Multi-layer evolution schemes for the finite-dimensional quantum systems in external fields.

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This talk is prepared to the 4th International Workshop "Quantum Physics and Communication", QPC 2007, Dubna, Russia, 15 - 19 October, 2007.

1. General formulation and operator-difference multi-layer calculation scheme

Let us consider the Cauchy problem for the time-dependent operator equation on the time interval $t \in [t_0, T]$

$$\imath \frac{\partial \Psi(t)}{\partial t} = H(t)\Psi(t), \quad \Psi(t_0) = \Psi_0, \tag{1}$$

where $H(t)$ is a linear self-adjoint operator. We rewrite Eq. (1) in terms of an unitary evolution operator $U(t, t_0, \lambda)$ with a complementary formal parameter λ carrying the initial state Ψ_0 to the solution $\Psi(t)$ in the form

$$\imath \frac{\partial U(t, t_0, \lambda)}{\partial t} = \lambda H(t) U(t, t_0, \lambda), \quad U(t, t, \lambda) = 1, \tag{2}$$

which considered in the uniform grid

$$\Omega_\tau[t_0, T] = \{t_0, t_{k+1} = t_k + \tau, t_K = T\} \tag{3}$$

with time step τ, in the time interval $[t_0, T]$. The complementary formal parameter λ will be replaced to be $\lambda = 1$ later. We express the unitary operator $U(t_{k+1}, t_k, \lambda)$ carrying the solution $\Psi(t_k)$ at $t = t_k$ to the one $\Psi(t_{k+1})$ at $t = t_{k+1}$ in the form [1] [2]

$$\begin{aligned} \Psi(t_{k+1}) &= U(t_{k+1}, t_k, \lambda)\Psi(t_k), \\ U(t_{k+1}, t_k, \lambda) &= \exp\left(-\imath\tau A_k^{(M)}(t_{k+1}, \lambda)\right) + O(\tau^{2M+1}). \end{aligned} \tag{4}$$

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[1] Puzynin I V, Selin A V and Vinitsky S I 1999 *Comput. Phys. Commun.* **123** 1–6

[2] Puzynin I V, Selin A V and Vinitsky S I 2000 *Comput. Phys. Commun.* **126** 158–161

We start with the power-series expansion of $A_k^{(M)}(t) \equiv A_k^{(M)}(t,\lambda)$ in terms of the formal parameter λ,

$$A_k^{(M)}(t,\lambda) = \frac{\imath}{\tau}\sum_{j=1}^{2M}\lambda^j A_{(j)k}(t), \quad A_k^{(M)}(t_k,\lambda) = 0, \tag{5}$$

where the coefficients $A_{(j)}(t) \equiv A_{(j)k}(t)$ are evaluated from the operator-identity [3]

$$-\imath\lambda H(t) = \sum_{n=1;q=0;l_1,\ldots,l_q=1}^{n+\Sigma_{i=1}^q l_i \le 2M} \frac{\lambda^{n+\Sigma_{i=1}^q l_i}}{(q+1)!}(adA_{(l_1)}(t))\ldots(adA_{(l_q)}(t))\ \dot{A}_{(n)}\ (t). \tag{6}$$

Here the linear operator $(adA) : \mathcal{L}(X) \to \mathcal{L}(X)$ ($\mathcal{L}(X)$ is the space of linear operators) is defined for operators $A, B \in \mathcal{L}(X)$ in the form $(adA)B = [A,B] \equiv AB - BA$ and have the following properties: $(adA)^0 B = B$, $(adA)^j B = (adA)^{j-1}(adA)B$. Note that the dot over the operator $A_{(n)}(t)$ means the partial derivation,
$\dot{A}_{(n)}\ (t) = \partial_t A_{(n)}(t)$, in t. Equating the coefficients at the same powers of λ in both sides of (6), we obtain a set of the first-order differential equations.

[3] Wilcox R M 1967 *J. Math. Phys.* **8** 962–982

For example, the first three equations reads as

$$\dot{A}_{(1)}(t) = -\imath H(t),$$
$$\dot{A}_{(2)}(t) = -\frac{(adA_{(1)}(t))\ \dot{A}_{(1)}(t)}{2}, \tag{7}$$
$$\dot{A}_{(3)}(t) = -\frac{(adA_{(2)}(t))\ \dot{A}_{(1)}(t)}{2} - \frac{(adA_{(1)}(t))^2\ \dot{A}_{(1)}(t)}{6} - \frac{(adA_{(1)}(t))\ \dot{A}_{(2)}(t)}{2},$$

we obtain

$$A_{(1)}(t) = -\imath\Upsilon^1_1(t), \quad A_{(2)}(t) = \frac{1}{2}\Upsilon^2_{21}(t), \quad A_{(3)}(t) = \frac{\imath}{6}\left(\Upsilon^3_{123}(t) + \Upsilon^3_{321}(t)\right). \tag{8}$$

The fourth-order term is similarly calculated. We find

$$A_{(4)}(t) = \frac{1}{12}\left(\Upsilon^4_{1432}(t) + \Upsilon^4_{1234}(t) + \Upsilon^4_{4312}(t) + \Upsilon^4_{2341}(t)\right). \tag{9}$$

Here

$$\Upsilon^n_{l_1,\ldots,l_n}(t) = \int_{t_k}^{t} dt_1 \int_{t_k}^{t_1} dt_2 \ldots \int_{t_k}^{t_{n-1}} dt_n (adH(t_{l_1}))\ldots(adH(t_{l_{n-1}}))H(t_{l_n}). \tag{10}$$

Solving sequentially the set of equations thus obtained, we are led to the effective Hamiltonians $A_k^{(M)}(t)$ connected with the original one $H(t)$ via the Magnus expansion [4] written in the terms of repeated integrals [5]. We wish to express the truncation $A_k^{(M)}(t)$ given in terms of $H(t)$, its partial derivative in time and the higher ones. Putting the Taylor expansion of $H(t)$ in a vicinity of $t_c = t_k + \tau/2$ as

$$H(t) = \sum_{j=0}^{2M} \frac{(t - t_c)^j}{j!} \partial_t^j H(t_c) + O\left(\tau^{2M+1}\right) \tag{11}$$

into the integrals, one can find an analytical (meaning non-numerical) expression of operators, $A_k^{(1)}(t), A_k^{(2)}(t), \ldots, A_k^{(M)}(t)$, with help of a symbolic algorithm GATEO (Generation of Approximations of the Time-Evolution Operator) [6]. Indeed, for $A_k^{(1)}(t)$, we have only to calculate the coefficient of λ^1, and then obtain

$$A_k^{(1)}(t_{k+1}) = \int_0^1 d\xi H(t_k + \xi\tau) = H(t_c) + O(\tau^2). \tag{12}$$

[4] Magnus W 1954 *Commun. Pure Appl. Math.* **7** 649–673

[5] Wilcox R M 1967 *J. Math. Phys.* **8** 962–982

[6] Gusev A, Gerdt V, Kaschiev M, Rostovtsev V, Samoylov V, Tupikova T, Uwano Yo and Vinitsky S 2005 *Lecture Notes in Computer Science* **3718** 244–258

To show the complexity of calculations, we present the first three approximations of the exponential (4) for the final effective Hamiltonians $A_k^{(M)} \equiv A_k^{(M)}(t_{k+1})$ in the form $A_k^{(M)} = \hat{A}_k^{(M)} + \imath \breve{A}_k^{(M)}$

$$
\begin{aligned}
\hat{A}_k^{(1)} &= H, \\
\breve{A}_k^{(1)} &= 0, \\
\hat{A}_k^{(2)} &= \hat{A}_k^{(1)} + \frac{\tau^2}{24}\ \ddot{H}, \\
\breve{A}_k^{(2)} &= \breve{A}_k^{(1)} + \frac{\tau^2}{12}(adH)\ \dot{H}, \\
\hat{A}_k^{(3)} &= \hat{A}_k^{(2)} + \frac{\tau^4}{1920}\ \ddddot{H} - \frac{\tau^4}{720}(adH)^2\ \ddot{H} - \frac{\tau^4}{240}(ad\ \dot{H})^2 H, \\
\breve{A}_k^{(3)} &= \breve{A}_k^{(2)} - \frac{\tau^4}{480}(ad\ \dddot{H})H + \frac{\tau^4}{480}(ad\ \ddot{H})\ \dot{H} + \frac{\tau^4}{720}(adH)^3\ \dot{H},
\end{aligned}
\tag{13}
$$

where $H \equiv H(t_c)$, $\dot{H} \equiv \partial_t H(t)|_{t=t_c}, \ldots$

1.1. Generalized $[M/M]$ Padé approximation

Application to the exponential operator of the generalized $[M/M]$ Padé approximation yields

$$\exp\left(-\imath\tau A_k^{(M)}\right) = \prod_{\zeta=M}^{1} T_{\zeta k} + O(\tau^{2M+1}), \tag{14}$$

$$T_{\zeta k} = \left(I + \frac{\tau\overline{\alpha}_\zeta^{(M)} A_k^{(M)}}{2M}\right)^{-1} \left(I + \frac{\tau\alpha_\zeta^{(M)} A_k^{(M)}}{2M}\right),$$

where I is the unit operator and the overline indicates the complex conjugate operation. The coefficients, $\alpha_\zeta^{(M)}$ $(\zeta = 1, \ldots, M,\ M \geq 1)$, stand for the roots of the polynomial equation, ${}_1F_1(-M, -2M, 2M\imath/\alpha) = 0$, where ${}_1F_1$ is the confluent hypergeometric function.

Table: The real and imaginary parts of the coefficients $\alpha_\zeta^{(M)}$, $M = 1, 2, 3$, $\zeta = 1, \ldots, M$

M	ζ	$\Re\alpha_\zeta^{(M)}$	$\Im\alpha_\zeta^{(M)}$
1	1	+0.0	−1.0
2	1	−0.57735026918962576450914878050	−1.0
2	2	+0.57735026918962576450914878050	−1.0
3	1	−0.81479955424892281841473623156	−0.85405673065166346526579940886
3	2	+0.0	−1.29188653869667306946840118228
3	3	+0.81479955424892281841473623156	−0.85405673065166346526579940886

Table 1 lists the values of the coefficients, $\alpha_\zeta^{(M)}$ for $M = 1, 2, 3$, in GATEO. The coefficients $\alpha_\zeta^{(M)}$ have the following properties: $\Im\alpha_\zeta^{(M)} < 0$ and $0.6 < |\alpha_\zeta^{(M)}| < \mu^{-1}$, where $\mu \approx 0.28$ is the root of equation $\mu \exp(\mu + 1) = 1$ [7]. Note that the condition $\tau < 2M\mu||A_k^{(M)}(t)||^{-1}$ guarantees the validity of the approximation (14) for any bounded operator $A_k^{(M)}(t)$.

[7] Puzynin I V, Selin A V and Vinitsky S I 1999 *Comput. Phys. Commun.* **123** 1–6

1.2. The operator-difference scheme of the evolution operator

We are now in a position to obtain the transition from $\Psi(t_k)$ to $\Psi(t_{k+1})$, by using the approximation (14) of the evolution operator in (4). To make it, we rewrite the transition in terms of the auxiliary functions defined by

$$\psi_k^0 = \Psi(t_k),$$
$$\left(I + \frac{\tau\overline{\alpha}_\zeta^{(M)} A_k^{(M)}}{2M}\right)\psi_k^{\zeta/M} = \left(I + \frac{\tau\alpha_\zeta^{(M)} A_k^{(M)}}{2M}\right)\psi_k^{(\zeta-1)/M}, \quad \zeta = 1, \dots, M, \tag{15}$$
$$\Psi(t_{k+1}) = \psi_k^1.$$

Note that, this way preserves the unitarity of an approximate devolution operator since the truncated $A_k^{(M)}$ is always self-adjoint. The fact that $\Im\alpha_\zeta^{(M)} \neq 0$ yields the operators, $T_{\zeta k}$, to be isometric, so that all the $\|\psi_k^{\zeta/M}\|$ have an equal norm, $\|\psi_k^0\| = \|\psi_k^{1/M}\| = \cdots = \|\psi_k^1\|$.

1.3. The operator-difference scheme with a partial splitting of the evolution operator

To generate schemes with extraction symmetric part $\tilde{A}_k^{(M)}(t)$ of the operator $A_k^{(M)}(t)$, we apply a gauge transformation $\tilde{\psi} = \exp\left(\imath S_k^{(M)}(t)\right)\psi$, that leads to a new operator

$$\tilde{A}_k^{(M)}(t) = \exp\left(\imath S_k^{(M)}(t)\right) A_k^{(M)}(t) \exp\left(-\imath S_k^{(M)}(t)\right), \tag{16}$$

in accordance with well-known formula

$$\exp(A)B\exp(-A) = \sum_{j=0} \frac{1}{j!}(adA)^j B. \tag{17}$$

We will find $S_k^{(M)}(t)$ in the form of a series by powers of τ

$$S_k^{(M)}(t) = \sum_{j=0}^{2M} \tau^j S_{(j)}(t), \tag{18}$$

where unknown coefficients $S_k^{(M)} \equiv S_k^{(M)}(t_{k+1})$ are calculated from an additional condition

$$\breve{\tilde{A}}_k^{(M)} = \exp\left(\imath S_k^{(M)}\right) \breve{A}_k^{(M)} \exp\left(-\imath S_k^{(M)}\right) = O(\tau^{2M}). \tag{19}$$

Substituting the expansion of $S_k^{(M)}$ to the condition and equating at the same powers of τ, we obtain a set of algebraic (or operator) recurrence relations for evaluating unknown coefficients $S_{(j)}$ with the initial condition $S_{(0)} = 0$.

The first three approximations of (18) and (16) have the form

$$S_k^{(1)} = 0,$$
$$S_k^{(2)} = S_k^{(1)} + \frac{\tau^2}{12}\ \dot{H},$$
$$S_k^{(3)} = S_k^{(2)} + \frac{\tau^4}{480}\ \dddot{H} + \frac{\tau^4}{720}(adH)^2\ \dot{H}, \quad \text{for} \quad (ad\ \ddot{H})\ \dot{H} \equiv 0, \tag{20}$$

and

$$\tilde{A}_k^{(1)} = \hat{A}_k^{(1)} = H,$$
$$\tilde{A}_k^{(2)} = \hat{A}_k^{(2)} = \tilde{A}_k^{(1)} + \frac{\tau^2}{24}\ \ddot{H},$$
$$\tilde{A}_k^{(3)} = \hat{A}_k^{(3)} + \frac{\tau^4}{288}(ad\ \dot{H})^2 H = \tilde{A}_k^{(2)} + \frac{\tau^4}{1920}\ \ddddot{H} - \frac{\tau^4}{720}(adH)^2\ \ddot{H} - \frac{\tau^4}{1440}(ad\ \dot{H})^2 H. \tag{21}$$

Taking into account the above procedures at each k-th time step of the grid $\Omega_\tau[t_0, T]$ ($k = 0, 1, \ldots, K-1$), we are led to the operator-difference scheme with a partial splitting of the evolution operator

$$\tilde{\psi}_k^0 = \exp\left(\imath S_k^{(M)}\right) \Psi(t_k),$$

$$\left(I + \frac{\tau\overline{\alpha}_\zeta^{(M)} \tilde{A}_k^{(M)}}{2M}\right) \tilde{\psi}_k^{\zeta/M} = \left(I + \frac{\tau\alpha_\zeta^{(M)} \tilde{A}_k^{(M)}}{2M}\right) \tilde{\psi}_k^{(\zeta-1)/M}, \quad \zeta = 1, \ldots, M, \tag{22}$$

$$\Psi(t_{k+1}) = \exp\left(-\imath S_k^{(M)}\right) \tilde{\psi}_k^1.$$

Hence, the auxiliary functions $\tilde{\psi}_k^{\zeta/M}$ in Eq. (22) can be treated as a kind of approximate solutions on a set of the fractional time steps $t_{k+\zeta/M} = t_k + \tau\zeta/M$, $\zeta = 1, \ldots, M-1$ in the time interval $[t_k, t_{k+1}]$. The scheme (22) is an implicit one of order $2M$ preserving the norm of the difference solution, so that this scheme is stable. Further, the scheme (22) provides an approximation of the order $O(\tau^{2M})$.

We wish to make the generalized $[L/L]$ Padé approximation for $\exp\left(\imath S_k^{(M)}\right)$ analogy to (14). This approximation has the order $O\left(\tau^{4L+2}\right)$ and should be $4L+2 \geq 2M$, so that we can choose $L = \left[\frac{M}{2}\right]$. In this case we obtain the modified numerical scheme of the (22)

$$\begin{aligned}
&\psi_k^0 = \Psi(t_k),\\
&\left(I - \frac{\overline{\alpha}_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{\eta/L} = \left(I - \frac{\alpha_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{(\eta-1)/L}, \quad \eta = 1,\dots,L,\\
&\tilde{\psi}_k^0 = \psi_k^1,\\
&\left(I + \frac{\tau\overline{\alpha}_\zeta^{(M)} \tilde{A}_k^{(M)}}{2M}\right)\tilde{\psi}_k^{\xi/M} = \left(I + \frac{\tau\alpha_\zeta^{(M)} \tilde{A}_k^{(M)}}{2M}\right)\tilde{\psi}_k^{(\xi-1)/M}, \quad \zeta = 1,\dots,M, \qquad (23)\\
&\psi_k^0 = \tilde{\psi}_k^1,\\
&\left(I + \frac{\overline{\alpha}_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{\eta/L} = \left(I + \frac{\alpha_\eta^{(L)} S_k^{(M)}}{2L}\right)\psi_k^{(\eta-1)/L}, \quad \eta = 1,\dots,L,\\
&\Psi(t_{k+1}) = \psi_k^1.
\end{aligned}$$

2. Application of calculation scheme for TDSE

Let us consider d dimensional TDSE with a Hamiltonian $H(t) \equiv H(\mathbf{r}, t)$

$$\imath \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = H(\mathbf{r}, t)\Psi(\mathbf{r}, t), \quad \Psi(\mathbf{r}, t_0) = \Psi_0(\mathbf{r}), \tag{24}$$

where

$$H(\mathbf{r}, t) = H_0(\mathbf{r}) + f(\mathbf{r}, t), \quad H_0(\mathbf{r}) = -\frac{1}{2}\nabla^2_{\mathbf{r}} + U(\mathbf{r}), \quad f(\mathbf{r}, t_0) \equiv 0. \tag{25}$$

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

$$\|\Psi\|^2 = \int |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1, \quad t \in [t_0, T]. \tag{26}$$

Thus, we rewrite the operators $\tilde{A}_k^{(M)}$ and $S_k^{(M)}$ in the forms

$$\begin{aligned}
&\tilde{A}_k^{(1)} = H, \quad S_k^{(1)} = 0, \\
&\tilde{A}_k^{(2)} = \tilde{A}_k^{(1)} + G^{(2)}, \quad S_k^{(2)} = S_k^{(1)} + Z^{(2)}, \qquad (27)\\
&\tilde{A}_k^{(3)} = \tilde{A}_k^{(2)} + G^{(3)} - \frac{\tau^4}{720} \nabla_{\mathbf{r}} \left(\nabla_{\mathbf{r}}^2 \ddot{f} \right) \nabla_{\mathbf{r}}, \quad S_k^{(3)} = S_k^{(2)} + Z^{(3)} + \frac{\tau^4}{720} \nabla_{\mathbf{r}} \left(\nabla_{\mathbf{r}}^2 \dot{f} \right) \nabla_{\mathbf{r}},
\end{aligned}$$

where

$$\begin{aligned}
&G^{(2)} = \frac{\tau^2}{24} \ddot{f}, \\
&Z^{(2)} = \frac{\tau^2}{12} \dot{f}, \qquad (28)\\
&G^{(3)} = \frac{\tau^4}{1920} \ddddot{f} + \frac{\tau^4}{1440} \left(\nabla_{\mathbf{r}} \dot{f} \right)^2 - \frac{\tau^4}{720} \left(\nabla_{\mathbf{r}} \ddot{f} \right) \left(\nabla_{\mathbf{r}} (U + f) \right) - \frac{\tau^4}{2880} \left(\nabla_{\mathbf{r}}^4 \ddot{f} \right), \\
&Z^{(3)} = \frac{\tau^4}{480} \dddot{f} + \frac{\tau^4}{720} \left(\nabla_{\mathbf{r}} \dot{f} \right) \left(\nabla_{\mathbf{r}} (U + f) \right) + \frac{\tau^4}{2880} \left(\nabla_{\mathbf{r}}^4 \dot{f} \right),
\end{aligned}$$

and $f \equiv f(\mathbf{r}, t_c)$, $\dot{f} \equiv \partial_t f(\mathbf{r}, t)|_{t=t_c}, \ldots, U \equiv U(\mathbf{r})$. We can see from (27) the operators $\tilde{A}_k^{(3)}$ and $S_k^{(3)}$ don't contained the operator $\nabla_{\mathbf{r}}$ at $\left(\nabla_{\mathbf{r}}^2 f\right) = 0$. In further we will use of the cases $M \leq 3$, because the considering calculation schemes are rather cumbersome for a practical utilization at $M \geq 4$.

2.1. Kantorovich approach

In the close coupling approximation, known in mathematics as the Kantorovich method the partial wave function $\Psi(\mathbf{r},t)$ is expanded over the one-parametric basis functions $\{B_j(\Omega;r)\}_{j=1}^{N}$

$$\Psi(\mathbf{r},t)=\sum_{j=1}^{N}B_j(\Omega;r)\chi_j(r,t). \tag{29}$$

In Eq. (29), the vector-function $\boldsymbol{\chi}(r,t)=(\chi_1(r,t),\ldots,\chi_N(r,t))^T$ 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. In the Kantorovich approach, the functions $B_j(\Omega;r)$ are determined as solutions of the following parametric eigenvalue problem

$$\left(-\frac{1}{2r^2}\hat{\boldsymbol{\Lambda}}_{\Omega}^2+U(\mathbf{r})\right)B_j(\Omega;r)=E_j(r)B_j(\Omega;r), \tag{30}$$

where $\hat{\boldsymbol{\Lambda}}_{\Omega}^2$ 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

$$\left\langle B_i(\Omega;r)\middle|B_j(\Omega;r)\right\rangle_{\Omega}=\int\overline{B}_i(\Omega;r)B_j(\Omega;r)d\Omega=\delta_{ij}, \tag{31}$$

where δ_{ij} is the Kronecker symbol.

After minimizing the Rayleigh-Ritz variational functional, and using the expansion (29) the equation (24) is reduced to a finite set of N ordinary second-order differential equations

$$\imath \mathbf{I}\frac{\partial \boldsymbol{\chi}(r,t)}{\partial t} = \mathbf{H}(r,t)\boldsymbol{\chi}(r,t), \quad \boldsymbol{\chi}(r,t_0) = \boldsymbol{\chi}_0(r), \tag{32}$$

with

$$\mathbf{H}(r,t) = -\frac{1}{2r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\mathbf{I}\frac{\partial}{\partial r} + \mathbf{V}(r,t) + \mathbf{Q}(r)\frac{\partial}{\partial r} + \frac{1}{r^{d-1}}\frac{\partial r^{d-1}\mathbf{Q}(r)}{\partial r}. \tag{33}$$

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

$$\begin{aligned} V_{ij}(r,t) = V_{ji}(r,t) &= \frac{E_i(r)+E_j(r)}{2}\delta_{ij} + \frac{1}{2}\left\langle \frac{\partial B_i(\Omega;r)}{\partial r}\middle| \frac{\partial B_j(\Omega;r)}{\partial r}\right\rangle_\Omega \\ &+ \left\langle B_i(\Omega;r)\middle| f(\mathbf{r},t)\middle| B_j(\Omega;r)\right\rangle_\Omega, \quad I_{ij} = \delta_{ij}, \\ Q_{ij}(r) = -Q_{ji}(r) &= -\frac{1}{2}\left\langle B_i(\Omega;r)\middle| \frac{\partial B_j(\Omega;r)}{\partial r}\right\rangle_\Omega . \end{aligned} \tag{34}$$

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

$$\begin{aligned}
&\tilde{A}_k^{(M)} \to \tilde{\mathbf{A}}_k^{(M)}, \quad \tilde{A}_{k,ij}^{(M)} = \left\langle B_i(\Omega;r) \middle| \tilde{A}_k^{(M)} \middle| B_j(\Omega;r) \right\rangle_{\Omega}, \\
&S_k^{(M)} \to \tilde{\mathbf{S}}_k^{(M)}, \quad \tilde{S}_{k,ij}^{(M)} = \left\langle B_i(\Omega;r) \middle| \tilde{S}_k^{(M)} \middle| B_j(\Omega;r) \right\rangle_{\Omega}, \\
&I \to \mathbf{I}, \quad I_{ij} = \delta_{ij}.
\end{aligned} \tag{35}$$

2.2. High-order approximation of the finite-element method

To solve problem (32) on the time grid $\Omega_\tau[t_0, T]$, the boundary conditions and normalization condition with respect to the space variable r on an infinite interval are replaced with appropriate conditions on a finite interval $\hat{\Omega}_r[r_{\min}, r_{\max}]$. Then, at each k-th step of the time grid $\Omega_\tau[t_0, T]$, we consider the discrete representation of solution $\boldsymbol{\chi}(r, t_k)$ to problem (32) with the help of FEM on the grid $\hat{\Omega}_h^p = \{r_0 = r_{\min}, r_j = r_{j-1} + h_j, r_n = r_{\max}\}$ in the form of a finite sum of local functions $N(r)$

$$\chi_\mu(r, t_k) = \sum_{l=0}^{np} \chi_\mu^l(t_k)\, N_l^p(r), \quad \mu = 1, \ldots, N, \tag{36}$$

where $\chi_\mu^l(t_k)$ are node values of the unknown function $\chi_\mu(r, t_k)$, with respect to which the initial problem is numerically solved. The local functions $N_l^p(r)$ are piecewise continuous polynomials of order p equal to one at one of the nodes r_μ and zero at the other nodes of the grid $\hat{\Omega}_h^p$; i.e., $N_l^p(r_\nu) = \delta_{l\nu}$, $l, \nu = 0, \ldots, np$. The coefficients $\chi_\mu^l(t_k)$ are formally related to the values of the vector $\chi_\mu(r, t_k)$ of the problem at the Lagrangian node points

$$r_{j,i}^p = r_{j-1} + \frac{h_j}{p} i, \quad h_j = r_j - r_{j-1}, \quad i = \overline{0, p}, \tag{37}$$

by the relations $\chi_\mu^l(t_k) \equiv \chi_\mu^l(r_{j,i}^p, t_k), \quad l = i + p(j-1)$.

Substituting (36) into matrix operator-difference scheme, multiplying it from the left by $N_l^p(r)$ and integrating over the interval $\hat{\Omega}_r[r_{\min}, r_{\max}]$ considering scheme is reduced to a system algebraic equations for $\left\{\{\chi_\mu^l(r_{j,i}^p, t_k)\}_{l=0}^{np}\right\}_{\mu=1}^N$ at given M

$$\tilde{\mathbf{A}}_k^{(M)} \to \mathbf{A}_k^p, \quad A_{k,ij}^p = A_{k,ji}^p = \int_{r_{\min}}^{r_{\max}} N_i^p(r) \tilde{\mathbf{A}}_k^{(M)} N_j^p(r) r^{d-1} dr, \quad (38)$$

$$\tilde{\mathbf{S}}_k^{(M)} \to \mathbf{S}_k^p, \quad S_{k,ij}^p = S_{k,ji}^p = \int_{r_{\min}}^{r_{\max}} N_i^p(r) \tilde{\mathbf{S}}_k^{(M)} N_j^p(r) r^{d-1} dr,$$

$$\mathbf{I} \to \mathbf{B}^p, \quad B_{ij}^p = B_{ji}^p = \int_{r_{\min}}^{r_{\max}} N_i^p(r) \, \mathbf{I} \, N_j^p(r) r^{d-1} dr.$$

3. Numerical tests

3.1. One dimensional model

The TDSE for a one-dimensional harmonic oscillator with an explicitly time-dependent frequency in the finite time interval $t \in [0, T]$ has the form

$$\mathbf{H}(x,t) = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{\omega^2(t)x^2}{2}, \quad \psi_0(x) = \sqrt[4]{\frac{1}{\pi}} \exp\left(-\frac{1}{2}(x-\sqrt{2})^2\right), \tag{39}$$

with $\omega^2(t) = 4 - 3\exp(-t)$ [8]. The exact solution of Eq. (39) reads

$$\psi_{ext}(x,t) = \sqrt[4]{\frac{1}{\pi}} \exp\left(-X(t)x^2 + 2Y(t)x - Z(t)\right), \tag{40}$$

where the functions $X(t)$, $Y(t)$ and $Z(t)$ satisfy to the Cauchy problem

$$\begin{aligned} \imath\frac{d}{dt}X(t) &= 2X^2(t) - \frac{\omega^2(t)}{2}, \quad X(0) = \frac{1}{2}, \\ \imath\frac{d}{dt}Y(t) &= 2X(t)Y(t), \quad Y(0) = \frac{\sqrt{2}}{2}, \\ \imath\frac{d}{dt}Z(t) &= -X(t) + 2Y^2(t), \quad Z(0) = 1. \end{aligned} \tag{41}$$

[8] Puzynin I V, Selin A V and Vinitsky S I 1999 *Comput. Phys. Commun.* **123** 1–6

To approximate the solution $\psi(x,t)$ in the variable x, we used the finite element grid $\hat{\Omega}_x[x_{\min}, x_{\max}] = \{x_{\min} = -10, (100), x_{\max} = 10\}$ and time step $\tau = .9765625e-2$, 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

$$Er^2(t,j) = \int_{x_{\min}}^{x_{\max}} |\psi(x,t) - \psi^{\tau_j}(x,t)|^2 dx, \tag{42}$$

and the Runge coefficient

$$\beta(t) = \log_2 \left| \frac{Er(t,1) - Er(t,2)}{Er(t,2) - Er(t,3)} \right|, \tag{43}$$

where $\psi^{\tau_j}(x,t)$ are the numerical solutions with the time step $\tau_j = \tau/2^{j-1}$. For the function $\psi(x,t)$ 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, that strongly correspond to theoretical ones $\beta(t) \equiv \beta_M(t) \approx 2M$.

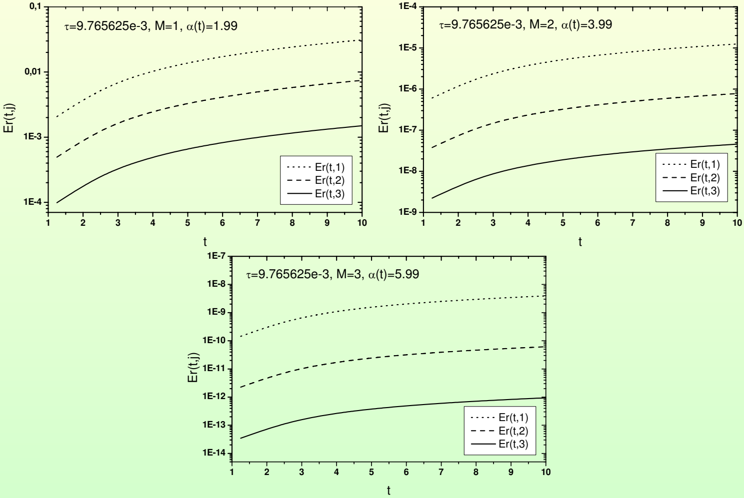

Figure: Values of discrepancy functions $Er(t,j)$ for $j = 1, 2, 3$ and $M = 1, 2, 3$.

3.2. 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 $E_2(t)$ in the finite time interval $t \in (0, T]$ has the form

$$\imath \frac{\partial}{\partial t}\phi(x_1, y_1, t) = -\frac{1}{2}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2}\right)\phi(x_1, y_1, t) + \frac{\imath\omega}{2}\left(x_1\frac{\partial}{\partial y_1} - y_1\frac{\partial}{\partial x_1}\right)\phi(x_1, y_1, t)$$
$$+\frac{\omega^2}{8}(x_1^2 + y_1^2)\phi(x_1, y_1, t) - (x_1 E_1(t) + y_1 E_2(t))\phi(x_1, y_1, t). \quad (44)$$

The transformation to a rotated coordinate system with frequency $\omega/2$

$$x_1 = x\cos\left(\frac{\omega t}{2}\right) + y\sin\left(\frac{\omega t}{2}\right), \quad y_1 = y\cos\left(\frac{\omega t}{2}\right) - x\sin\left(\frac{\omega t}{2}\right), \quad (45)$$

and $x = r\cos(\theta)$, $y = r\sin(\theta)$, leads to the following equation

$$\imath \frac{\partial}{\partial t}\phi(r, \theta, t) = -\frac{1}{2}\left(\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right)\phi(r, \theta, t) \quad (46)$$
$$+\frac{\omega^2 r^2}{8}\phi(r, \theta, t) + r(f_1(t)\cos(\theta) + f_2(t)\sin(\theta))\phi(r, \theta, t),$$

$$f_1(t) = -E_1(t)\cos\left(\frac{\omega t}{2}\right) + E_2(t)\sin\left(\frac{\omega t}{2}\right), \quad (47)$$
$$f_2(t) = -E_1(t)\sin\left(\frac{\omega t}{2}\right) - E_2(t)\cos\left(\frac{\omega t}{2}\right).$$

Using the Galerkin projection of solutions by means of the basis of the angular functions $B_j(\theta)$

$$\phi(r,\theta,t) = \sum_{j=1}^{N} B_j(\theta)\chi_j(r,t), \tag{48}$$

$$B_1(\theta) = \frac{1}{\sqrt{2\pi}}, \quad B_{2j}(\theta) = \frac{\sin(j\theta)}{\sqrt{\pi}}, \quad B_{2j+1}(\theta) = \frac{\cos(j\theta)}{\sqrt{\pi}}, \quad j \geq 1, \tag{49}$$

we arrive at the matrix equation (32) 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 $t=0$ (in the case $f_1(0) = f_2(0) = 0$) are chosen in the form

$$\chi_1(r,0) = \sqrt{\omega}\exp\left(-\frac{1}{4}\omega r^2\right), \quad \chi_j(r,0) \equiv 0, \quad j \geq 2. \tag{50}$$

Note that, this problem has an exact solution for a partial choice of the field

$$E_j(t) = a_j \sin(\omega_j t) \tag{51}$$

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. The needed projections of an exact solution to the radial ones have the form

$$\chi_j^{ext}(r,t) = \int_0^{2\pi} B_j(\theta)\phi_{ext}(r,\theta,t)d\theta. \tag{52}$$

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 $\phi(x, y, t)$ is should be periodically with period $T = 2$, i.e., $|\phi(x, y, t)| = |\phi(x, y, t + T)|$.
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 $\tau = 0.00625$, 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 analogy to (42)

$$Er^2(t, j) = \sum_{\nu=1}^{N} \int_0^{r_{\max}} |[\chi_\nu(r, t) - \chi_\nu^{\tau_j}(r, t)]|^2 r dr, \quad j = 1, 2, 3, \tag{53}$$

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 $\tau_4 = \tau/8$.

Table: The test results of the discrepancy functions $Er(t, j)$ $(j = 1, 2, 3)$ for the approximations $M = 1, 2, 3$. Here number of the used differential equations $N = 30$, time step $\tau = 0.00625$, and t is some times.

t	M=1			
	$Er(t,1)$	$Er(t,2)$	$Er(t,3)$	$\beta_1(t)$
0.4	0.7399(-02)	0.1777(-02)	0.3562(-03)	1.984
0.8	0.4054(-01)	0.9773(-02)	0.1960(-02)	1.977
1.2	0.7351(-01)	0.1777(-01)	0.3566(-02)	1.972
1.6	0.7630(-01)	0.1844(-01)	0.3700(-02)	1.973
2.0	0.8103(-01)	0.1957(-01)	0.3925(-02)	1.974

t	M=2			
	$Er(t,1)$	$Er(t,2)$	$Er(t,3)$	$\beta_2(t)$
0.4	0.6811(-05)	0.4261(-06)	0.2509(-07)	3.993
0.8	0.6156(-04)	0.3858(-05)	0.2273(-06)	3.991
1.2	0.1228(-03)	0.7700(-05)	0.4537(-06)	3.989
1.6	0.1256(-03)	0.7882(-05)	0.4645(-06)	3.988
2.0	0.1313(-03)	0.8254(-05)	0.4866(-06)	3.986

t	M=3			
	$Er(t,1)$	$Er(t,2)$	$Er(t,3)$	$\beta_3(t)$
0.4	0.5064(-08)	0.9193(-10)	0.3799(-10)	6.526
0.8	0.6363(-07)	0.1008(-08)	0.6168(-10)	6.047
1.2	0.1438(-06)	0.2262(-08)	0.7341(-10)	6.015
1.6	0.1723(-06)	0.2719(-08)	0.8136(-10)	6.007
2.0	0.2634(-06)	0.4209(-08)	0.1039(-09)	5.981

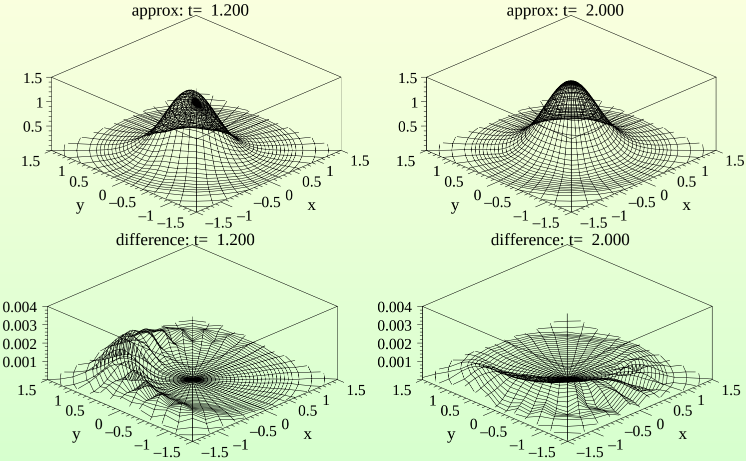

Figure: The absolute values of the numerical solution $|\phi(x,y,t)|$ and difference $|\phi_{ext}(x,y,t) - \phi(x,y,t)|$ at $t = 1.2$ and $t = 2$. Here $N = 30$, $\tau_4 = \tau/8 = 0.00078125$ and $M = 3$.

3.3. Three dimensional model

As known, the δ-shaped pulses are a widely used approximation for electric-field pulses that are much shorter than the classical orbital period. The Hamiltonian of the kicked hydrogen atom in a magnetic field reads

$$H = H_0 + V_{ext},\ H_0 = -\frac{1}{2}\Delta_{\mathbf{r}} - \frac{1}{r} + \frac{\beta^2 r^2}{8}\sin^2(\theta),\ V_{ext} = \mathbf{r}\,\mathbf{F}\sum_{k=1}^{S}\delta(t-kT), \quad (54)$$

where S is the number of kicks applied, T its period, $\beta = B_0/B$ is a dimensionless parameter which determines the field strength B, and $\mathbf{F} = (0, 0, F)$ is the external field. Between the pulses the wave packet evolves according to the TDSE

$$\imath\,\frac{\partial\psi(\mathbf{r},t)}{\partial t} = H_0\psi(\mathbf{r},t). \quad (55)$$

We use following formula for calculation of wave function $\psi(\mathbf{r}, sT_+)$ directly after the pulse $t = sT_+$

$$\psi(\mathbf{r}, sT_+) = \exp\left(-\imath\,\mathbf{r}\mathbf{F}\right)\psi(\mathbf{r}, sT_-). \quad (56)$$

via the wave function $\psi(\mathbf{r}, sT_-)$ immediately before the pulse.

Using the Kantorovich expansion of solutions by means of the basis functions $B_j(\theta; r)$

$$\psi(\mathbf{r}, t) = \frac{\exp(\imath\, m\varphi)}{\sqrt{2\pi}} \sum_{j=1}^{N} B_j(\theta; r)\chi_j(r, t). \tag{57}$$

The functions $B_j(\eta = \cos(\theta); r)$ are determined as solutions of the following parametric eigenvalue problem [9] [10]

$$\left(-\frac{1}{2r^2}\left(\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} - \frac{m^2}{1-\eta^2}\right) - \frac{1}{r} + \frac{\beta^2 r^2}{8}(1-\eta^2)\right) B_j(\eta; r) = E_j(r) B_j(\eta; r). \tag{58}$$

[9] Chuluunbaatar O, Gusev A A, Gerdt V P, Rostovtsev V A, Vinitsky S I, Abrashkevich A G, Kaschiev M S and Serov V V 2007 accepted in Comput. Phys. Commun. doi:10.1016/j.cpc.2007.09.005.

[10] Chuluunbaatar O, Gusev A A, Derbov V L, Kaschiev M S, Serov V V, Melnikov L A and Vinitsky S I 2007 J. Phys. **A 40** 11485–11524.

$$\beta = 0; \quad F = 0.002; \qquad T \equiv T_{n=9} = 5357: \tag{59}$$

$$P_n(t) = \sum_{l=0}^{n-1} |\langle nl0|\psi(\mathbf{r},t)\rangle|^2 \quad \text{the probability function}: \tag{60}$$

$$C(t) = |\langle\psi(\mathbf{r},t)|\psi_0(\mathbf{r})\rangle| \quad \text{the autocorrelation function}: \tag{61}$$

$$|\psi_0(\mathbf{r})\rangle = |n = 9k = 0m = 0\rangle^{11}: \tag{62}$$

$$r \to r/n; \quad t \to t/n^2; \quad \hat{T} = \hat{T}_n = T_n/n^2 \sim 66: \tag{63}$$

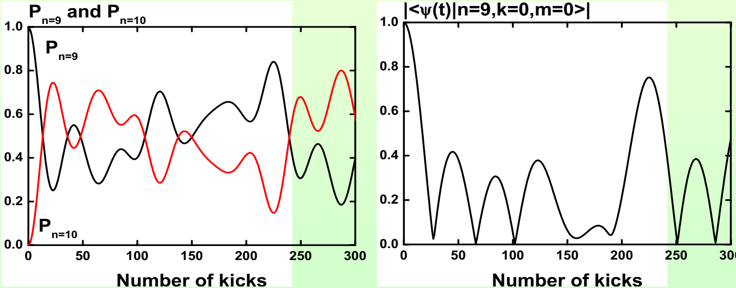

Figure: The dynamics of physical quantities of a kicked hydrogen atom.

[11] Klews M and Schweizer W 2001 Phys. Rev. A, **64** 053403-1-053403-5.

$$\beta = 0.1472e-4; \quad F = 0.002; \qquad T \equiv T_{n=9} = 5357: \qquad (64)$$

Table: The eigenvalues E_{calc} calculated by the code KANTBP [12] of the magnetic states $n = 9, v, m = 0$, $\delta E_{calc} = (E_{calc} - E^{(0)})/\beta^2$ corresponds to the first order corrections $E^{(1)}_{pt}$ by of a perturbation calculation $E_{pt} = E^{(0)} + \beta^2 E^{(1)}_{pt}$. Below, the factor x in the brackets means $(x) \equiv 10^x$.

v	E_{calc}	E^0	δE_{calc}	E^1_{pt}
0	-6.172 798(-3)	-6.172 839 (-3)	1529.11	1529.16
1	-6.172 797(-3)	-6.172 839 (-3)	1545.01	1545.04
2	-6.172 747(-3)	-6.172 839 (-3)	3384.07	3384.10
3	-6.172 728(-3)	-6.172 839 (-3)	4080.42	4080.47
4	-6.172 689(-3)	-6.172 839 (-3)	5536.15	5536.38
5	-6.172 641(-3)	-6.172 839 (-3)	7315.02	7315.33
6	-6.172 582(-3)	-6.172 839 (-3)	9476.34	9476.83
7	-6.172 514(-3)	-6.172 839 (-3)	12006.50	12007.13
8	-6.172 435(-3)	-6.172 839 (-3)	14902.72	14903.51

[12] Chuluunbaatar O, Gusev A A, Abrashkevich A G, Amaya-Tapia A, Kaschiev M S, Larsen S Y and Vinitsky S I 2007 Comput. Phys. Commun. **177** 649–675.

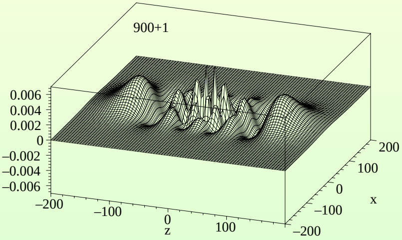

Figure: The three dimensional plots of the normalized even wave functions in zx plane of states $|n = 9v = 0m = 0\rangle$ and $|n = 9v = 8m = 0\rangle$[13].

[13] Chuluunbaatar O, Gusev A A, Derbov V L, Kaschiev M S, Serov V V, Melnikov L A and Vinitsky S I 2007 J. Phys. **A 40** 11485–11524.

$|\psi_0(\mathbf{r})\rangle = |n = 9 v = 0 m = 0\rangle$ $\quad$ $|\psi_0(\mathbf{r})\rangle = |n = 9 v = 8 m = 0\rangle$

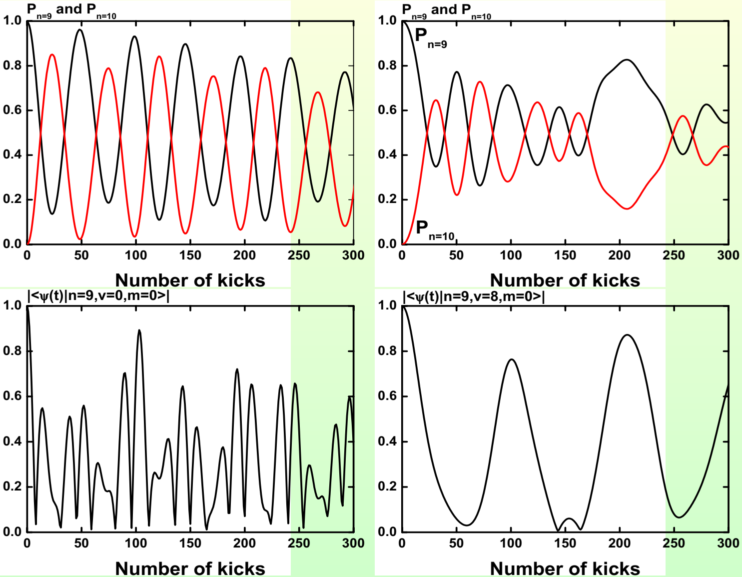

Figure: The dynamics of physical quantities of a kicked hydrogen atom in the magnetic field.

4. Conclusions

We have presented a new computational approach to solve the TDSE, in which partial (unitary) splitting of evolution operator and the FEM are combined together effectively. Especially, to realize our approach in an explicit form, we have derived the second-, fourth-, and sixth-order approximations with respect to time step. Several numerical results have been also given which turn out to agree with the theoretical ones to a good extent.