W}_2^1(\mathbf{R}^d)$. 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:

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

The coefficients, $\alpha_\zeta^{(M)}$ ($\zeta = 1, \dots, M$, $M \geq 1$), stand for the roots of the polynomial equation, ${}_1F_1(-M, -2M, 2M\iota/\alpha) = 0$, 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 $M \leq 3$, 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

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

where $f \equiv f(\mathbf{r}, t_c)$, $\dot{f} \equiv \partial_t f(\mathbf{r}, t)|_{t=t_c}, \dots$, $U \equiv U(\mathbf{r})$ 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 $\{B_j(\Omega; r)\}_{j=1}^N$

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

In Eq. (6), the vector-function $\chi(r, t) = (\chi_1(r, t), \dots, \chi_N(r, t))^T$ is unknown, and the surface function $\mathbf{B}(\Omega; r) = (B_1(\Omega; r), \dots, B_N(\Omega; r))^T$ 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]:

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

where the generalized self-adjoint angular momentum operator $\hat{\mathbf{L}}_{\Omega}^2$ 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:

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

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

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

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

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

The boundary conditions and normalization condition have the form

$$\begin{aligned} \boldsymbol{\chi}(0, t) &= 0, \quad \text{if} \quad \min_{1 \leq j \leq N} \lim_{r \rightarrow 0} r^{d-1} |V_{jj}(r, t)| = \infty, \\ \lim_{r \rightarrow 0} r^{d-1} \left(\mathbf{I} \frac{\partial}{\partial r} - \mathbf{Q}(r) \right) \boldsymbol{\chi}(r, t) &= 0, \quad \text{if} \quad \min_{1 \leq j \leq N} \lim_{r \rightarrow 0} r^{d-1} |V_{jj}(r, t)| < \infty, \\ \lim_{r \rightarrow \infty} \boldsymbol{\chi}(r, t) &= 0, \end{aligned} \quad (11)$$

$$\int_0^{\infty} (\bar{\boldsymbol{\chi}}(r, t))^T \boldsymbol{\chi}(r, t) r^{d-1} dr = 1. \quad (12)$$

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)

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

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

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

The operator $\mathbf{C}_k^{(3)}$ is equal to zero for $(\nabla_{\mathbf{r}}^2 f) = 0$ 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

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

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]

$$\begin{aligned} i \frac{\partial}{\partial t} \phi(x_1, y_1, t) &= -\frac{1}{2} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} \right) \phi(x_1, y_1, t) + \frac{i\omega}{2} \left(x_1 \frac{\partial}{\partial y_1} - y_1 \frac{\partial}{\partial x_1} \right) \phi(x_1, y_1, t) + \\ &\quad + \frac{\omega^2}{8} (x_1^2 + y_1^2) \phi(x_1, y_1, t) - (x_1 E_1(t) + y_1 E_2(t)) \phi(x_1, y_1, t). \quad (17) \end{aligned}$$

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:

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

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

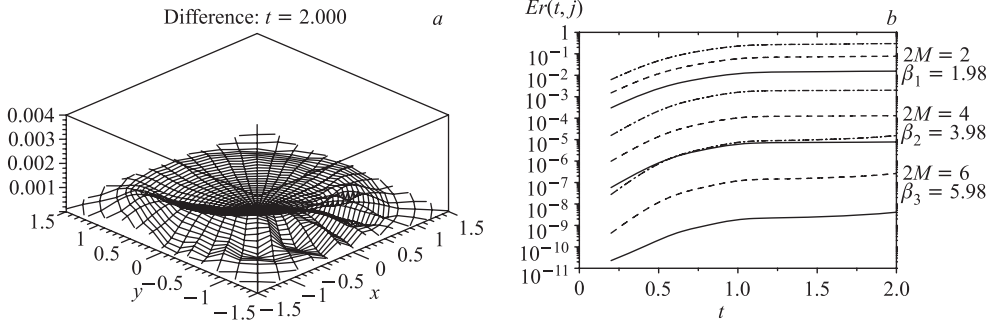


Fig. 1. The absolute values of the difference $|\phi_{\text{ext}}(x, y, t) - \phi(x, y, t)|$ at $t = 2$ (a) and the test results of the discrepancy functions $Er(t, j)$, $j = 1, 2, 3$ (dash-dotted, dashed and solid curves) for the approximations of order $M = 1, 2, 3$ with the time step $\tau = 0.00625$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

functions $B_j(\theta)$

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

$$B_{2j}(\theta) = \frac{\sin(j\theta)}{\sqrt{\pi}}, \quad B_{2j+1}(\theta) = \frac{\cos(j\theta)}{\sqrt{\pi}},$$

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

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

Note that Eq.(17) has an exact solution $\phi_{\text{ext}}(x, y, t)$ 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 $\hat{\Omega}_r[r_{\min}, r_{\max}] = \{r_{\min} = 0, (120), 1.5, (60), r_{\max} = 4\}$ 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 $\beta(t)$

$$Er^2(t, j) = \sum_{\nu=1}^N \int_0^{r_{\max}} |\chi_\nu(r, t) - \chi_\nu^{\tau_j}(r, t)|^2 r dr, \quad (21)$$

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

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 $|\phi_{\text{ext}}(x, y, t) - \phi(x, y, t)|$ 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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