ATOM PHYSICS AND PHYSICS OF CLUSTERS AND NANOSTRUCTURES

Original article
DOI: https://doi.org/10.18721/JPM.18405

APPLICATION OF PARABOLIC WAVE PACKETS TO SOLVING THE EVOLUTION PROBLEM OF A HYDROGEN ATOM EXPOSED TO LONG LASER PULSES

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Abstract. The article studies the features of application of the parabolic wave packets (PWP) (we proposed) to the solution of the Time-Dependent Schrцdinger Equation (TDSE) for a hydrogen atom exposed to a long laser pulse. Within the framework of the Time-Dependent Variational Principle, the TDSE is transformed into a system of first-order differential equations with respect to the PWP parameters. The efficiency of the proposed scheme has been studied using an exactly solvable example of pulses of arbitrary (including complex) amplitude and duration. The case of ultraviolet radiation was also considered, for which our calculations were compared with the results obtained by other authors. Possible reasons for the observed discrepancy between the results of applying our approach and those obtained by standard methods were listed.

Keywords: parabolic wave packets, time-dependent Schrцdinger equation, time-dependent variational principle, hydrogen atom

Funding: Formalism development of using PWP for description of the action of long laser pulses on a hydrogen atom as well as the action of narrow high-power pulses of coherent XUV on this atom was funded by Russian Science Foundation (project No. 23-72-01072, https://rscf.ru/project/23-72-01072/).

The computational part of the work was supported by the Ministry of Science and Higher Education of Russian Federation within the project FEME-2024-0005.

Citation: Zaytsev A. S., Zaytsev S. A., Zaytseva D. S., Kramar E. I., Application of parabolic wave packets to solving the evolution problem of a hydrogen atom exposed to long laser pulses, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 18 (4) (2025) 61–74. DOI: https://doi.org/10.18721/JPM.18405

Научная статья
УДК 539.1, 539.18
DOI: https://doi.org/10.18721/JPM.18405

ПРИМЕНЕНИЕ ПАРАБОЛИЧЕСКИХ ВОЛНОВЫХ ПАКЕТОВ К РЕШЕНИЮ ЗАДАЧИ ЭВОЛЮЦИИ АТОМА ВОДОРОДА ПОД ДЕЙСТВИЕМ ДЛИТЕЛЬНЫХ ЛАЗЕРНЫХ ИМПУЛЬСОВ

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Аннотация. Исследованы особенности применения предложенных нами параболических волновых пакетов (PWP) к решению нестационарного уравнения Шрёдингера (TDSE) для атома водорода, находящегося под действием длительного лазерного импульса. В рамках нестационарного вариационного принципа (TDVP) уравнение TDSE преобразуется в систему дифференциальных уравнений первого порядка относительно параметров PWP. Эффективность предлагаемой схемы исследована на точно решаемом примере импульсов произвольной (в том числе комплексной) амплитуды и длительности. Рассмотрен также случай воздействия ультрафиолетового излучения, для которого выполнено сопоставление наших расчетных данных с результатами других авторов. Перечислены возможные причины наблюдаемого расхождения между результатами применения нашего подхода и результатами использования стандартных методов.

Ключевые слова: параболические волновые пакеты, уравнение Шрёдингера, вариационный принцип, атом водорода, импульсный лазер

Финансирование. Разработка формализма применения PWP для описания действия длительных лазерных импульсов на атом водорода, а также действия на него коротких интенсивных импульсов когерентного экстремального ультрафиолетового (XUV) излучения поддержана Российским научным фондом (проект № 23-72-01072, https://rscf.ru/project/23-72-01072/).

Вычислительная часть работы поддержана Министерством науки и высшего образования Российской Федерации в рамках проекта FEME0005-2024-.

Ссылка для цитирования: Зайцев А. С., Зайцев С. А., Зайцева Д. С., Крамарь Е. И. Применение параболических волновых пакетов к решению задачи эволюции атома водорода под действием длительных лазерных импульсов // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2025. Т. 18. № 4. С. 61–74. DOI: https://doi.org/10.18721/JPM.18405

Introduction

The advances made in developing attosecond pulse sources of X-ray and ultraviolet radiation [1] have opened up new possibilities for studying time-dependent phenomena in atoms and molecules. Such experiments make it possible to observe the dynamics of ultrafast electrons in real time [2, 3], to study the generation of high harmonics [4], etc. In turn, interpreting these new experimental data theoretically has driven intense research to develop efficient numerical methods for solving the Time-Dependent Schrцdinger Equation (TDSE) [5]. In the case of weak fields, Coulomb scattering states modified by laser radiation are accurately described analytically within the framework of the strong field approximation [6], the Bunkin–Fedorov approach [7] and the Coulomb–Volkov model [8].

The shift toward laser radiation with higher power has fueled the development of more precise methods based on direct numerical solution of the TDSE. The most widespread is the Crank–Nicolson method [9], which is an implicit-explicit finite-difference scheme, and its modifications [10]. An additional approach, based on Dirac's variational principle, is the Time-Dependent Variational Principle (TDVP) [11]. The parameters of the trial functions used to represent the TDSE solution satisfy the TDVP. A successful application of TDVP was developed in [12], where the TDSE solution is sought as Gaussian Wave Packets (GWP).

We previously proposed a method for solving the TDSE [13] describing a hydrogen atom exposed to linearly polarized laser radiation. Our approach assumes that the solution is expanded in the space of so-called parabolic wave packets (PWP) with time-dependent parameters. The axial symmetry is taken into account within our PWP approach by using parabolic coordinates with the z axis directed along the polarization vector. Thus, the initially three-dimensional problem is reduced to finding a solution on the plane (ξ,η).

The advantage of the method is that it can yield solutions in an unbounded space, so that the numerical procedure is free from spurious boundary reflections typical for approaches that rely on a computational domain with explicitly set boundaries

The method also has a number of drawbacks. The main one is that the order of the numerical scheme must be sufficient to provide the accuracy required for the stability of the procedure. For example, the relatively stable Crank–Nicolson method is the most frequently used in evolution problems that apply the finite element method or the grid-based spatial discretization method [9]. Unfortunately, this method turned out to be insufficiently accurate in our case: the matrix of the equation became singular at the first steps of the procedure.

This study concentrates on expanding the capabilities of the PWP approach to make it applicable to pulses with the duration of about 10 optical cycles. This was achieved by using an eighth-order Dormand–Prince method consisting of 13 stages [14], belonging to the Runge–Kutta family. The developed numerical scheme was tested for a complex pulse allowing for an exact solution as a single PWP function. Notably, choosing the values of the pulse parameters yields solutions that become non-normalizable at certain times. This behavior, which falls outside standard boundary conditions, provides an additional test of the numerical scheme's robustness.

We also calculated the photoelectron spectra for pulses of different durations, comparing our results with those obtained earlier by other authors. In particular, we considered cases of short intense pulses of coherent extreme ultraviolet (XUV) radiation [15], as well as single-cycle and 7-cycle pulses [16, 17]. While the results of our earlier work [13] showed full agreement with other studies for short few-cycle pulses, the situation is different for longer pulses. For instance, the photoionization spectrum calculated by the standard method for such radiation exhibits relatively regular oscillations with increasing electron energy. On the other hand, according to our calculations, the curve characterizing the spectrum of the electron ejected by the pulse contains several peaks followed by a monotonic decrease. To determine the reasons for this discrepancy, we analyzed the error of our numerical scheme, as well as the convergence of the results with decreasing time step and with increasing basis set size.

Atomic units (a.u./a.e.) $\hbar = e = m_e = 1$ are used in the paper, unless otherwise specified.

Quantum-mechanical theory of the phenomenon under consideration

Consider a TDSE of the form

$$i\frac{\partial}{\partial t}\Psi(t) = \hat{\mathcal{H}}(t)\Psi(t), \tag{1}$$

where the complete Hamiltonian of the system

$$\hat{\mathcal{H}}(t) = \hat{H}_C + \hat{U}(t), \tag{2}$$

is represented by the sum of the Coulomb Hamiltonian $\hat{H}_C$ and the perturbation energy $\hat{U}(t)$ induced by the laser field.

The Coulomb Hamiltonian is defined as

$$\hat{H}_C = -\frac{1}{2M}\nabla_{\mathbf{r}}^2 + \frac{Z}{r}, \tag{3}$$

where **r** is the radius vector of a particle with mass M; in the case of the hydrogen atom, $M = 1$ and the particle charge $Z = -1$.

In the case of a linearly polarized laser pulse, the natural choice for the direction of the z axis is parallel to the polarization vector.

Thus, the perturbation operator takes the following form in the dipole approximation and the length gauge:

$$\hat{U}(t) = E(t)z, \tag{4}$$

where $E(t)$ is the field.

Axial symmetry necessitates parabolic coordinates ξ, η, φ, which are related to the Cartesian coordinates by the formulas

$$x = \sqrt{\xi\eta}\cos\varphi, y = \sqrt{\xi\eta}\sin\varphi, z = \frac{1}{2}(\xi - \eta). \tag{5}$$

Thus, the TDSE expressed by Eq. (1) is reduced to the following equation on the plane (ξ,η):

$$i\frac{(\xi+\eta)}{4}\frac{\partial}{\partial t}\Psi(t,\xi,\eta) = \left[-\frac{1}{2M}\left(\frac{\partial}{\partial\xi}\xi\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}\eta\frac{\partial}{\partial\eta}\right) + \frac{Z}{2} + \frac{E(t)}{8}\left(\xi^2 - \eta^2\right)\right]\times \\ \times\Psi(t,\xi,\eta). \tag{6}$$

Parabolic wave packets. We seek the solution to Eq. (1) as the following expansion [13]:

$$\Psi(t) = \sum_{\kappa}\sum_{j=1}^{N} u_j^{\kappa}(t), \tag{7}$$

with respect to the basis functions

$$\left\langle \xi,\eta,\phi \middle| u^{\kappa}(t)\right\rangle = \frac{e^{i\kappa\phi}}{\sqrt{2\pi}}[\xi\eta]^{\frac{\lambda}{2}} g(t,\xi,\eta), \lambda = |\kappa|, \tag{8}$$

where

$$g(t,\xi,\eta) = \exp\left[\gamma(t) - a(t)\xi - b(t)\eta\right]. \tag{9}$$

We call the trial functions (9) parabolic wave packets (PWP) by analogy with the Gaussian wave packets (GWP) known in the literature [12].

Variational principle. If a basis set of N vectors (9) is used, the wave function of the system is represented by a vector of length $3N$, whose components are nonlinear parameters

$$\{\gamma_j(t), a_j(t), b_j(t)\}, j = 1,\ldots N,$$

ordered as follows:

$$\mathbf{q} = \begin{bmatrix} \{\gamma_1(t)\gamma_2(t),\ldots,\gamma_N(t)\}, \\ \{a_1(t), a_2(t),\ldots,a_N(t)\}, \\ \{b_1(t), b_2(t),\ldots,b_N(t)\} \end{bmatrix}. \tag{10}$$

Thus, the time dependence of the PWP parameters determines the evolution of the atomic system. The equation for the components of the parameter vector is obtained by substituting expansion (7) into Eq. (1), followed by the application of the McLachlan TDVP [11].

As a result, the initial TDSE is transformed into a system of first-order ordinary differential equations (see, for example, [12]) with respect to the parameters

$$i\mathrm{M}\dot{\mathbf{q}} = \mathbf{v}. \tag{11}$$

Here M is a positive definite Hermitian matrix of size $3N \times 3N$, whose elements are determined by the formula

$$\mathrm{M}_{jj'} = \left\langle \frac{\partial \Psi}{\partial q_j} \middle| \frac{\partial \Psi}{\partial q_{j'}} \right\rangle, \tag{12}$$

where **v** is a complex vector of length $3N$ with the following elements:

$$v_j = \left\langle \frac{\partial \Psi}{\partial q_j} \middle| \hat{\mathcal{H}}\Psi \right\rangle. \tag{13}$$

The initial values of the parameters $q(0)$ are determined by diagonalization of Hamiltonian (3) for the hydrogen atom.

Exactly solvable case. Benchmark solutions are essential for validating the proposed numerical scheme. As such, we constructed the following auxiliary field [13]:

$$E(t) = F(t) + i\frac{s(t)}{r}, \tag{14}$$

where $F(t) = 0$ for $t \le 0$ and

$$s(t) = \int_0^t F(t')\,dt', \tag{15}$$

which allows for an exact solution in the form of a single PWP (9). Indeed, if we substitute expression (9) into Eq. (6), we obtain an equation of the form

$$i\frac{(\xi+\eta)}{4}\frac{\partial}{\partial t}g(t,\xi,\eta) = -\frac{1}{2}\left[\frac{\partial}{\partial \xi}\xi\frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta}\eta\frac{\partial}{\partial \eta} + 1 - \frac{F(t)}{4}\left(\xi^2 - \eta^2\right) - i\frac{s(t)}{2}\right]\times \\ \times g(t,\xi,\eta), \tag{16}$$

A system of equations with respect to the PWP parameters follows from Eq. (16):

$$\begin{aligned} a(t) + b(t) &= 1, \\ \frac{\partial}{\partial t}a(t) &= \frac{i}{2}F(t), \\ \frac{\partial}{\partial t}b(t) &= -\frac{i}{2}F(t), \\ \frac{\partial}{\partial t}\gamma(t) &= s(t) + 2ia^2(t) = -s(t) + 2ib^2(t). \end{aligned} \tag{17}$$

Finally, assuming for the ground state of the hydrogen atom

$$a(0) = b(0) = \frac{1}{2} \text{ and } \gamma(0) = \frac{1}{2}\ln 2,$$

we obtain the following system of equations:

$$\begin{aligned} a(t) &= \frac{1}{2}\left[1 + is(t)\right], \\ b(t) &= \frac{1}{2}\left[1 - is(t)\right], \\ \gamma(t) &= \frac{1}{2}\ln 2 + \frac{i}{2}\left[t - \int_0^t s^2(t')\,dt'\right]. \end{aligned} \tag{18}$$

We should note that the function $F(t)$ can be arbitrary, which means that perturbation theory may be inapplicable to such a pulse for arbitrary values of its carrier frequency and amplitude.

In the case of benchmark problem (14), (15) admitting the existence of a solution as a single PWP (see Eq. (9)), the (3×3)-matrix $\mathcal{M}$ (12) takes the following explicit form:

$$\mathrm{M} = \frac{e^{\omega}}{4u^2v^2}\begin{bmatrix} u+v & -\dfrac{u+2v}{u} & -\dfrac{2u+v}{v} \\ -\dfrac{u+2v}{u} & 2\dfrac{u+3v}{u^2} & 2\dfrac{u+v}{uv} \\ -\dfrac{2u+v}{v} & 2\dfrac{u+v}{uv} & 2\dfrac{3u+v}{v^2} \end{bmatrix}, \tag{19}$$

where $u = a + a^*$, $v = b + b^*$ and $\omega = \gamma + \gamma^*$ (the asterisk indicates the operation of complex conjugation).

In turn, expression (13) for the vector $\mathbf{v}$ also takes the simple form:

$$v = \frac{e^{\omega}}{2uv}\begin{bmatrix} -1 + a + b - \dfrac{2a^2 - is(t)}{2u} - \dfrac{2b^2 - is(t)}{2v} + \dfrac{E(t)}{2}\left(\dfrac{1}{u^2} - \dfrac{1}{v^2}\right) \\ \dfrac{1-a-b}{u} + \dfrac{2a^2 - is(t)}{u^2} + \dfrac{2b^2 + is(t)}{2uv} - \dfrac{E(t)}{2}\left(\dfrac{3}{u^3} - \dfrac{1}{uv^2}\right) \\ \dfrac{1-a-b}{v} + \dfrac{2a^2 - is(t)}{2uv} + \dfrac{2b^2 + is(t)}{v^2} - \dfrac{E(t)}{2}\left(\dfrac{1}{u^2v} - \dfrac{3}{v^3}\right) \end{bmatrix}. \tag{20}$$

Note, however, that matrix equation (11) cannot be reduced to system (17) by symbolic transformations, so to validate the approach based on Eqs. (11)–(13), we are left with the option of the numerical scheme from [13]. We validate our approach for the examples presented in the following sections.

Ionization amplitude. The solution of TDSE (1) can be used to obtain information about energy and angle distributions of photoelectrons produced by the laser pulse. In our case, the characteristic under study is the ionization amplitude, defined as follows.

The perturbation $\hat{U}(t)$ vanishes at $t > t_f$, so that the solution $\Psi(t)$ can be formally expanded in terms of eigenfunctions of the Hamiltonian $\hat{H}_{\mathrm{C}}$:

$$\Psi(t, \mathbf{r}) = \int d\mathbf{k} C(\mathbf{k}) \psi_k^-(\mathbf{r}) e^{-i\frac{k^2}{2M}(t - t_f)} + \psi_b(t - t_f, \mathbf{r}), \tag{21}$$

where ψ_k^- is the continuum state wave function of the atomic system, momentum-normalized to the δ-function; ψ_b denotes the contribution of all bound states of the atom.

The coefficients $C(\mathbf{k})$ in expression (21) determine the amplitude of the electron transition to the continuum state ψ_k^-, namely, the ionization amplitude.

As shown in [18], to extract the amplitude $C(\mathbf{k})$, it is sufficient to apply Green's function of the Coulomb system

$$\hat{G}_C^{(+)}(Z,M,k) \equiv \left[\frac{k^2}{2M} + i\varepsilon - \hat{H}_C\right]^{-1}$$

to the solution $\Psi(t)$ at the end of the pulse, i.e., at time $t = t_f$.

Indeed, it follows from the properties of Green's function for $r \to \infty$ [19] that the required amplitude appears in the asymptotic expression for $\hat{G}_C^{(-)}\Psi(t_f)$ as a coefficient for a divergent Coulomb wave:

$$\left\langle \mathbf{r} \left| \hat{G}_C^{(+)}(Z,M,k) \right| \Psi(t_f) \right\rangle \simeq -\sqrt{2\pi} C(k\hat{\mathbf{r}}) \frac{\exp\left\{ i\left[kr - \beta \ln(2kr) \right] \right\}}{r}, \tag{22}$$

where β is the Sommerfeld parameter, $\beta = ZM/k$.

On the other hand, we proved in [13] that

$$\left\langle \mathbf{r} \left| \hat{G}_C^{(+)}(Z,M,k) \right| \frac{g_j(t,\xi,\eta)}{\sqrt{2\pi}} \right\rangle \simeq -\sqrt{2\pi} C_j(k\hat{\mathbf{r}}) \frac{\exp\left\{ i\left[kr - \beta \ln(2kr) \right] \right\}}{r}, \tag{23}$$

where

$$\begin{aligned} C_j(\mathbf{k}) \equiv C_j^0(\mathbf{k}) = \frac{M}{\pi} \frac{\exp\{\gamma_j\}}{\left[4a_j b_j\right]^2} \Gamma(i\beta+1) e^{-\frac{\pi\beta}{2}} \frac{1}{c_j + s_j} \left(\frac{(1+p_j)(1+q_j)}{c_j + s_j} \right)^{i\beta} \times \\ \times \left\{ a_j + b_j + b_j \left(\frac{1-p_j}{1+p_j} \right) \left[1 + (1+i\beta) \frac{4\rho_j}{(1-p_j)^2} \frac{c_j}{c_j + s_j} \right] + \right. \\ \left. + a_j \left(\frac{1-q_j}{1+q_j} \right) \left[1 + (1+i\beta) \frac{4q_j}{(1-q_j)^2} \frac{s_j}{c_j + s_j} \right] \right\} \Bigg|_{t=t_f}. \end{aligned} \tag{24}$$

where

$$\begin{aligned} p = -ik/2a,\ q = -ik/2b, \\ c = (1-p)(1+q)\cos^2(\theta/2), \\ s = (1+p)(1-q)\sin^2(\theta/2), \end{aligned} \tag{25}$$

$$c_\nu^{(n,\lambda)} = (-1)^\nu \frac{(n+\lambda)!}{(n-\nu)!(\nu+\lambda)!\nu!}. \tag{26}$$

Thus, the ionization amplitude is represented as a sum

$$C(\mathbf{k}) = \sum_{j=1}^{N} C_j(\mathbf{k}). \tag{27}$$

In turn, the ionization probability (or the photoelectron spectrum) is then calculated by integrating the squared amplitude over all possible electron emission angles:

$$\frac{dP}{dE} = k \int \left| C(\mathbf{k}) \right|^2 d\Omega_{\mathbf{k}}. \tag{28}$$

Numerical implementation for the solution of the matrix equation

The solution of matrix equation (11) in this paper is obtained by an eighth-order Runge–Kutta scheme with a constant step depending on the size of the matrix. Differential system (11) is stiff, so the number of steps must be increased with increasing size of the basis. We believe that this is because experience shows that the exponents $a_j(t)$, $b_j(t)$ corresponding to different g_j (see expression (9)) can differ by several orders of magnitude. The difference in parameters increases rather quickly. Consequently, the equation matrix becomes singular at the first steps of the procedure even with small values of N ($N \approx 10$), and the solution process terminates prematurely.

We also achieved the required accuracy for the numerical stability of this procedure. This was possible with the help of an eight-order Dormand–Prince method consisting of 13 stages [14]. The chosen scheme also yields a solution for pulses with the duration of about 10 optical cycles. We analyzed the error of the numerical scheme, as well as the convergence of the method both with increasing basis set size and with increasing number of time steps (decreasing step size).

Results and discussion

Exactly solvable problems. The case when the strength of the external laser field is comparable to that of the intra-atomic field is of particular interest. Since perturbation theory turns out to be inapplicable, this situation serves as a convenient test for our numerical approach.

We considered two exactly solvable examples of the auxiliary field $E(t)$ (14), when the function $F(t)$ follows different expressions:

$$\text{I. } F_{\text{I}}(t) = \sin(t); \text{ II. } F_{\text{II}}(t) = [(1 + i)/2] \sin(t).$$

As follows from system of equations (18), the function $s(t)$ in Example I is real, so that

$$\text{Re}[(a(t)] = \text{Re}[(b(t)] = 1/2,$$

and thus the solution $g(t,\xi,\text{nn})$ remains normalized at each point in time. Preserving the unit norm is one of the standard requirements for solving the TDSE for the initially bound state of a quantum system.

The pulse amplitude in Example II is complex, which leads to unusual behavior of the real part of the parameter $a(t)$, which now vanishes at points $t_j = \pi(2j + 1)$. Therefore, the solution $g(t,\xi,\text{h})$ ceases to be normalized with respect to the variable ξ at these points in time. This deviation from the behavior typical for quantum systems can serve as an additional test of the stability of the numerical scheme based on Eq. (11).

The absolute deviations of the calculated parameters $\gamma(t)$, $a(t)$ and $b(t)$ from their exact values (18) are shown in Fig. 1. The calculations used different versions of the schemes, i.e., the fourth-order Runge–Kutta scheme and the Dormand–Prince scheme. It follows from the results in Fig. 1 that the accuracy of the calculations expectedly increases by 6–8 orders of magnitude with the Dormand–Prince scheme.

Our main finding is that the error remains stable over time, allowing our approach to be used with the Dormand–Prince scheme for long pulses. Finally, these results validate our approach for high-power laser radiation, i.e., under conditions where neither field (atomic nor external) can be treated within perturbation theory.

Ultraviolet radiation. The PWP approach was also validated for the case of a weak field where perturbation theory is applicable. In particular, we calculated the photoelectron spectrum for a hydrogen atom exposed to a laser pulse with the following shape [16, 17]:

$$E(t) = E_0 \sin[\omega(t - t_0)] \sin^2 \frac{\pi t}{T_f}, t_0 = \frac{T_f - \pi}{2}, 0 \le t \le T_f, \tag{29}$$

where $\omega = 1.71$; $T_f = 3.67$ or 25.72 for the cases of one or seven optical cycles, respectively.

The amplitude E_0 of the field linearly polarized along the z axis was assumed to be 0.05 (small compared to the intra-atomic field strength).

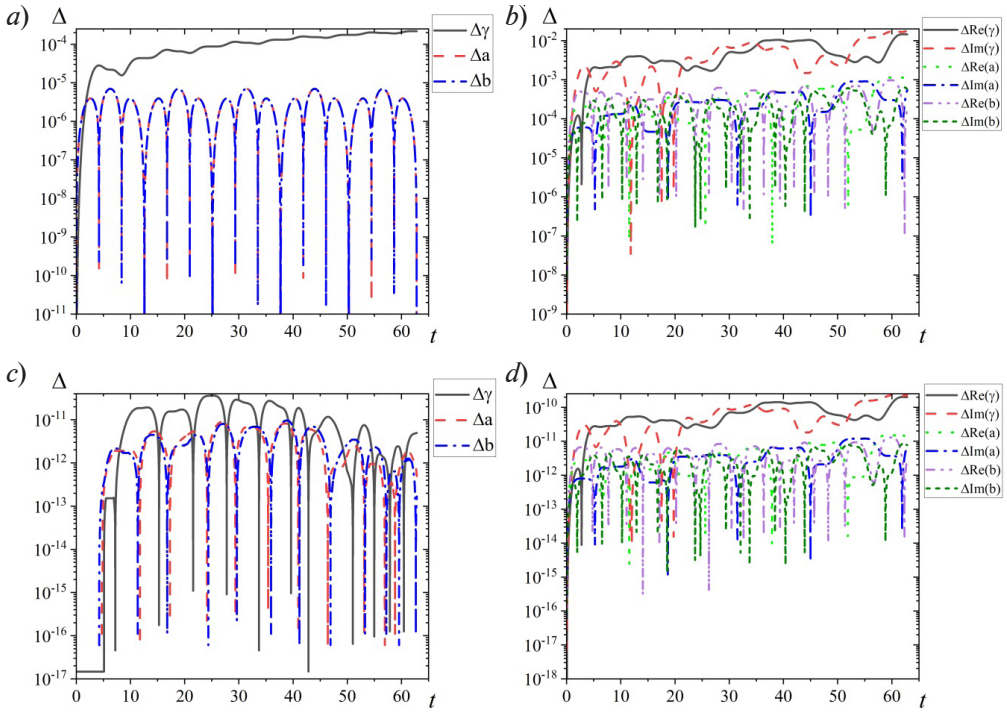

Fig. 1. Time evolutions of absolute deviations Δ of parameters γ, *a*, and *b* (solutions of system (12) taking into account (19) and (20)) from their exact values (18): fourth-order Runge–Kutta (*a*, *c*) and Dormand–Prince (*b*, *d*) schemes were used The corresponding PWP (9) satisfies Eq. (16) with pulse (14), (15), where the function $F(t)$ follows the expressions $F_{\mathrm{I}}(t)$ (*a*, *b*) and $F_{\mathrm{II}}(t)$ (*c*, *d*)

The calculation results for the ionization probability are shown in Fig. 2, *a* and *b*, respectively, for pulse durations of one or seven optical cycles (the data obtained by us are also compared with the results from [16, 17]).

A basis set of PWP (8) of size $N = 54$ was used for a single-cycle pulse whose shape is represented by expression (29). We also analyzed the dependence of the ionization probability on the time step h, which was varied in the range of $7.34\cdot(10^{-5}–10^{-6})$.

As follows from Fig. 2,*a*, convergence of ionization probability density is achieved fairly quickly: the corresponding curves become indistinguishable starting from $h = 7.34\cdot10^{-5}$. The calculation results obtained in [16] are also shown for comparison in Fig. 2,*a*. The ionization probability density for a 7-cycle pulse compared with the results from [17] is also shown in Fig. 2,*b*. The convergence properties were analyzed in this case using basis sets of size $N = 54$ and 78. Taking into account the increase in pulse duration, the initial time step was also increased to $h = 1.29\cdot10^{-4}$. The time step h was decreased to $2.57\cdot10^{-5}$. As seen from Fig. 2,*b*, convergence occurs already at $h = 1.29\cdot10^{-4}$. A similar pattern is observed with an increase in the number of PWP used, which reached 78 in our calculations.

Finally, we considered the case when a hydrogen atom is exposed to a 9-cycle pulse [15]:

$$E(t) = f(t)\, E_0 \sin(\omega t) \tag{30}$$

with a fairly common shape of the envelope $f(t)$:

$$f(t) = \begin{cases} \sin^2\left(\dfrac{\pi t}{2n_1 T}\right), & 0 \le t \le n_1 T, \\ 1, & n_1 T \le t \le (n_1 + n_2)T, \\ \sin^2\left(\dfrac{\pi t}{2n_3 T}\right), & (n_1 + n_2)T \le t \le t_f. \end{cases} \tag{31}$$

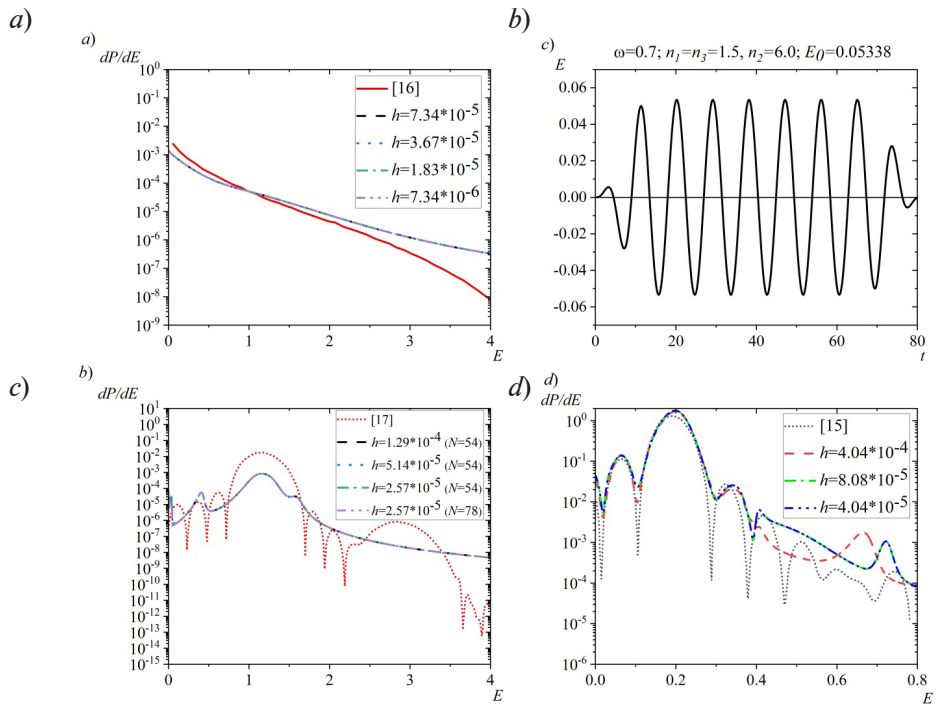

Fig. 2. Probability density for ionization (28) of hydrogen atoms exposed to XUV pulses (29) (*a*, *b*) and (30) with envelope (31) (*d*); the data were obtained using the Dormand–Prince scheme for different time steps:
for single-cycle ($T_f = 3.67$) (*a*), 7-cycle ($T_f = 25.72$) (*b*) pulses; shape of 9-cycle pulse with the corresponding parameters (*c*), probability density obtained for this (c) pulse (*d*). The corresponding results from [16] (*a*), [17] (*b*) and [15] (*d*) are presented for comparison

where T is the period of one cycle of the central frequency, $T = 2\pi/\omega$; n_1, n_2, n_3 are the shape parameters that set the number of cycles corresponding to the phases of ramp-on, plateau and ramp-off of the pulse, respectively.

As a result, the quantity $t_f = (n_1 + n_2 + n_3)T$ determines the total duration of the pulse. We used the characteristic values of the parameters [15]: $n_1 = n_3 = 1.5$; $n_2 = 6.0$. The amplitude and frequency of the pulse are also taken from [15]: $\omega = 0.7$; $E_0 = 0.05338$. The shape of the pulse is shown in Fig. 2, *c*.

In this case, we also used 54 PWP (see Eq. (8)). It follows from the results obtained for the ionization probability (Fig. 2,*d*) that convergence is achieved with a time step $h = 8.08 \cdot 10^{-5}$; note that further reduction of the step size produces a negligible effect.

Our results for all cases considered in this section are generally consistent with the corresponding results obtained by other authors.

Analysis of discrepancies with the results in the literature. The clear discrepancies observed require further analysis of their possible origin. Firstly, full agreement with the results in [11] was reached in the cases we previously calculated for ultrashort half-cycle pulses [13]. Thus, it is natural to assume that the discrepancies observed for pulses of longer duration (a higher number of cycles) are explained by a loss of accuracy with a corresponding increase in the number of time steps. To eliminate this possible cause, we used the Dormand–Prince scheme, providing higher accuracy (by 6–8 orders of magnitude) than the fourth-order Runge–Kutta method (see Fig. 1); we used the latter in [13].

The second possible reason is an inappropriate choice of time step. To account for this, our calculations included a convergence study with a decreasing time step, similar to the one conducted in [13]. Recall that the good agreement of our calculations with the results in [10] for a 4-cycle pulse, achieved at a step of 0.0001 a.u., deteriorates as the step decreases. Note that time-step convergence was achieved in our calculations (both in the previous paper [13] and in this work). On the other hand, we have not encountered such analysis in the literature mentioned above.

Finally, the representation of the angular part of the solution deserves separate discussion. Notably, if spherical coordinates are used, a large number of partial waves (ranging from 15 to 60) is typically required to describe the solution. In other words, the angular dependence has the form of polynomials including functions $\sin\theta$ and $\cos\theta$ of rather high degree. As follows from Eqs. (24) and (25) for the ionization amplitude, the dependence of this amplitude on the angle θ in our representation is a rational function, and it cannot always be approximated even by the number of Legendre polynomials typically used in calculations with spherical coordinates. Thus, in the general case, it is impossible to compare our method with standard approaches.

Conclusion

This paper aimed to extend the PWP method developed in [13] to make it applicable to pulses of about 10 optical cycles in duration. This was possible with the help of an eighth-order Dormand–Prince method consisting of 13 stages [14]. The developed numerical scheme was tested for a model pulse allowing for an exact solution as a single PWP. Notably, selecting the values of the pulse parameters makes it possible to obtain solutions that become non-normalizable at certain times, which falls outside standard boundary conditions and can serve as an additional test of the numerical scheme's robustness.

We also performed calculations of photoelectron spectra for weak fields considered by other authors. In particular, the results were obtained for pulses with a duration of 1 [16], 7 [16, 17] and 9 [15] optical cycles.

Despite the general agreement of our calculations with the results of [15–17], there are significant differences. For example, the photoionization spectrum calculated by other authors shows oscillations with increasing electron energy. In our case, the spectrum only contains several peaks, after which it decreases monotonically. We believe that there are two main reasons for this difference. Firstly, the angular part of the solution is described by radically different means in our PWP approach and in standard methods using spherical coordinates. The PWP amplitude uses rational expressions containing the functions $\sin\theta$ and $\cos\theta$, whereas the standard methods use the expansion of the amplitude in terms of Legendre polynomials.

Therefore, it is difficult to compare these two approaches, for example, because the expansion of the PWP amplitude may require an exceedingly large number of Legendre polynomials. Furthermore, our calculations include a convergence study for the results with a significantly decreased time step. Unfortunately, such a study is not available in [15–17], so it is not yet possible to compare methods at this level.

In the future, we plan an in-depth comparison of the methods, considering various aspects of standard approaches.

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Received 09.04.2025. Approved after reviewing 27.05.2025. Accepted 27.05.2025.
Статья поступила в редакцию 09.04.2025. Одобрена после рецензирования 27.05.2025. Принята 27.05.2025.