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

O. Chuluunbaatar, V. P. Gerdt, A. A. Gusev, M. S. Kaschiev, V. A. Rostovtsev, Y. Uwano, and S. I. Vinitsky

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 TDSE’s are devised by using a set of appropriate basis angular functions and a finite element method in nonuniform spatial grids. The efficiency, convergence and accuracy of the numerical schemes are demonstrated in the case of an exactly solvable model of the two-dimensional oscillator in time-depended electric fields.

PACS number: 03.67.Ac; 01.30.Cc; 03.67.-a

DOI: 10.1134/S15474771109070127

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 split-interval [9] rewriting after factorization of a gauge transformation, in the time interval $[t_0, T]$, of the following symmetric form:

$$\Psi(t_k) = \Psi(t_0) e^{-iL},$$

and a governing function $f(r, t)$ on the time interval $t \in [t_0, T]$:

$$f(r, t) = f(r, t_0), \
\psi(r, t_0) = \psi_0(r), \
\frac{\partial\psi(r, t)}{\partial t} = H(r, t)\psi(r, t), \
\|\psi\|^2 = \int |\psi(r, t)|^2 dr = 1, \
\psi(r, t_0) = \psi_0(r), \
H(r, t) = H_0(r) + f(r, t), \
H_0(r) = -\frac{1}{2}\nabla^2 r + U(r),$$

We also require continuity of derivatives of the control function $f(r, t)$ and continuity of the solutions $\Psi(r, t) \in W^1_2(\mathbb{R}^d \otimes [t_0, T])$ and $\psi_0(r) \in W^1_2(\mathbb{R}^d)$. We solve the above Cauchy problem (1), (2) in the uniform grid $\Omega_{[t_0, T]}$ with time step $\tau$, 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:

$$\psi_k = \psi(t_k),$$

$$\left( I - \frac{\alpha_n \tilde{S}_k^{(M)}}{2L} \right) \psi_n^{(n-1)/L},$$

$$\eta = 1, ..., L,$$

$$\psi_k^{(\eta)} = \psi_k,$$

$$\left( I + \frac{\tau A_k^{(M)}}{2M} \right) \psi_k^{(\zeta)/M},$$

$$\zeta = 1, ..., M,$$
ψ_0^k = \tilde{\psi}_1^k,
(1 + \frac{\alpha_n^{(L)} S^{(M)}}{2L})\psi_{\eta/L}^k = (1 + \frac{\alpha_n^{(L)} S^{(M)}}{2L})\psi_{(\eta-1)/L}^k,
\eta = 1, \ldots, L,
\Psi(t_{i+1}) = \psi^k_1.

The coefficients, \(\alpha_n^{(M)} (\zeta = 1, \ldots, M, M \geq 1)\), stand for the roots of the polynomial equation, \(\int P_1(-M, -2M, 2M/\alpha) = 0\), where \(P_1\) is the confluent hypergeometric function. This scheme has the accuracy of order \(O(\alpha^{2M})\) with respect to time step \(\tau\), if we choose \(L = [M/2]\). Below we consider the scheme with \(M \leq 3\), that sufficient for a practical utilization. For the Hamiltonian given in (2) the operators \(\tilde{A}_k^{(M)}\) and \(S_k^{(M)}\) read as

\[ \tilde{A}_k^{(1)} = H, \quad S_k^{(1)} = 0, \]
\[ \tilde{A}_k^{(2)} = \tilde{A}_k^{(1)} + G^{(2)}, \quad S_k^{(2)} = S_k^{(1)} + Z^{(2)}, \]
\[ \tilde{A}_k^{(3)} = \tilde{A}_k^{(2)} + G^{(3)} - \frac{\tau^4}{720} \nabla_r (\nabla_r f) \nabla_r, \]
\[ S_k^{(3)} = S_k^{(2)} + Z^{(3)} + \frac{\tau^4}{720} \nabla_r (\nabla_r f) \nabla_r, \]
\[ G^{(2)} = \frac{\tau^2}{24} f^{(2)}, \quad Z^{(2)} = \frac{\tau^2}{12} f^{(2)}, \]
\[ G^{(3)} = \frac{\tau^4}{1920} + \frac{\tau^4}{1440} (\nabla_r f)^2 - \frac{\tau^4}{720} (\nabla_r f) \]
\times (\nabla_r (U + f)) - \frac{\tau^4}{2880} (\nabla_r f),
\[ Z^{(3)} = \frac{\tau^4}{480} f^{(3)} + \frac{\tau^4}{720} (\nabla_r f) (\nabla_r (U + f)) + \frac{\tau^4}{2880} (\nabla_r f), \]
where \(f \equiv f(r, t_c), f^{(2)} \equiv \partial f(r, t_c) / \partial t_c, \ldots, U \equiv U(r)\) and \(t_c = t + \tau/2\).

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 \(\Psi(r, t)\) is expanded over the one-parametric basis functions \(\{B_j(\Omega; r)\}_{j=1}^N\)

\[ \Psi(r, t) = \sum_{j=1}^N B_j(\Omega; r) \chi_j(r, t). \]

In Eq. (6), the vector-function \(\chi_j(r, t) = (\chi_{j1}(r, t), \ldots, \chi_{jN}(r, t))^T\) are unknown, and the surface function \(B(\Omega; r) = (B_1(\Omega; r), \ldots, B_N(\Omega; r))^T\) is an orthonormal basis with respect to the set of angular coordinates \(\Omega\) 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]

\[ (- \frac{1}{2r^2} \tilde{A}_\Omega^2 + U(r)) B_j(\Omega; r) = E_j(r) B_j(\Omega; r), \]

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

\[ \langle B_j(\Omega; r) | B_j(\Omega; r) \rangle_\Omega = \int B_j(\Omega; r) B_j(\Omega; r) d\Omega = \delta_{jj}, \]

where \(\delta_{ij}\) 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

\[ t \frac{\partial \chi(r, t)}{\partial t} = H(r, t) \chi(r, t), \quad \chi(r, t_0) = \chi_0(r), \]
\[ H(r, t) = - \frac{1}{2r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} + V(r, t) \]
\[ + Q(r) \frac{\partial}{\partial r} + \frac{1}{2r^{d-1}} \frac{\partial^2}{\partial r^2} Q(r). \]

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

\[ V_{ij}(r, t) = \frac{E_i(r) + E_j(r)}{2} \delta_{ij} \]
\[ + \frac{1}{2} \left( \frac{\partial B_i(\Omega; r)}{\partial r} \right) \left( \frac{\partial B_j(\Omega; r)}{\partial r} \right)_\Omega \]
\[ + \langle B_i(\Omega; r) | f(r, t) | B_j(\Omega; r) \rangle_\Omega, \]
\[ I_{ij} = \delta_{ij}, \quad Q_{ij}(r) = \frac{1}{2} \langle B_i(\Omega; r) | \frac{\partial B_j(\Omega; r)}{\partial r} \rangle_\Omega. \]

The boundary conditions and normalization condition have the form

\[ \chi(0, t) = 0, \quad \text{if} \quad \lim_{r \to 0} r^{d-1} |V_{ij}(r, t)| = \infty, \]
\[ \lim_{r \to 0} r^{d-1} \left( \frac{\partial}{\partial r} - Q(r) \right) \chi(r, t) = 0, \quad \text{if} \quad \min_{1 \leq j \leq N} \lim_{r \to 0} r^{d-1} |V_{ij}(r, t)| < \infty, \]
\[ \lim_{r \to \infty} \chi(r,t) = 0, \]
\[ \int_{0}^{1} (\tilde{\chi}(r,t))^T \chi(r,t) r^{d-1} dr = 1. \] (12)

In this case we obtain the finite \( N \times N \) matrix operator-difference scheme for unknown vector-functions \( \chi(r,t) \), analogy to (3)
\[ I \longrightarrow \tilde{I}, \quad \tilde{A}^{(M)}_k \longrightarrow A^{(M)}_k, \quad S^{(M)}_k \longrightarrow \tilde{S}^{(M)}_k, \] (13)

where \( \tilde{A}^{(M)}_k \) and \( \tilde{S}^{(M)}_k \) are matrix operators of dimension \( N \times N \) given by the relation
\[ \tilde{A}^{(1)}_k = H(r,t), \quad \tilde{S}^{(1)}_k = 0, \]
\[ \tilde{A}^{(2)}_k = \tilde{A}^{(1)}_k + G^{(2)}, \quad \tilde{S}^{(2)}_k = \tilde{S}^{(1)}_k + \tilde{Z}^{(2)}, \]
\[ \tilde{A}^{(3)}_k = \tilde{A}^{(2)}_k + G^{(3)} + C^{(3)}_k, \]
\[ \tilde{S}^{(3)}_k = \tilde{S}^{(2)}_k + \tilde{Z}^{(3)} - C^{(3)}_k, \]
\[ \tilde{G}^{(M)}_{ij} = \langle B_i(\Omega;r)|G^{(M)}|B_j(\Omega;r)\rangle_{\Omega}, \]
\[ \tilde{Z}^{(M)}_{ij} = \langle B_i(\Omega;r)|Z^{(M)}|B_j(\Omega;r)\rangle_{\Omega}. \] (14)

The operator \( C^{(3)}_k \) equal to zero for \( \langle V^2_{r,f} \rangle = 0 \) and in other cases has the form
\[ C^{(3)}_k = \frac{\tau^4}{720} \left\{ -\frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \tilde{D}(r) \frac{\partial}{\partial r} + \tilde{V}(r) \right\} - \tilde{Q}^T \left( \frac{\partial}{\partial r} + \frac{1}{r^{d-1}} \frac{\partial}{\partial r} \tilde{Q}(r) \right), \] (15)

where \( \tilde{D}(r), \tilde{V}(r) \) and \( \tilde{Q}(r) \) are matrices of dimension \( N \times N \) whose elements are given by the relations
\[ \tilde{D}_{ij}(r) = \langle B_i(\Omega;r)|\langle V^2_{r,f} \rangle|B_j(\Omega;r)\rangle_{\Omega}, \]
\[ \tilde{V}_{ij}(r) = \langle \frac{\partial B_i(\Omega;r)}{\partial r} |\langle V^2_{r,f} \rangle| \frac{\partial B_j(\Omega;r)}{\partial r} \rangle_{\Omega}, \]
\[ + \frac{1}{r^2} \langle \hat{A}_\Omega B_i(\Omega;r)|\langle V^2_{r,f} \rangle|\hat{A}_\Omega B_j(\Omega;r)\rangle_{\Omega}, \]
\[ \tilde{Q}_{ij}(r) = -\langle B_i(\Omega;r)|\langle V^2_{r,f} \rangle| \frac{\partial B_j(\Omega;r)}{\partial r} \rangle_{\Omega}. \] (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]
\[ \frac{1}{2} \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} \phi(x_1,y_1,t) \]
\[ + \frac{\omega^2}{8} (x_1^2 + y_1^2) \]
\[ \times \phi(x_1,y_1,t) - (x_1 E_1(t) + y_1 E_2(t)) \phi(x_1,y_1,t). \] (17)

The transformation to a rotated coordinate system with frequency \( \omega/2 \), \( x_1 = \cos(\omega/2) + \sin(\omega/2), \)
\[ \omega = \cos(\omega/2) - \sin(\omega/2), \]
and polar coordinates \( x = r \cos(\theta), y = r \sin(\theta), \) leads to the following equation
\[ \dot{\phi}(r,\theta,t) = \left( -\frac{11 \frac{\partial}{\partial r}}{2 r^2 \partial^2 - \frac{\partial}{\partial r} - \frac{11 \partial^2}{2 r^2 \partial \theta^2} \right) \phi(r,\theta,t), \] (18)

where \( f(t) = -E_1(t)\cos(\omega t/2) + E_2(t)\sin(\omega t/2), f_1(t) = -E_1(t)\sin(\omega t/2) - E_2(t)\cos(\omega t/2). \)

Using the Galerkin projection of solutions by means of the angular basis functions \( B_j(\theta) \)
\[ \phi(r,\theta,t) = \sum_{j=1}^{N} B_j(\theta) \chi_j(r,t), \]
\[ B_1(\theta) = \frac{1}{\sqrt{2\pi}}, \]
\[ B_{2j}(\theta) = \frac{\sin(j \theta)}{\sqrt{\pi}}, \quad B_{2j+1}(\theta) = \frac{\cos(j \theta)}{\sqrt{\pi}}, \] (19)

we arrive at the matrix Eq. (9) with \( Q(r) \equiv 0 \) for unknown coefficients \( \chi_j(r,t) \) in the interval \( t \in [0, T] \). The initial functions \( \chi_j(r,t) \) at \( t = 0 \) are chosen in the form
\[ \chi_i(r,0) = \sqrt{\omega} \exp \left( -\frac{1}{4} \omega r^2 \right), \] (20)
\[ \chi_j(r,0) \equiv 0, \quad j \geq 2. \]

Note that, Eq. (17) has an exact solution \( \phi_{ex}(x,y,t) \) 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 \( \phi(r,\theta,t) \) 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 \( \Omega_r \), \( r_{\text{min}} \leq r_{\text{max}} \leq r_{\text{min}} = 0, \]
\( (120), 1.5, (60), r_{\text{max}} = 4 \) 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 $\beta(t)$

$$Er^2(t, j) = \sum_{\nu = 1}^{N} \int_{0}^{r_{\text{max}}} \left| \chi_{\nu}(r, t) - \chi_{\nu}^{\tau_{j}}(r, t) \right|^2 rdr,$$

$$\beta(t) = \log_{10} \left( \frac{\|Er(t, 1)\|}{\|Er(t, 2) - Er(t, 3)\|} \right),$$

where $\chi_{\nu}^{\tau_{j}}(r, t)$ are the numerical solutions with the time step $\tau_{j} = \pi/2^{j-1}$. For the function $\chi_{\nu}(r, t)$ one can use the numerical solution with the time step $\tau_{4} = \pi/8$. Hence, we obtain the numerical estimates for the convergence order of the numerical scheme (13), that strongly correspond to theoretical ones $\beta(t) \equiv \beta_m(t) = 2M$. Figure 1 display absolute values of the difference $|\phi_{\text{ex}}(x, y, t) - \phi(x, y, t)|$ 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].

ACKNOWLEDGMENTS

This work was partly supported by Grant I-1402/2004-2007 of the Bulgarian Foundation for Scientific Investigations, the theme 09-6-1060-2005/2009 “Mathematical support of experimental and theoretical studies conducted by JINR” and Scientific Center for Applied Research of JINR.

REFERENCES