

## Two-dimensional oscillator in time-dependent fields: Comparison of some exact and approximate calculations

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Operator-difference multilayer schemes for solving the time-dependent Schrödinger equation up to sixth order of accuracy in the time step are presented. Reduced schemes for solving a set of coupled time-dependent Schrödinger equations with respect to the hyper-radial variable are devised using expansion of a wave packet over the set of appropriate basis angular functions. Further discretization of the resulting problem is realized by means of the finite-element method. The convergence of the expansion with respect to the number of basis functions and the efficiency of the numerical schemes are demonstrated in the exactly solvable model of an electric-field-driven two-dimensional oscillator (or a charged particle in a constant uniform magnetic field), in which we explicitly observed an effect of the periodical focusing and defocusing of the probability density flux.

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Numerical solution of the time-dependent Schrödinger equation (TDSE) with prescribed accuracy is necessary for solving control problems in finite-dimensional quantum systems [1], decay problems in nuclear physics [2], deexcitation of antihydrogen atoms [3], problems of ionization of atoms and molecules by short-pulse fields, or impact collisions beyond the dipole approximation [4]. For solving the TDSE in a finite-dimensional spatial domain it is common to seek a wave-packet solution expanded over an appropriate angular basis and then apply a certain discrete numerical scheme to the resulting hyper-radial equations, for example, finite-difference [4,5], finite-element [6,7], spline [8–10] methods, etc.

Usually the rate of convergence with respect to the number of angular basis functions is controlled by solving the corresponding stationary Schrödinger equation (SSE) [11]. However, some special cases of long-range potentials acting in asymptotic regions, like confinement potentials, require additional analysis [5,12], which is the *key problem*. Numerical solution of TDSEs describing exactly solvable models can provide useful information for such analysis.

In this Brief Report, a computational method is applied to solve the TDSE, in which the unitary splitting algorithm with uniform time grids [13] is combined with the Kantorovich or Galerkin reduction to a set of hyper-radial TDSEs [7], the finite-element method (FEM) [14], and interpolation on non-uniform spatial grids [7]. The efficiency, convergence, and accuracy of the numerical schemes developed are confirmed by benchmark calculations of an exactly solvable model, namely, the driven two-dimensional oscillator [1].

The  $d$ -dimensional TDSE with the self-adjoint Hamiltonian  $H(\mathbf{r}, t)$  and the governing function  $f(\mathbf{r}, t)$  in the time interval  $t \in [t_0, T]$  has the form

$$i\partial\Psi(\mathbf{r}, t)/\partial t = H(\mathbf{r}, t)\Psi(\mathbf{r}, t), \quad \Psi(\mathbf{r}, t_0) = \Psi_0(\mathbf{r}),$$

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

We require continuity of derivatives of  $F(\mathbf{r}, t)$  and the solutions  $\Psi(\mathbf{r}, t) \in \mathbf{W}_2^1(\mathbf{R}^d \otimes [t_0, T])$  and  $\Psi_0(\mathbf{r}) \in \mathbf{W}_2^1(\mathbf{R}^d)$ . The normalization condition is

$$\|\Psi\|^2 = \int |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1. \quad (2)$$

The Cauchy problem (1) is solved on the uniform grid  $\Omega_{\tau}[t_0, T] = \{t_0, t_{k+1} = t_k + \tau, t_K = T\}$  with time step  $\tau$  in the time interval  $[t_0, T]$  by means of the operator-difference multilayer calculation scheme [13]. Using the factorization of the additional gauge transformation operator  $\exp(\pm i\tau\tilde{S}_k^{(M)})$ , we calculate the required operators  $\tilde{S}_k^{(M)}$  and arrive at a new symmetric  $(M+2L)$ -layer scheme for transforming  $\Psi(\mathbf{r}, t_k)$  ( $k=0, K-1$ ) into  $\Psi(\mathbf{r}, t_{k+1})$ :

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

where  $I$  is the unit operator, the overbar denotes the complex conjugate,  $\zeta=1, M$ , and  $\eta=1, L$ . The auxiliary functions  $\tilde{\psi}_k^{\zeta/M}$ ,  $\zeta=1, M-1$ , in Eq. (3) can be treated as a kind of approximate solution on a set of fractional time steps  $t_{k+\zeta/M} = t_k + \tau\zeta/M$ , in the time interval  $[t_k, t_{k+1}]$ . The additional functions  $\psi_k^{\eta/L}$ ,  $\eta=1, L-1$ , will provide an approximation of the above gauge transformation operator  $\exp(\pm i\tau\tilde{S}_k^{(M)})$  at points  $t_k$  and  $t_{k+1}$ , respectively. The coefficients  $\alpha_{\zeta}^{(M)}$  are the roots of the polynomial equation  ${}_1F_1(-M, -2M, 2Mi/\alpha) = 0$ , where  ${}_1F_1$  is the confluent hypergeometric function, and have the following properties:  $\text{Im} \alpha_{\zeta}^{(M)} < 0$  and  $0.6 < |\alpha_{\zeta}^{(M)}| < \mu^{-1}$ , where  $\mu \approx 0.28$  is the root of the equation  $\mu \exp(\mu+1) = 1$  [15]. This scheme has accuracy  $O(\tau^{2M})$  with respect to the time step  $\tau$  if we choose  $L = \lceil \frac{M}{2} \rceil$ , where  $\lceil x \rceil$  is the integer part of  $x$ . Below we consider the scheme with  $M \leq 3$  sufficient for

practical utilization. For the Hamiltonian in Eq. (1) the operators  $\tilde{A}_k^{(M)}$  and  $\tilde{S}_k^{(M)}$  are given by

$$\tilde{A}_k^{(1)} = H(\mathbf{r}, t_c), \quad \tilde{S}_k^{(1)} = 0,$$

$$\tilde{A}_k^{(2)} = \tilde{A}_k^{(1)} + (\tau^2/24)\ddot{F}, \quad \tilde{S}_k^{(2)} = \tilde{S}_k^{(1)} + (\tau^2/12)\dot{F},$$

$$\begin{aligned} \tilde{A}_k^{(3)} = & \tilde{A}_k^{(2)} + (\tau^4/1920)\ddot{\ddot{F}} + (\tau^4/1440)(\nabla_r \dot{F})^2 - (\tau^4/2880)(\nabla_r^4 \dot{F}) \\ & - (\tau^4/720)(\nabla_r \ddot{F})(\nabla_r F) - (\tau^4/720)\nabla_r(\nabla_r^2 \dot{F})\nabla_r, \end{aligned}$$

$$\begin{aligned} \tilde{S}_k^{(3)} = & \tilde{S}_k^{(2)} + (\tau^4/480)\ddot{\ddot{F}} + (\tau^4/720)(\nabla_r \dot{F})(\nabla_r F) \\ & + (\tau^4/2880)(\nabla_r^4 \dot{F}) + (\tau^4/720)\nabla_r(\nabla_r^2 \dot{F})\nabla_r, \end{aligned} \quad (4)$$

where  $F \equiv F(\mathbf{r}, t)$ ,  $\dot{F} \equiv (\partial F(\mathbf{r}, t)/\partial t)|_{t=t_c}, \dots$ , and  $t_c = t_k + \tau/2$ . The condition  $\tau < 2M\mu\|\tilde{A}_k^{(M)}\|^{-1}$  guarantees the validity of the scheme (3) for any bounded operator  $\tilde{A}_k^{(M)}$ . From the condition  $\text{Im } \alpha_k^{(M)} \neq 0$  it follows that the auxiliary and additional functions  $\tilde{\psi}_k^{\xi/M}$  and  $\psi_k^{\eta/L}$  have equal norms. In the case  $M=1$ , the scheme (3) corresponds to the well-known Crank-Nicolson scheme [16].

Let us consider a formal adiabatic expansion of the partial solution  $\Psi(\mathbf{r}, t)$  of Eq. (1) over one-parametric basis functions  $\{B_j(\Omega; r)\}_{j=1}^N$ ,

$$\Psi(\mathbf{r}, t) = \sum_{j=1}^N B_j(\Omega; r)\chi_j(r, t). \quad (5)$$

The vector function  $\chi(r, t) = (\chi_1(r, t), \dots, \chi_N(r, t))^T$  is unknown; the orthonormal basis surface functions  $B_j(\Omega; r) \in \mathcal{F}_r \sim \mathbf{L}_2(S^{d-1}(\Omega))$  and the potential curves  $E_j(r)$  are solutions of the one-parametric eigenvalue problem [11, 17] with respect to angular variables  $\Omega$ ,

$$[-(1/2r^2)\hat{\Lambda}_\Omega^2 + U(\mathbf{r})]B_j(\Omega; r) = E_j(r)B_j(\Omega; r). \quad (6)$$

Here  $\hat{\Lambda}_\Omega^2$  is the generalized self-adjoint angular momentum operator corresponding to the  $d$ -dimensional Laplace operator  $\nabla_r^2$ . The eigenfunctions satisfy the same angular boundary conditions as  $\Psi(\mathbf{r}, t)$  and are normalized as follows:

$$\langle B_i(\Omega; r)|B_j(\Omega; r)\rangle_\Omega = \int \bar{B}_i(\Omega; r)B_j(\Omega; r)d\Omega = \delta_{ij}, \quad (7)$$

where  $\delta_{ij}$  is the Kronecker symbol.

By using the expansion (5) we reduce the initial problem (1) to a boundary problem for a set of  $N$  coupled second-order ordinary differential equations that determine the vector function  $\chi(r, t)$  of the expansion (6) in the finite interval  $r \in [0, r_{\max}]$ :

$$i\mathbf{I}[\partial\chi(r, t)/\partial t] = \mathbf{H}(r, t)\chi(r, t), \quad \chi(r, t_0) = \chi_0(r),$$

$$\begin{aligned} \mathbf{H}(r, t) = & -(1/2r^{d-1})\mathbf{I}(\partial/\partial r)r^{d-1}(\partial/\partial r) + \mathbf{V}(r, t) + \mathbf{Q}(r)(\partial/\partial r) \\ & + (1/r^{d-1})[\partial r^{d-1}\mathbf{Q}(r)/\partial r]. \end{aligned} \quad (8)$$

Here  $\mathbf{V}(r, t)$ ,  $\mathbf{Q}(r)$ , and  $\mathbf{I}$  are  $N \times N$  matrices with the elements

$$\begin{aligned} V_{ij}(r, t) = & E_j(r)\delta_{ij} + \frac{1}{2}\langle [\partial B_i(\Omega; r)/\partial r][\partial B_j(\Omega; r)/\partial r] \rangle_\Omega \\ & + \langle B_i(\Omega; r)|f(\mathbf{r}, t)|B_j(\Omega; r)\rangle_\Omega, \end{aligned}$$

$$Q_{ij}(r) = -\frac{1}{2}\langle B_i(\Omega; r)|[\partial B_j(\Omega; r)/\partial r] \rangle_\Omega, \quad I_{ij} = \delta_{ij}. \quad (9)$$

The boundary and normalization conditions have the form

$$\chi(0, t) = 0 \quad \text{if} \quad \min_{1 \leq j \leq N} \lim_{r \rightarrow 0} r^{d-1}|V_{jj}(r, t)| = \infty,$$

$$\begin{aligned} \lim_{r \rightarrow 0} r^{d-1}[\mathbf{I} \partial/\partial r - \mathbf{Q}(r)]\chi(r, t) = 0 \\ \text{if} \quad \min_{1 \leq j \leq N} \lim_{r \rightarrow 0} r^{d-1}|V_{jj}(r, t)| < \infty, \end{aligned} \quad (10)$$

$$\lim_{r \rightarrow \infty} \chi(r, t) = 0 \mapsto \chi(r_{\max}, t) = 0,$$

$$\int_0^{r_{\max}} (\bar{\chi}(r, t))^T \chi(r, t) r^{d-1} dr = 1. \quad (11)$$

In this case we arrive at the finite  $N \times N$  matrix operator-difference scheme for the unknown vector function  $\chi(r, t)$  analogous to (3),

$$I \mapsto \mathbf{I}, \quad \tilde{A}_k^{(M)} \mapsto \tilde{\mathbf{A}}_k^{(M)}, \quad \tilde{S}_k^{(M)} \mapsto \tilde{\mathbf{S}}_k^{(M)}, \quad (12)$$

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

$$\tilde{A}_{k;ij}^{(M)} = \langle B_i(\Omega; r)|\tilde{A}_k^{(M)}|B_j(\Omega; r)\rangle_\Omega,$$

$$\tilde{S}_{k;ij}^{(M)} = \langle B_i(\Omega; r)|\tilde{S}_k^{(M)}|B_j(\Omega; r)\rangle_\Omega. \quad (13)$$

Moreover,  $\tilde{\mathbf{A}}_k^{(1)} = \mathbf{H}(r, t_c)$ ,  $\tilde{\mathbf{S}}_k^{(1)} = \mathbf{0}$ .

In the dipole approximation and atomic units the TDSE for a two-dimensional charged oscillator (or a charged particle in a constant uniform magnetic field) driven by an external electric field with the components  $\mathcal{E}_1(t)$  and  $\mathcal{E}_2(t)$  in the time interval  $t \in [0, T]$  has the form [1]

$$\begin{aligned} i \frac{\partial \phi(x_1, y_1, t)}{\partial t} = & \left[ -\frac{1}{2} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} \right) + \frac{i\omega}{2} \left( x_1 \frac{\partial}{\partial y_1} - y_1 \frac{\partial}{\partial x_1} \right) \right. \\ & \left. + \frac{\omega^2}{8} (x_1^2 + y_1^2) - [x_1 \mathcal{E}_1(t) + y_1 \mathcal{E}_2(t)] \right] \phi(x_1, y_1, t). \end{aligned} \quad (14)$$

The transformation to the coordinate system rotating with the angular frequency  $\omega/2$ ,

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} \cos(\omega t/2) & \sin(\omega t/2) \\ -\sin(\omega t/2) & \cos(\omega t/2) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \quad (15)$$

and polar coordinates  $x = r \cos(\theta)$ ,  $y = r \sin(\theta)$  yields the equation

$$\begin{aligned} i \partial \phi(r, \theta, t) / \partial t = & \left\{ -\frac{1}{2}(1/r)(\partial/\partial r)r(\partial/\partial r) - \frac{1}{2}(1/r^2)(\partial^2/\partial \theta^2) \right. \\ & + \omega^2 r^2/8 + r[f_1(t)\cos(\theta) \\ & \left. + f_2(t)\sin(\theta)] \right\} \phi(r, \theta, t), \end{aligned} \quad (16)$$

where

$$\begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix} = \begin{pmatrix} -\cos(\omega t/2) & \sin(\omega t/2) \\ -\sin(\omega t/2) & -\cos(\omega t/2) \end{pmatrix} \begin{pmatrix} \mathcal{E}_1(t) \\ \mathcal{E}_2(t) \end{pmatrix}. \quad (17)$$

Using the Galerkin projection of the solutions by means of the angular basis functions  $\{B_j(\theta)\}_{j=1}^N$ ,

$$\phi(r, \theta, t) = \sum_{j=1}^N B_j(\theta) \chi_j(r, t),$$

$$B_1(\theta) = \frac{1}{\sqrt{2\pi}}, \quad B_{2j}(\theta) = \frac{\sin(j\theta)}{\sqrt{\pi}}, \quad B_{2j+1}(\theta) = \frac{\cos(j\theta)}{\sqrt{\pi}}, \quad (18)$$

we arrive at the matrix Eq. (8) with  $V_{ij}(r, t) = \langle B_i(\theta) | -\frac{1}{2}(1/r^2)(\partial^2/\partial\theta^2) + F(r, \theta, t) | B_j(\theta) \rangle_\theta$  and  $Q_{ij}(r) \equiv 0$  for unknown coefficients  $\{\chi_j(r, t)\}_{j=1}^N$ . The initial functions  $\chi_j(r, t)$  at  $t=0$  are chosen in the form

$$\chi_j(r, 0) = \sqrt{\omega} \exp[-(\omega/4)r^2] \delta_{j1}, \quad (19)$$

which corresponds to the ground-state wave packet of the free oscillator,

$$\phi_0(x, y) = \sqrt{\omega/2\pi} \exp[-(\omega/4)(x^2 + y^2)]. \quad (20)$$

Note that for the particular choice of the field  $\mathcal{E}_j(t) = a_j \sin(\omega_j t)$  the initial problem (14) and (20) has an analytical solution  $\phi_{\text{ext}}(x, y, t)$  that provides a good example to test the efficiency of numerical algorithms and the rate of convergence of the projection with the number  $N$  of radial equations and with the time  $t$ . This closed-form solution is

$$\phi_{\text{ext}}(x, y, t) = \sqrt{\omega/2\pi} \exp[-(\omega/4)(x^2 + y^2) + 2Y_1(t)x + 2Y_2(t)y - Z_1(t) - Z_2(t)], \quad (21)$$

where the functions  $Y_j(t)$  and  $Z_j(t)$  satisfy the Cauchy problem

$$i(d/dt)Y_j(t) = (\omega/2)Y_j(t) + f_j(t)/2, \quad Y_j(0) = 0,$$

$$i(d/dt)Z_j(t) = -\omega/4 + 2Y_j^2(t), \quad Z_j(0) = 0. \quad (22)$$

We choose  $\omega = 4\pi$ ,  $\omega_1 = 3\pi$ ,  $\omega_2 = 5\pi$ ,  $a_1 = 24$ ,  $a_2 = 9$ . For these parameters the absolute value  $\phi(x, y, t)$  should be periodic in time with the period  $T = 2$ .

To approximate the solution  $\chi_j(r, t)$  as a function of  $r$ , we used the finite-element grid  $\hat{\Omega}_r[r_{\min}, r_{\max}] = \{r_{\min} = 0, (120), 1.5, (60), r_{\max} = 4\}$ , where the numerals in parentheses denote the number of finite elements in the subinterval. Between each two nodes we apply Lagrange interpolation polynomials up to the order  $p = 8$ . The applicability, stability, and efficiency of the FEM and Lagrange interpolation with nonuniform steps in the spatial variable  $r$  were demonstrated for solving the SSE with a long-range potentials [18] and the TDSE with a long-range potential using masking functions [6].

To analyze the convergence of a sequence of three time grids with the initial time step  $\tau = 0.0125$  and each next time step being half of the previous one, we introduce the auxiliary time-dependent discrepancy functions  $E(t, j)$ ,  $j = 1, 2, 3$ , and the Runge coefficient  $\beta(t)$ ,

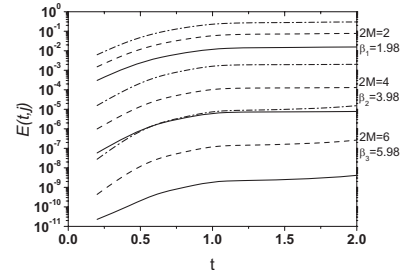


FIG. 1. Discrepancy functions  $E(t, j)$ ,  $j = 1, 2, 3$  (dash-dotted, dashed, and solid curves), for approximations of the order  $2M = 2, 4, 6$ , respectively, with the time step  $\tau = 0.0125$  and  $N = 30$ .

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

$$\beta(t) = \log_2 \left[ \frac{E(t, 1) - E(t, 2)}{E(t, 2) - E(t, 3)} \right], \quad (23)$$

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 a numerical solution with the time step  $\tau_4 = \tau/8$ .

Figure 1 displays the behavior of the discrepancy functions  $E(t, j)$ ,  $j = 1, 2, 3$ , for approximations of the order  $2M = 2, 4, 6$  and  $N = 30$ . For each triplet of curves, the average value of the convergence rates  $\beta(t) \equiv \beta_M(t)$  over all values of  $\beta_M(t_k) \approx 2M$  on the grid  $\Omega_r[0, 2]$  is depicted. As a result, theoretical estimates for the order convergence of the proposed scheme (12) of the second, fourth, and sixth order of accuracy,  $O(\tau^{2M})$ , respectively, are confirmed. Figure 2 displays the absolute value of the difference  $\phi_{\text{ext}}(x, y, t=2) - \phi(x, y, t=2)$  for the approximation of the order  $2M = 6$  with the time step  $\tau_4 = 0.0015625$  and  $N = 20$  [Fig. 2(a)] and 30 [Fig. 2(b)].

Figure 2 illustrates the possibility of solving the key problem, namely, the necessary number  $N$  of angular basis functions should be controlled not only by solving the SSE [11]

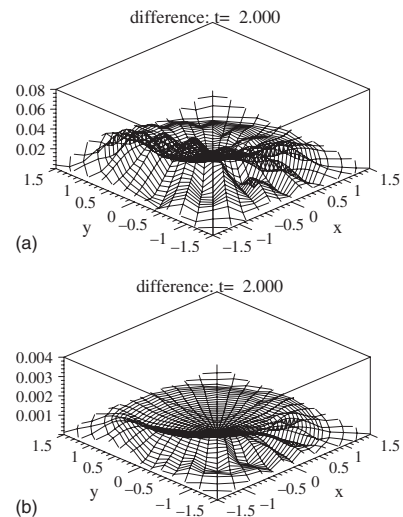


FIG. 2. Absolute value of the difference  $\phi_{\text{ext}}(x, y, t=2) - \phi(x, y, t=2)$  for the approximation of the order  $2M = 6$  with the time step  $\tau_4 = 0.0015625$  and  $N = 20$  (a) and 30 (b).

but also by solving the exact solvable TDSE. Such benchmark calculations allow one to trace the moving spatial regions in which the time-dependent wave packet, expanded over the angular basis, is essentially nonzero.

If the initial state of a free harmonic oscillator is taken to be a Gaussian wave packet, differing in width from the ground eigenstate, then the evolution consists in periodic oscillations of the packet width, i.e., repeated focusing and defocusing in the coordinate and momentum space. Similar behavior is observed in Gaussian light beams in parabolic gradient waveguides (see, e.g., [20] and references therein). Recently this oscillator property was discussed as a key point in relation to the important problem of channeling and super-focusing of light nuclear beams in thin doped films [21].

We calculated the time dependence of the wave packet shape in the model of a two-dimensional oscillator driven by an external field. Figure 3 shows the temporal dynamics of a closed loop in the  $x, y$  plane, within which the probability density  $|\phi(x, y, t)|^2$  is not less than one-half of its maximal value at given  $t$ . For calculations we took the frequencies to be the same as above and considered two cases:  $a_1 = a_2 = 0$  [Fig. 3(a)] and  $a_1 = 24, a_2 = 9$  [Fig. 3(b)]. In both cases the wave function at the initial moment of time was  $\phi_0(x, y) = \sqrt{\omega/(20\pi)} \exp[-\omega(x^2 + y^2)/40]$ . Periodic restoration of the initial wave packet shape (20) is seen to occur, wherever the packet center is at rest [Fig. 3(a)] or rotating [Fig. 3(b)].

To summarize, we have presented a computational approach to solve the TDSE, in which the partial (unitary) splitting of the evolution operator and the FEM are efficiently combined. In particular, to implement our approach in the explicit form (3) and (4) using the factorization of the additional operator  $\exp(\pm i\tilde{S}_k^{(M)})$  at the end points of the sub-intervals, we derived the second-, fourth-, and sixth-order approximations with respect to the time step. These factorizations are one of the key points of the proposed approach. The advantage of the FEM over the usual finite-difference technique consists in the explicit symmetry of the scheme (3) in matrix form (12) without additional calculation of the first

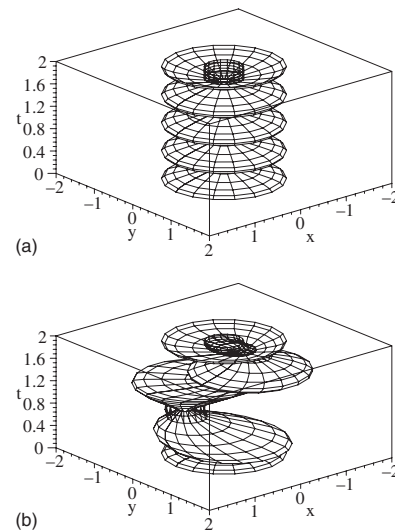


FIG. 3. Temporal dynamics of the loop in the  $x, y$  plane within which the probability density  $|\phi(x, y, t)|^2$  is greater than one-half of its maximal value, i.e.,  $|\phi(x, y, t)|^2 \geq \max_{x, y} |\phi(x, y, t)|^2 / 2$ .

spatial derivative of the matrix  $\mathbf{Q}(r) \neq \mathbf{0}$  [7]. The schemes developed provide a useful tool for calculations of threshold phenomena in the formation and ionization of (anti)hydrogenlike atoms and ions in magnetic traps [12], quantum dots in a magnetic field [19], channeling processes [21,22], potential scattering with confinement potentials [5], and control problems for finite-dimensional quantum systems [1].

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