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Multi-Layer Evolution Schemes for the Finite-Dimensional Quantum Systems in External Fields[1]

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Abstract—The operator-difference multi-layer (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 TDSE's are devised by using a set of appropriate basis angular functions and a finite element method with respect to a hyper-radial 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-depended electric fields.

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1. INTRODUCTION

Solving the TDSE with a required accuracy are 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 of appropriate angular basis functions and further discretization of hyper-radial equations, for example, the finite-difference [4], finite-element [5], spline [6] methods and 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 hyper-radial 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 is confirmed by benchmark calculations of an exactly solvable model of the two-dimensional oscillator in time-depended external fields [1].

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2. 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 $t \in [t_0, T]$:

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

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

We also require continuity of derivatives of the control function $f(\mathbf{r}, t)$ and continuity of the 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] rewriting after factorization of a gauge transformation, with operator S, in the following symmetric form:

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

$$\psi_k^0 = \tilde{\psi}_k^1,$$
$$\left(I + \frac{\bar{\alpha}_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{\eta/L} = \left(I + \frac{\alpha_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{(\eta-1)/L},$$
$$\eta = 1,\ldots,L,$$
$$\Psi(t_{k+1}) = \psi_k^1.$$

The coefficients, $\alpha_\zeta^{(M)}$ ($\zeta = 1, \ldots, M, M \ge 1$), 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 $M \le 3$, that sufficient for a practical utilization. For the Hamiltonian given in (2) the operators $\tilde{A}_k^{(M)}$ and $S_k^{(M)}$ read as

$$\begin{aligned}
\tilde{A}_k^{(1)} &= H, \quad S_k^{(1)} = 0,\\
\tilde{A}_k^{(2)} &= \tilde{A}_k^{(1)} + G^{(2)}, \quad S_k^{(2)} = S_k^{(1)} + Z^{(2)},\\
\tilde{A}_k^{(3)} &= \tilde{A}_k^{(2)} + G^{(3)} - \frac{\tau^4}{720}\nabla_{\mathbf{r}}(\nabla_{\mathbf{r}}^2 \dot{f})\nabla_{\mathbf{r}},\\
S_k^{(3)} &= S_k^{(2)} + Z^{(3)} + \frac{\tau^4}{720}\nabla_{\mathbf{r}}(\nabla_{\mathbf{r}}^2 \dot{f})\nabla_{\mathbf{r}},
\end{aligned} \tag{4}$$

$$\begin{aligned}
G^{(2)} &= \frac{\tau^2}{24}\ddot{f}, \quad Z^{(2)} = \frac{\tau^2}{12}\dot{f},\\
G^{(3)} &= \frac{\tau^4}{1920}\ddddot{f} + \frac{\tau^4}{1440}(\nabla_{\mathbf{r}}\dot{f})^2 - \frac{\tau^4}{720}(\nabla_{\mathbf{r}}\ddot{f})\\
&\times(\nabla_{\mathbf{r}}(U+f)) - \frac{\tau^4}{2880}(\nabla_{\mathbf{r}}^4 \ddot{f}),\\
Z^{(3)} &= \frac{\tau^4}{480}\dddot{f} + \frac{\tau^4}{720}(\nabla_{\mathbf{r}}\dot{f})(\nabla_{\mathbf{r}}(U+f)) + \frac{\tau^4}{2880}(\nabla_{\mathbf{r}}^4 \dot{f}),
\end{aligned} \tag{5}$$

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

3. 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 $\chi(r, t) = (\chi_1(r, t), \ldots, \chi_N(r, t))^T$ are 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]

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

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

$$\begin{aligned}
&\langle B_i(\Omega;r)|B_j(\Omega;r)\rangle_\Omega\\
&= \int \bar{B}_i(\Omega;r)B_j(\Omega;r)d\Omega = \delta_{ij},
\end{aligned} \tag{8}$$

where δ_{ij} is the Kronecker symbol.

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

$$\begin{aligned}
&\imath\mathbf{I}\frac{\partial\chi(r,t)}{\partial t} = \mathbf{H}(r,t)\chi(r,t), \quad \chi(r,t_0) = \chi_0(r),\\
&\mathbf{H}(r,t) = -\frac{1}{2r^{d-1}}\mathbf{I}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r} + \mathbf{V}(r,t)\\
&+ \mathbf{Q}(r)\frac{\partial}{\partial r} + \frac{1}{r^{d-1}}\frac{\partial r^{d-1}\mathbf{Q}(r)}{\partial r}.
\end{aligned} \tag{9}$$

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

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

The boundary conditions and normalization condition have the form

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

$$\lim_{r\to\infty}\chi(r,t) = 0,$$
$$\int_0^\infty (\bar{\boldsymbol{\chi}}(r,t))^T\boldsymbol{\chi}(r,t)r^{d-1}dr = 1. \quad (12)$$

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

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

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

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

The operator $\mathbf{C}_k^{(3)}$ 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

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

4. 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 the 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]

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

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

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

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

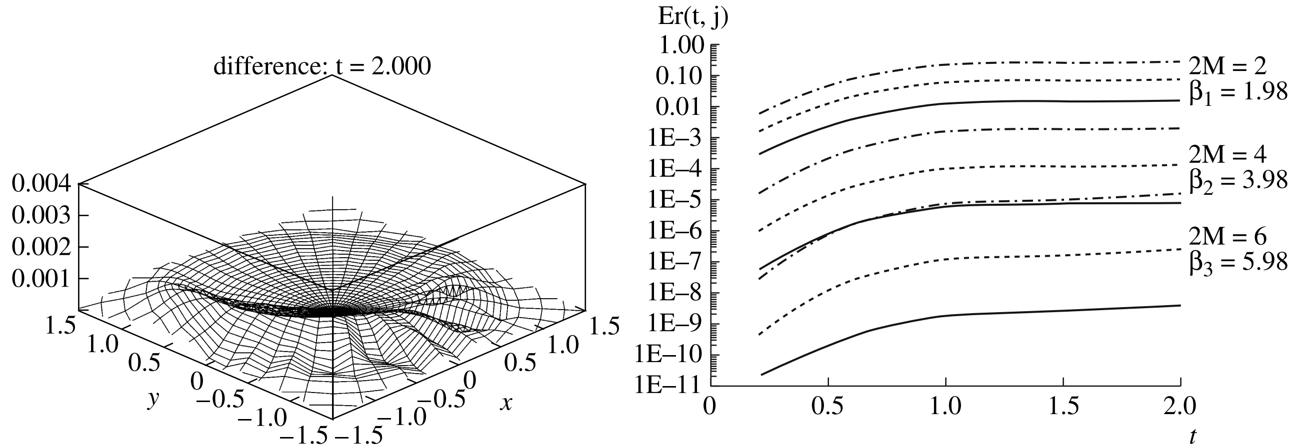
$$\begin{aligned}
\phi(r,\theta,t) &= \sum_{j=1}^N B_j(\theta)\chi_j(r,t), \quad B_1(\theta) = \frac{1}{\sqrt{2\pi}},\\
B_{2j}(\theta) &= \frac{\sin(j\theta)}{\sqrt{\pi}}, \quad B_{2j+1}(\theta) = \frac{\cos(j\theta)}{\sqrt{\pi}},
\end{aligned} \quad (19)$$

we arrive at the matrix Eq. (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

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

Note that, Eq. (17) has an exact solution $\phi_{ext}(x, y, t)$ for a partial choice of the field $E_j(t) = a_j\sin(\omega_j t)$ which that 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 $\phi(r, \theta, t)$ is should be periodically 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



The absolute values of the difference $|\phi_{ext}(x, y, t) - \phi(x, y, t)|$ at $t = 2$ 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 $\tau = 0.00625$.

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 $\beta(t)$

$$Er^2(t,j) = \sum_{\nu=1}^{N} \int_0^{r_{\max}} \left|\chi_\nu(r,t) - \chi_\nu^{\tau_j}(r,t)\right|^2 r dr,$$
$$\beta(t) = \log_2 \left|\frac{Er(t,1) - Er(t,2)}{Er(t,2) - Er(t,3)}\right|, \qquad (21)$$

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 display absolute values of the difference $|\phi_{ext}(x, y, t) - \phi(x, y, t)|$ is shown at $t = 2$ and behavior of the discrepancy functions $Er(t; j)$, $j = 1, 2, 3$, 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.

CONCLUSIONS

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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