A hydrogen atom in strong elliptically polarized laser fields within discrete variable representation

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Abstract
The nondirect product discrete variable representation (npDVR) is developed for the time-dependent Schrödinger equation with nonseparable angular variables and is applied to a hydrogen atom in elliptically polarized strong laser fields. The 2D npDVR is constructed on spherical harmonics orthogonalized on the 2D angular grids of the Popov and Lebedev 2D cubatures for the unit sphere. With this approach we have investigated the dynamics of a hydrogen atom initially in its ground state in elliptically polarized laser fields with the intensity up to \(I = 10^{14}\) W cm\(^{-2}\) and a wavelength of \(\lambda = 800\) nm. For these parameters of the laser field and the entire range of ellipticity variation, we have calculated the total excitation and ionization yields of the atom. The performed analysis of the method convergence shows that the achieved accuracy of our calculations significantly exceeds the accuracy of recent works of other authors relevant to the problem, due to the high efficiency of the 2D npDVR in approximating the angular part of the 3D time-dependent Schrödinger equation. We also propose a new simple procedure for infinite summation of the transition probabilities to the bound states of the hydrogen atom when calculating the total excitation yield and prove its accuracy by comparison with conventional methods. The obtained results show the potential prospects of the 2D npDVR for investigating atomic dynamics in stronger laser fields.

Keywords: Schrödinger equation, strong laser field, elliptically polarized laser, discrete variable representation, Lebedev quadrature, nondirect product grid

(Some figures may appear in colour only in the online journal)

1. Introduction

In the past, great progress has been made in the development of high-power laser technology, and many laser-driven non-linear processes have been discovered and investigated, such as high harmonic generation (HHG) [1, 2], above threshold ionization (ATI) [3, 4] and laser-induced tunneling [5, 6] (see, for example, [7–9] and references therein). An adequate quantitative description of all these processes required the development of special methods that take into account the features of quantum dynamics of an electron in a combined Coulomb and time-dependent laser field. Thus, the electron motion should be described in a very extended space and during long time-scales [10]. The polarization of the laser field here plays the role of an additional control parameter, but it also complicates the problem. While the problem of a hydrogen atom in a linearly polarized laser field is two-dimensional (2D) due to cylindrical symmetry and a large set of efficient methods has been developed to solve the corresponding 2D Schrödinger

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equation, in an elliptically polarized field the problem becomes three-dimensional (3D) and requires special consideration.

Different aspects of strong laser–atom interactions induced by elliptically polarized laser fields were investigated using the semi-analytical models [11–14] and numerical simulations of the corresponding 3D time-dependent Schrödinger equation (3D TDSE) [15–18]. Thus, the HHG of a hydrogen atom in an elliptically polarized laser field was achieved in the best recent calculations of other authors [16, 17]. We also suggest a novel approach to infinite summation over the bound states of a hydrogen atom when calculating the total excitation probability and prove its accuracy by comparing with conventional methods for linearly polarized laser fields. The demonstrated efficiency of our method for these problems makes it promising in stronger fields for solving the corresponding 3D TDSE with the nonseparable angular part.

In the next section, our approaches to numerical integration of the 3D TDSE with the 2D Gaussian DVR and 2D Popov and Lebedev npDVRs are presented. We also describe the formulas for calculating the ionization yield and the procedure for approximating infinite summation over the states of the discrete spectrum of the hydrogen atom when calculating the total excitation probability. In section 3, the results of calculations and discussions are presented. The concluding remarks are given in the last section.

2. Theoretical method

2.1. Time-dependent Schrödinger equation in 2D DVR

To study the dynamics of a hydrogen atom in an arbitrarily polarized laser field, we need to solve the corresponding TDSE (the atomic units \( m = e = \hbar = 1 \) are used throughout the text unless stated otherwise),

\[
i \frac{\partial}{\partial t} \psi(r, t) = [H_0 + V(r, t)] \psi(r, t)
\]

with the Hamiltonian \( H_0 = -\frac{i}{2} \Delta - \frac{1}{2} \) of the hydrogen atom in free space. We describe the interaction of the atomic electron with the laser field

\[
E(t) = \frac{f(t)}{\sqrt{1 + \varepsilon^2}} E_0 (\hat{x} \cos \omega t + \hat{y} \sin \omega t)
\]

in the length gauge under the dipole approximation

\[
V(r, t) = -r \cdot E(t),
\]

where \( E_0, 0 \leq \varepsilon \leq 1 \) and \( \omega \) are the electric field amplitude, ellipticity and frequency of the laser field, respectively. The pulse envelope function is considered as

\[
f(t) = \cos^2 \left( \frac{\pi t}{n_T T} \right), \quad -n_T T/2 < t < n_T T/2,
\]

where \( n_T \) optical cycles of the period \( T = 2\pi/\omega \) are included during the pulse.
To solve the TDSE, we follow the 2D DVR method [19, 20, 36, 37], where the electron wavefunction $\psi(r, \Omega)$ in the spherical coordinates $(r, \Omega) = (r, \theta, \phi)$ is expanded as

$$ \psi(r, \Omega) = \frac{1}{r} \sum_{\mu=1}^{N_\Omega} f_j(\Omega) u_j(r,t) $$

over the basis $f_j(\Omega)$ associated with a 2D angular grid $\Omega_j (j = 1, 2, \ldots, N_\Omega)$ on the unit sphere $\Omega$. In the works of Melezhik on 2D DVR in application to the TDSE, the angular grids $\Omega_j = (\theta_j, \phi_j)$ were constructed as direct products of the nodes $\theta_j, \phi_j$ of the 1D Gaussian quadratures over the $\theta$ and $\phi$ variables, respectively, where $j = 1, \ldots, N_\theta, j_\phi = 1, \ldots, N_\phi$ and $N_\Omega = N_\theta \times N_\phi$. [19, 20, 36]. This construction turned out to be very efficient in integration of the TDSE with three [19, 36, 38] and four [39–41] spatial variables. Particularly, with this approach, the polarization of the high harmonics generated by hydrogen atoms was successfully investigated in elliptically polarized laser fields [19]. Recently [24], we have improved the computational scheme for the 3D stationary Schrödinger equation by implementing the 2D Popov and Lebedev non-direct product DVRs on the unit sphere $\Omega_j = (\theta_j, \phi_j)$ instead of the Gaussian 2D DVR. When integrating the stationary 3D Schrödinger equation for the hydrogen atom in a crossed magnetic and electric fields, it was shown that the use of the 2D npDVR essentially accelerated the convergence of the computational scheme over $N_\Omega$ with respect to the 2D DVR scheme based on the Gaussian 1D quadratures with $N_\Omega = N_\theta \times N_\phi$. This result motivated us to extend the 2D npDVR based on the Popov and Lebedev curatures to the TDSE (1) for the hydrogen atom in a strong elliptically polarized laser field, where convergence of the computational scheme becomes crucial due to the complexity of the problem to be solved.

When angular grid points $\Omega_j = (\theta_j, \phi_j)$ are chosen as nodes of 1D Gaussian quadratures over the $\theta$ and $\phi$ variables, the basis functions $f_j(\Omega)$ are defined as

$$ f_j(\Omega) = \sum_{\mu=1}^{N_\Omega} Y_{\nu}(\Omega) |Y^{-1}|_{\nu j}. $$

Here, the index $\nu$ numerates the pair $\{l, m\}$ $m = -(N_\phi - 1)/2, \ldots, + (N_\phi - 1)/2$ and $l = |m|, \ldots, |m| + N_\theta - 1$ related to the modified spherical harmonic

$$ Y_{\nu}(\Omega) = Y_{lm}(\Omega) = e^{i\nu\phi} \sum_{l'} c_{l'}^{l} P_{l'}^{\nu}(\theta), $$

where $P_{l'}^{\nu}(\theta)$ are the associated Legendre polynomials. For the majority of $l$ and $l'$ from a given above set, except the largest $l$ and $l'$, $c_{l'}^{l} = \delta_{ll'}$ and $Y_{lm}(\Omega)$ coincide with the spherical harmonics. The non-zero $c_{l'}^{l}$ for the largest $l$ and $l'$ are found using the Gram–Schmidt orthogonalization procedure for $Y_{lm}(\Omega)$ on the grid $\Omega_j$ [42]. The matrix $Y^{-1}$ is inverse to the $N_\Omega \times N_\Omega$ matrix $Y_{\mu l} = \sqrt{w_l} Y_{l}(\Omega_j)$, where $w_l = (2\pi w_l')/N_\phi$ and $w_l'$ are the weights of the Gaussian quadrature over the $\theta$ variable.

On the other hand, if the Popov or Lebedev curature is used to generate the angular grid points $\Omega_j = (\theta_j, \phi_j)$ with $j = 1, \ldots, N_\Omega$, then $f_j(\Omega)$ is defined as

$$ f_j(\Omega) = \sum_{\nu=1}^{N_\Omega} \sqrt{4\pi w_l} \Phi_{\nu}(\Omega) \Phi_{\nu}^{*}(\Omega_j), $$

where $w_l$ is the Popov or Lebedev weight ($\sum_{\nu=1}^{N_\Omega} w_l = 1.0$) for Popov and Popov grid points and weights see [43] and [25–27], respectively. The function $\Phi_{\nu}(\Omega)$ is a special linear combination of the spherical harmonics, $\Phi_{\nu}(\Omega) = \sum_{\mu} S_{\nu \mu} Y_{\nu}(\Omega)$, obtained within the method described in our previous work [24]. Here, $S$ refers to a $N_\Omega \times N_\Omega$ matrix (with $\mu = 1, \ldots, N_\Omega \geq N_\Omega$), which makes the set of $N_\Omega$ basis functions $\Phi_{\nu}(\Omega)$ orthonormal over the grid points $\Omega_j$ in the sense of the Popov or Lebedev curatures.

Thus, the problem is reduced to a system of Schrödinger-type equations which should be solved for the unknown $N_\Omega$-dimensional vector $u(r,t) = \{\sqrt{w_l}u_l(r)\}_{l=1}^{N_\Omega}$

$$ \frac{\partial}{\partial t} u(r,t) = \left[H_0(r) + V(r,t)\right] u(r,t), $$

where the elements of the $N_\Omega \times N_\Omega$ matrices $H_0(r)$ and $V(r,t)$ are represented as

$$ H_{0ij}(r) = -\frac{1}{2} \left( \delta_{ij} \frac{d^2}{dr^2} - \frac{L_{ij}^2}{r^2} \right) - \frac{1}{r} \delta_{ij}, $$

$$ V_{ij}(r,t) = V(r,\Omega_j, t) \delta_{ij}. $$

In the Gaussian case, the elements of the $L^2$ matrix are defined as

$$ L_{ij}^2 = \sum_{\nu=1}^{N_\Omega} \sqrt{w_l} w_l' Y_{\nu}(\Omega_j) l(l+1) \bar{Y}_{\nu}^{*}(\Omega_{j'}). $$

whereas in the Popov and Lebedev cases, they are written as

$$ L_{ij}^2 = 4\pi \sum_{\nu=1}^{N_\Omega} \sqrt{w_l} w_l' \sum_{\mu=1}^{N_\Omega} S_{\nu \mu} Y_{\nu}(\Omega_j) \bar{Y}_{\nu}^{*}(\Omega_{j'}), $$

with $N_\Omega \geq N_\Omega$ and $\mu = \{l_\mu, m_\mu\}$ defined in [24].

To propagate the wavefunction in time $t_n \rightarrow t_{n+1} = t_n + \Delta t$, the component-by-component split-operator method [44] is applied as

$$ u(r, t_n + \Delta t) = \exp \left[-\frac{i}{2} \Delta t V(r, t_n) \right] \exp[-i\Delta t H_0(r)] \times \exp \left[-\frac{i}{2} \Delta t V(r, t_n) \right] u(r, t_n). $$

Since the interaction potential $V(r, t)$ is diagonal in our 2D DVRs over both angular grid distributions (either Gaussian...
\( \Omega_j = (\theta_j, \phi_j) \) or Popov (Lebedev) \( \Omega_j = (\theta_j, \phi_j) \), the first and last steps of the procedure (14) represent simple multiplications of the vectors \( \exp[-(i/2)\Delta t\hat{A}(r, \Omega_j, t)] \) and \( u(r, t) \) which results in \( u(r, t + \frac{1}{2}\Delta t) \). The intermediate step is performed after diagonalizing the nondiagonal part (\( \hat{L}^2 \) operator), which transforms \( \hat{H}_0 \) to a diagonal matrix \( \hat{A} \). Then we can approximate its related exponential expression according to
\[
\exp[-i\Delta t\hat{A}] \approx \left(1 + \frac{i}{2}\Delta t\hat{A}\right)^{-1} \left(1 - \frac{i}{2}\Delta t\hat{A}\right) \tag{15}
\]
which ensures the desired accuracy of the numerical algorithm (14).

Thus, we reach the following initial value problem for the intermediate step:
\[
\left(1 + \frac{i}{2}\Delta t\hat{A}\right) u(t_0 + \frac{3}{4}\Delta t) = \left(1 - \frac{i}{2}\Delta t\hat{A}\right) u(t_0 + \frac{1}{4}\Delta t), \tag{16}
\]
\[
u = 0, t_0 + \frac{3}{4}\Delta t = u(r = r_m, t_0 + \frac{3}{4}\Delta t) = 0, r_m \to \infty. \tag{17}
\]
Here, the transformed wavefunction \( \tilde{u} \) and operator \( \tilde{A} \) are defined based on the transformation method, which is used to diagonalize the \( \hat{L}^2 \) operator. When using Gaussian grid points, we apply a simple unitary transformation \( M_{\nu\nu'} = \sqrt{w_{\nu}}Y_{\nu}(\Omega_j) \) [20, 36], then
\[
\tilde{u} = \tilde{M}u, \tag{18}
\]
\[
\tilde{A}_{\nu\nu'} = \left(M\hat{H}_0\tilde{M}^\dagger\right)_{\nu\nu'} = \left[\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{1}{r}\right] \delta_{\nu\nu'}, \tag{19}
\]
with \( \nu = \{l, m\} \).

In the Popov and Lebedev cases, we use the conventional numerical diagonalization method. We find the eigenvectors and eigenvalues of the \( \hat{L}^2 \) matrix in these representations. Then, the transformation matrix \( W \) is constructed from the numerically calculated eigenvectors, which are stored on its columns so that \( W^{-1}\hat{L}^2W = J \), where \( J \) is the diagonal matrix of the acquired eigenvalues \( J_{\nu} \). Thus, \( \tilde{u} \) and \( \tilde{A} \) are represented as
\[
\tilde{u} = W^{-1}u, \tag{20}
\]
\[
\tilde{A}_{\nu\nu'} = \left(W^{-1}\hat{H}_0W\right)_{\nu\nu'} = \left[\frac{1}{2}\frac{d^2}{dr^2} + \frac{J_{\nu}}{r^2} - \frac{1}{r}\right] \delta_{\nu\nu'}, \tag{21}
\]
with \( \nu = 1, 2, \ldots, N_\Omega \).

Finally, before applying the last operation in (14), \( \tilde{u} \) should be transformed to \( u \) through the operation \( u = \tilde{M}^\dagger\tilde{u} (u = \tilde{W}u) \) while using Gaussian (Popov or Lebedev) quadratures (cubatures).

It should be emphasized that both transformation matrices (either \( M \) or \( \tilde{W} \)) are independent of \( r \) and \( t \).

To approximate the Schrödinger equation (9) over the radial variable \( r \) the six-order finite-difference approximation is used on a quasi-uniform grid \( \{r_j\}^N_r \) on the interval \( r \in [0, r_m] \) constructed by mapping the \( r \) variable to \( x \in [0, 1] \) with the formula \( r = r_m[\exp(4x) - 1]/[\exp(4) - 1] \). To avoid the artificial reflection of the electron at the radial grid boundary, the wave function is multiplied after each time step by the absorbing ‘mask function’ suggested in [45]. The total number of operations at each time step (14) in our algorithm is \( N_r(2N^2_\Omega + \alpha N_{\Omega}) \), where \( \alpha = (2 \times 7)^2 \simeq 200 \) is given by the width of the band of the band matrices \( A \) in (19) and (21) with the finite-difference approximation of the radial derivatives with respect to the variable \( r \). Here, we have an obvious advantage with respect to the Tong computational scheme [16] for numerical integration of the Schrödinger equation (1), where the number of operations at each time step is \( N_rN_\Omega N_g(N_r + N_\Omega + N_g) \), i.e. quadratically dependent on the number of radial grid points \( N_r \). The computational time of our scheme linearly depends on \( N_r \) and \( \sim N^2_\Omega \) with \( 1 \leq \gamma < 2 \) approaching 1 for not very big \( N_\Omega \) [20]. Linear dependence of the computational time on \( N_r \) permits computations on the radial grids up to \( r_m = 1000 \) and \( \Delta r = 1/N_r = 0.00025 \). The time step of integration is chosen to be \( \Delta t = 0.05 \) (1/2200 of one optical cycle).

Once the wavefunction \( \psi(r, t) \) is calculated, one can investigate the physical properties of the atom in the laser field, such as photoelectron momentum spectra, photoexcitation or HHG. Here, we focus on the ionization and excitation probabilities.

2.2. Ionization and excitation

We calculate the transition probabilities in the hydrogen atom due to interaction with a laser pulse by projecting the electron wave packet at the end of the pulse \( \psi(r, t = nT) \) on the bound
\[
P_{nlm} = |\langle \phi_{nlm} | \psi \rangle|^2 = |d_{nlm}|^2 \tag{22}
\]
and continuum
\[
\frac{dP_{lm}}{dE} = |\langle \phi_{klm} | \psi \rangle|^2 = |e_{klm}|^2 \tag{23}
\]
states of the atomic spectrum in free space. The hydrogen eigenfunctions in the above formulas (22) and (23) of the bound
\[
\phi_{nlm}(r) = R_{nl}(r)Y_{lm}(\Omega) \tag{24}
\]
and continuum
\[
\phi_{klm}(r) = \sqrt{\frac{2}{\pi k}} \frac{F_{l}(\eta, kr)}{r} Y_{lm}(\Omega) \tag{25}
\]
spectrum form an orthonormal and complete basis set, which can be used for expansion of the electron wave packet \( \psi(r, t) \) after interaction with the laser pulse.
\[ \psi(r, t = nT) = \sum_{nlm} d_{nlm} \phi_{nlm}(r) + \sum_{lm} \int_0^{+\infty} c_{klm} \phi_{klm}(r) \, dE, \]

(26)

where \( E \) denotes the photoelectron energy, \( k = \sqrt{2E} \), \( \eta = -1/k \) and \( F(\eta, kr) \) is the Coulomb wave function regular as \( kr \to 0 \).

Thus, the population of the \( n \)th bound state and the ATI spectrum of the hydrogen atom after interaction with the laser pulse are described as

\[ P_n = \sum_{l=0}^{n-1} \sum_{m=-l}^{l} P_{nlm}, \]

(27)

and

\[ \frac{dP}{dE}(E) = \sum_{l=0}^{n_c} \sum_{m=-l}^{l} \frac{dp_{nlm}}{dE}(E). \]

(28)

Together with the above equations we also use the relation between the population probabilities

\[ \sum_{n=1}^{\infty} P_n + \int_0^{+\infty} \frac{dP}{dE} \, dE = \langle \psi|\psi \rangle \approx 1. \]

(29)

Due to the action of the absorbing ‘mask function’ at the edge of radial integration \( r_{ex} \), in our computation we have to take into account the effect that the normalization integral \( \sum_{j=1}^{\infty} \langle \psi|\psi \rangle \) decreases in time and deviates from the unit. Then, the total ionization yield is obtained by

\[ P_{ion} = \int_0^{+\infty} \frac{dP}{dE} \, dE + (1 - \langle \psi|\psi \rangle), \]

(30)

and \( \sum_{n=1}^{\infty} P_n = P_g + P_{ex} \), where \( P_g \) and \( P_{ex} \) denote the ground state population and total excitation probability, respectively.

To circumvent the seemingly intractable problem of calculating the populations \( P_n \) as \( n \to +\infty \), we propose an alternate method which does not require numerical analysis for very large \( n, l, m \) values. It is based on the known property of the Coulomb wave functions \( \phi_{nlm}(r) \) (24) and \( \phi_{klm}(r) \) (25): the functions \( n^{3/2} \phi_{nlm}(r) \) and \( \phi_{klm}(r) \) transform one to another as \( n \to +\infty \) and \( k \to 0 \) with the replacement \( n \leftrightarrow 1/(ik) \) [46, 47].

In this method, we stop calculating \( P_n \) at some rather large \( n = N' \)

\[ P_{ex} = \sum_{n=2}^{\infty} P_n = \sum_{n=2}^{N'} P_n + \sum_{n=N'+1}^{\infty} P_n, \]

(31)

and evaluate the remaining sum \( \sum_{n=N'+1}^{\infty} P_n \) in the above summation according to

\[ \sum_{n=N'+1}^{\infty} P_n \approx \int_{N'+1}^{+\infty} P_n \, dn = \int_{N'+1}^{+\infty} n^3 P_n \, d(\frac{1}{2n^2}) = \int_0^{E_f} \frac{dP}{dE}(E < 0) \, dE, \]

(32)

where \( E' = -\frac{1}{2N^2 + \eta^2} \), and \( n^3 P_n = \frac{dP}{dE}(E < 0) \). It is well known [48, 49] (see also [17]) that in the limit \( n \to +\infty \) the oscillator strength density \( \frac{dP}{dE}(E < 0) \) approaches the value \( \frac{dP}{dE}(0) \), coinciding with the limit \( \frac{dP}{dE}(+0) \) of the population of the states of the continuum spectrum at \( k \to 0(E \to +0) \).

Thus, by calculating \( \frac{dP}{dE}(E > 0) \) from equation (28) at some positive small values of \( E (E \to +0) \), where small \( l, m \) give a principal contribution, we can find a trend curve \( f(E) = \frac{dP}{dE}(0) + AE + BE^2 + \ldots \) passing through these points and the points \( n^3 P_n = \frac{dP}{dE}(E < 0) \) calculated on the negative side of \( E \) which belong to the \( n = N' \), \( N' - 1 \), \ldots, states. With the calculated \( f(E) \) we perform infinite summation in (32)

\[ \sum_{n=N'+1}^{\infty} P_n = \sum_{n=N'+1}^{\infty} \frac{f(E_n)}{n^3} + \int_{E_f}^{0} f(E) \, dE \]

(33)

where \( E_1 = E_{nlm+1} \) and \( n_m \) is chosen to be as large as 30 after which the difference between summation over \( n \) and integration over \( E \) becomes negligible. Finally, we can obtain \( P_{ex} \) using equation (31) and then the total ionization yield from

\[ P_{ion} = 1 - P_g - P_{ex}. \]

3. Results and discussion

Based on the computational schemes presented above, we investigate the dynamics of the hydrogen atom in an elliptically polarized laser field for different ellipticities \( 0 \leq \varepsilon \leq 1 \) with the laser intensity of \( I = 10^{14} \) W cm\(^{-2} \) and a wavelength of \( \lambda = 800 \) nm for the laser pulse duration of 20 fs (= 7.5 \times T).

3.1. Linearly polarized laser field

First, we consider a hydrogen atom in a laser field of linear polarization (\( \varepsilon = 0 \)). This permits the separation of the azimuthal angle \( \phi \) if the electric field is oriented along the z-axis and the 2D DVR basis constructed with the Gaussian scheme (6) reduces to the 1D DVR over \( \theta \) variable with \( N_{\Omega} = N_0 (l = 0, 1, \ldots, N_3 - 1, \) and \( m = 0) \). Such simplification of the problem gives us the possibility to get the most accurate result and use it as a test for the convergence of the 2D npDVRs constructed with the Popov and Lebedev cubatures where the separation of angular variables are not allowed, regardless of the chosen orientation of the electric field in space. In table 1, we demonstrate the convergence of the scheme based on the Gaussian 1D DVR with respect to the number of the basis function \( N_{\Omega} \) when calculating the populations \( P_n \) of the ground (\( n = 1 \)) and excited states up to \( n = 10 \). It is shown that including \( N_{\Omega} = 35 \) basis functions in the 1D DVR Gaussian scheme (where \( l \leq 34 \) and \( m = 0) \) fixes four significant digits after the decimal point in \( P_1 \) and gives the relative accuracy \( \sim 9% \) when calculating \( P_n \) for \( 2 \leq n \leq 10 \).

When increasing the number of basis functions to \( N_{\Omega} = 95 \) \( (l \leq 94, m = 0) \), eight significant digits are fixed in \( P_1 \), and the relative accuracy reaches the value \( \sim 0.5% \) in \( P_n \) for \( 2 \leq n \leq 10 \).

The distribution of the populations \( P_n \) over the angular momentum \( l \) is presented in figure 1. Here, the most probable angular momentum states are observed with \( l \leq 5 \).
Table 1. The transition probabilities $P_n$ to the bound states $n$ of the hydrogen atom calculated with the 1D DVR Gaussian scheme in the case of atomic interaction with the linearly polarized laser field along the $z$-axis. Here, $N_{\Omega} = N_{\Omega}$, and the contributing $l$ values in the basis functions are $l = 0, 1, \ldots, N_{\Omega} - 1$ ($m = 0$).

| $N_{\Omega}$ | 35     | 50     | 65     | 80     | 95     |
|-------------|--------|--------|--------|--------|--------|
| $n = 1$     | 0.9846 932 77 | 0.9846 771 92 | 0.9846 782 62 | 0.9846 782 90 | 0.9846 782 89 |
| $n = 2$     | $8.16 \times 10^{-5}$ | $7.89 \times 10^{-5}$ | $7.87 \times 10^{-5}$ | $7.87 \times 10^{-5}$ | $7.87 \times 10^{-5}$ |
| $n = 3$     | $8.83 \times 10^{-4}$ | $8.74 \times 10^{-4}$ | $8.69 \times 10^{-4}$ | $8.69 \times 10^{-4}$ | $8.69 \times 10^{-4}$ |
| $n = 4$     | $2.02 \times 10^{-4}$ | $2.20 \times 10^{-4}$ | $2.19 \times 10^{-4}$ | $2.19 \times 10^{-4}$ | $2.19 \times 10^{-4}$ |
| $n = 5$     | $1.23 \times 10^{-3}$ | $1.24 \times 10^{-3}$ | $1.24 \times 10^{-3}$ | $1.24 \times 10^{-3}$ | $1.24 \times 10^{-3}$ |
| $n = 6$     | $2.46 \times 10^{-4}$ | $2.34 \times 10^{-4}$ | $2.30 \times 10^{-4}$ | $2.31 \times 10^{-4}$ | $2.31 \times 10^{-4}$ |
| $n = 7$     | $1.27 \times 10^{-4}$ | $1.08 \times 10^{-4}$ | $1.18 \times 10^{-4}$ | $1.17 \times 10^{-4}$ | $1.17 \times 10^{-4}$ |
| $n = 8$     | $8.15 \times 10^{-5}$ | $7.14 \times 10^{-5}$ | $7.48 \times 10^{-5}$ | $7.37 \times 10^{-5}$ | $7.41 \times 10^{-5}$ |
| $n = 9$     | $5.45 \times 10^{-5}$ | $4.95 \times 10^{-5}$ | $4.95 \times 10^{-5}$ | $4.94 \times 10^{-5}$ | $4.94 \times 10^{-5}$ |
| $n = 10$    | $3.79 \times 10^{-5}$ | $3.54 \times 10^{-5}$ | $3.44 \times 10^{-5}$ | $3.46 \times 10^{-5}$ | $3.46 \times 10^{-5}$ |

Figure 1. The distribution of the population $P_n$ of the excited states of the hydrogen atom while the laser field is linearly polarized along the $z$-axis. The calculations are performed using the 1D npDVR Gaussian scheme with $N_{\Omega} = 95$. The vertical axis is in logarithmic scale.

In figure 2, we demonstrate the convergence $N_{\Omega} \rightarrow +\infty$ of the transition probabilities $\frac{d\rho}{d\Omega}(E)$ to the states of the continuum spectra of the hydrogen atom due to interaction with a laser pulse linearly polarized along the $z$-axis. The calculations are performed using the 1D DVR Gaussian scheme, where the $\phi$-variable is separated and $m = 0$. In the calculations, the highest angular momentum in equation (28) was fixed at $l_m = 35$ by the requirement that the error in cutting off summation (28) does not exceed the error when using the limited DVR basis. The spectrum contains several peaks, whose positions do not depend on the number of basis functions $N_{\Omega}$ and are almost placed at the peak positions $E_p$ of the energy spectrum in a multiphoton process [30–52]

$$E_p = \frac{p}{\hbar} \omega - U_{pe} - I,$$

where $I_i = 13.6$ eV is the ionization energy of the hydrogen atom, $\hbar \omega = 1.55$ eV is the photon energy, and $U_{pe} = I / (4 \omega^2) = 5.967$ eV is the ponderomotive energy of our laser field with intensity $I = 10^{14}$ W cm$^{-2}$. The calculated $\frac{d\rho}{d\Omega}(E)$ is qualitatively in agreement with [51], where a 25 fs laser pulse was used. For this high intensity, the first expected peak corresponding to the 13-photon ionization, $p = 13$ in equation (34), is split, just as in [51]. The various mechanisms leading to the doubling of the first ATI peak was intensively discussed earlier [33, 53–55]. In the considered case, apparently, the intermediate resonant population of some of the levels dressed by the strong laser field is responsible for this effect [33]. However, to clarify this issue, a detailed calculation of the level deformations by a strong laser pulse is required.

The distribution $\frac{d\rho}{d\Omega}(E)$ over the electron angular momentum $l$ in the continuum for different energies $E$ between successive peaks ($E = E_p + 0.01$ (in a.u.), where $p$ corresponds to 13, 14, 15, 16–photon ionization) is presented in figure 3. As can be seen in this figure, by increasing the electron energy, the contribution of higher $l$-values to the continuous spectrum is increased. However, the main contribution comes from the angular momenta $0 \leq l \leq 12$.

In table 2, the total ionization yield $P_{\text{ion}}$, which is calculated by integrating the transition probabilities $\frac{d\rho}{d\Omega}(E)$ over all
possible states of the ionized electron in its continuum (30), and the total excitation probability $P_{\text{ex}} = 1 - P_g - P_{\text{ion}}$ are presented. These results demonstrate the convergence of the computational scheme when calculating $P_{\text{ion}}$ and $P_{\text{ex}}$ at the accuracy level of the order of the fourth significant digit after the decimal point.

The total excitation probability $P_{\text{ex}}$ can also be calculated by direct summation of $P_{\text{ion}}$ over $n$ and $l$. However, this requires taking into account the contribution of large $n$ and $l$ values which, in some cases, can be considerable [34, 56, 57] and greatly complicates the problem computationally. Therefore, we propose an alternative method described in the previous section, equations (31) and (33), to calculate $P_{\text{ex}}$ without summation over large $n$ and $l$. To get the probability $P_{\text{ex}}$ according to these formulas (the procedure is illustrated in figure 4), we have calculated the populations $P_n$ of the hydrogen atom bound states up to $n = 7$, according to (27), and followed the method described in section 2.2, for calculating the populations of states with $n \geq 8$. The points $\frac{d}{dE}(E_n) = n^1 P_n$ on the negative side of the electron energy in figure 4 belong to $n = 6$ and $n = 7$ states. On the positive side, three $E$ points were chosen very close to the zero energy, where $\frac{d}{dE}(E)$ were calculated by equations (23) and (28). By these five points the polynomial function $f(E)$ was fixed to calculate $\sum_{n=8}^{\infty} P_n$, according to the relation (33). In figure 4 we see a good agreement between the calculated curve $f(E)$ and the corresponding values calculated for $n$ up to $n = 20$ by the direct method (22). It confirms that the choice of $n = 6$ and $n = 7$ when constructing

Table 2. The ionization yield $P_{\text{ion}}$ and the total excitation probability $P_{\text{ex}}$ as a function of $N_{12}$ in the Gaussian 1D DVR approach for the linearly polarized laser field along the $z$-axis. The $P_{\text{ex}}$ values are calculated by integrating the transition probabilities $\frac{d}{dE}(E)$ of the electron continuum over $E$ through equations (23), (28) and (30) and the excitation probabilities $P_{\text{ex}}$ by $P_{\text{ex}} = 1 - P_g - P_{\text{ion}}$.

| $N_{12}$ | 35   | 50   | 65   | 80   | 95   |
|----------|------|------|------|------|------|
| $P_{\text{ion}}$ | $1.298 \times 10^{-02}$ | $1.284 \times 10^{-02}$ | $1.301 \times 10^{-02}$ | $1.304 \times 10^{-02}$ | $1.304 \times 10^{-02}$ |
| $P_{\text{ex}}$ | $2.330 \times 10^{-03}$ | $2.484 \times 10^{-03}$ | $2.311 \times 10^{-03}$ | $2.286 \times 10^{-03}$ | $2.284 \times 10^{-03}$ |

Figure 3. The distribution of electrons $\frac{d}{dE}(E) = \sum_{m=-l}^{l} \frac{d}{dE}(E)$ over the angular momentum $l$ due to ionization of the hydrogen atom by a laser field linearly polarized along the $z$-axis (thus $m = 0$). Four different electron energy values $E$ above successive peaks $E = E_p + 0.01$ (in a.u.) are considered, where $E_p$ is obtained according to (34) and $p = 13, 14, 15, 16$ corresponds to $E_1$ (blue squares), $E_2$ (open red circles), $E_3$ (gray triangles) and $E_4$ (full green circles). Here, the calculations are performed with $N_{12} = 95$. The vertical axis is in logarithmic scale.

Figure 4. An illustration of the $P_{\text{ex}}$ calculation by formulas (31) and (33) when the laser field is linearly polarized along the $z$-axis. Two full circles $\frac{d}{dE}(E_n)$ on the negative part of the electron energy $E_n = -\frac{d}{dE}$ are calculated for $n = 6, 7$ by the relation $\frac{d}{dE}(E_n) = n^1 P_n$. Meanwhile, for three full circles on the positive side of $E$, we use the projection of the calculated electron wave packet at the end of the laser pulse onto Coulomb states of the continuum spectrum via equations (23) and (28). A cubic polynomial trend line (blue line) $f(E)$ passes through these circles. The open circles $\frac{d}{dE}(E_n)$ belong to the values calculated by the Gaussian 1D DVR scheme for $n = 8, 9, \ldots, 20$ and the green triangles show the corresponding interpolated $f(E_n)$. The calculations are performed within the Gaussian 1D DVR for $N_{12} = 65$. 

$\sum_{n=8}^{\infty} P_n$, according to the relation (33). In figure 4 we see a good agreement between the calculated curve $f(E)$ and the corresponding values calculated for $n$ up to $n = 20$ by the direct method (22). It confirms that the choice of $n = 6$ and $n = 7$ when constructing
schemes based on 2D npDVRs by calculating the population
is not allowed, regardless of the laser field orientation. In
Lebedev 2D npDVRs, where the separation of the
accuracy of the computational schemes based on the Popov and
results to investigate the convergence and evaluate the accur-
accuracy as
states of an electron in the continuum spectrum.
by integrating the electron transition probabilities over the
given accuracy, with the corresponding values obtained above
ionization yield
and ($\Omega$)
gives a good approximation, which can be used to eval-
pared $P_n$ for large $n$. The probabilities $P_{ex}$ calculated using
this method and $P_{ion} = 1 - P_g - P_{ex}$ as a function of $N_\Omega$ are
presented in table 3. By comparing the results presented in
tables 2 and 3, one can conclude that our proposed method (31)
and (33) for calculating the total excitation probability $P_{ex}$ and
ionization yield $P_{ion}$ generates values which coincide, within a
given accuracy, with the corresponding values obtained above
by integrating the electron transition probabilities over the
states of an electron in the continuum spectrum.
The values of $P_g$, $P_{ex}$ and $P_{ion}$, calculated above with high
accuracy as $N_\Omega = N_0 \rightarrow +\infty$ within the framework of the
Gaussian 1D DVR, hereinafter are used as ‘exact’ reference
results to investigate the convergence and evaluate the accuracy
of the computational schemes based on the Popov and
Lebedev 2D npDVRs, where the separation of the $\phi$-variable
is not allowed, regardless of the laser field orientation. In
figure 5, we demonstrate the convergence of the computational
schemes based on 2D npDVRs by calculating the population
of the ground state $P_g$ as a function of the number of the angular
grid points on the unit sphere $N_\Omega$ (the number of basis functions (8) in 2D npDVR expansion (5)). As can be seen in
this figure, the ground state population, calculated using the
Popov or Lebedev schemes, tends to the ‘exact’ value obtained
according to the Gaussian scheme (yellow dashed line). We
have also performed the calculation of $P_g(N_\Omega)$ for the nonsepa-able case of the Gaussian 2D DVR, when the laser field is
oriented along the $x$-axis and $N_\Omega = N_0 \times N_0$. Figure 5 displays
much faster convergence of the Popov and Lebedev schemes
compared to the Gaussian 2D DVR. The slowdown of the latter
can be explained by the known effect of clustering of
grid points $\Omega_j$ in the Gaussian scheme near the poles $z = 0$ as
$N_\Omega \rightarrow \infty$ [58] and a more adequate approximation of the angular
part of the 3D TDSE in 2D npDVRs.
A comparison of the different applied schemes for calculat-
ing $P_g$, $P_{ex}$ and $P_{ion}$ is summarized in table 4. Here, the
largest number of employed Popov and Lebedev grid points is
$N_{\Omega} = 672$ and 1202, respectively. A comparison of the most

| $N_\Omega$ | $\sum_{n=2}^{7} P_n$ | $\sum_{n=8}^{\infty} P_n$ | $P_{ex} = \sum_{n=2}^{\infty} P_n$ | $P_{ion} = 1 - P_g - P_{ex}$ |
|----------|-----------------|-----------------|-----------------|-----------------|
| 35       | $1.994 \times 10^{-03}$ | $3.047 \times 10^{-04}$ | $2.299 \times 10^{-03}$ | $1.301 \times 10^{-02}$ |
| 50       | $1.967 \times 10^{-03}$ | $2.856 \times 10^{-04}$ | $2.253 \times 10^{-03}$ | $1.307 \times 10^{-02}$ |
| 65       | $1.971 \times 10^{-03}$ | $2.864 \times 10^{-04}$ | $2.257 \times 10^{-03}$ | $1.306 \times 10^{-02}$ |
| 80       | $1.971 \times 10^{-03}$ | $2.882 \times 10^{-04}$ | $2.259 \times 10^{-03}$ | $1.306 \times 10^{-02}$ |
| 95       | $1.971 \times 10^{-03}$ | $2.872 \times 10^{-04}$ | $2.258 \times 10^{-03}$ | $1.306 \times 10^{-02}$ |

Figure 5. The population of the ground state $P_g$, calculated using the 2D npDVR schemes of Lebedev and Popov, as well as the Gaussian
2D and 1D DVR schemes for a hydrogen atom in a linearly polarized laser field, together with the results of [17]. The yellow dashed line
indicates the most accurate value $P_g$ obtained with the Gaussian 1D DVR scheme for the laser field polarization along the $z$-axis. The open
squares indicate the values $P_g$ calculated with the 2D Gaussian DVR for the laser field polarization along the $x$-axis, when the $\phi$ variable is
nonseparable and $N_\Omega = N_0 \times N_0$.

Table 3. The total excitation probability $P_{ex}$ and the ionization yield $P_{ion}$ as a function of $N_\Omega$ within the Gaussian 1D DVR scheme when
the laser field is linearly polarized along the $z$-axis. The $P_{ex}$ values are calculated, according to the formulas (31) and (33), approximating
the summation over all states of the discrete spectrum of the hydrogen atom (see text).

| $N_\Omega$ | $P_g$ | $P_{ex}$ | $P_{ion}$ |
|----------|-------|---------|---------|
|          | $0.9848$ | $0.9847$ | $0.9847$ |
|          | $1.90 \times 10^{-03}$ | $2.15 \times 10^{-03}$ | $2.26 \times 10^{-03}$ |
|          | $1.33 \times 10^{-02}$ | $1.32 \times 10^{-02}$ | $1.31 \times 10^{-02}$ |

Table 4. The ground state population $P_g$, total excitation probability $P_{ex}$ and total ionization yield $P_{ion}$ calculated with different 2DnpDVRs
and the Gaussian 1D DVR together with the results of [17] for a hydrogen atom in a linearly polarized laser field. Here, $P_{ex}$ were calculated
using formulas (31) and (33) of the method proposed in section 2.2, for infinite summation of the populations of the hydrogen bound states
and $P_{ion} = 1 - P_g - P_{ex}$.

| Methods          | Popov     | Lebedev   | Gaussian ($E = E \hat{z}$) | [17]     |
|------------------|-----------|-----------|---------------------------|----------|
| $P_g$            | $0.9848$  | $0.9847$  | $0.9847$                  | $0.9835$ |
| $P_{ex}$         | $1.90 \times 10^{-03}$ | $2.15 \times 10^{-03}$ | $2.26 \times 10^{-03}$ | $4.18 \times 10^{-03}$ |
| $P_{ion}$        | $1.33 \times 10^{-02}$ | $1.32 \times 10^{-02}$ | $1.31 \times 10^{-02}$ | $1.23 \times 10^{-02}$ |
Table 5. The transition probabilities $P_n$ to the bound states $n$ of the hydrogen atom in terms of increasing $r_m$ and $N_r$, while the ratio $\frac{r_m}{N_r} = 0.25$ is fixed. The calculations were performed with the Gaussian 1D DVR for $N_{ij} = N_{ij} = 95$ and the linearly polarized laser field along the z-axis.

| $n$ | $r_m = 250, N_r = 1000$ | $r_m = 500, N_r = 2000$ | $r_m = 1000, N_r = 4000$ |
|-----|-------------------------|-------------------------|-------------------------|
| 1   | 0.9846820               | 0.9846783               | 0.9846764               |
| 2   | $7.87 \times 10^{-05}$  | $7.87 \times 10^{-05}$  | $7.87 \times 10^{-05}$  |
| 3   | $6.69 \times 10^{-05}$  | $6.69 \times 10^{-05}$  | $6.69 \times 10^{-05}$  |
| 4   | $2.19 \times 10^{-04}$  | $2.19 \times 10^{-04}$  | $2.19 \times 10^{-04}$  |
| 5   | $1.24 \times 10^{-03}$  | $1.24 \times 10^{-03}$  | $1.24 \times 10^{-03}$  |
| 6   | $2.31 \times 10^{-04}$  | $2.31 \times 10^{-04}$  | $2.31 \times 10^{-04}$  |
| 7   | $1.17 \times 10^{-04}$  | $1.17 \times 10^{-04}$  | $1.17 \times 10^{-04}$  |
| 8   | $7.40 \times 10^{-05}$  | $7.41 \times 10^{-05}$  | $7.41 \times 10^{-05}$  |
| 9   | $4.95 \times 10^{-05}$  | $4.94 \times 10^{-05}$  | $4.95 \times 10^{-05}$  |
| 10  | $3.37 \times 10^{-05}$  | $3.46 \times 10^{-05}$  | $3.46 \times 10^{-05}$  |
| $P_{\text{ex}}$ | $2.28 \times 10^{-03}$  | $2.26 \times 10^{-03}$  | $2.26 \times 10^{-03}$  |
| $P_{\text{ion}}$ | $1.304 \times 10^{-02}$ | $1.306 \times 10^{-02}$ | $1.306 \times 10^{-02}$ |

Figure 6. The calculated ground state probabilities by the Popov and Lebedev 2D npDVR schemes for a hydrogen atom in a laser field of different polarizations $\varepsilon = 0.25, 0.5, 1.0$. The red horizontal lines show the corresponding values of Gao and Tong [17]. For circular polarization, the results obtained using the Gaussian 2D DVR scheme are also presented.

Table 5 shows accurate values obtained with the Lebedev 2D npDVR scheme at $N_{ij} = 1202$ with the ‘exact’ values calculated using the 1D Gaussian DVR for field polarization along the z-axis demonstrates the achieved absolute accuracy of this scheme of the order of $\sim 10^{-5}$ for $P_{\text{ex}}$ and $\sim 10^{-4}$ for $P_{\text{ion}}$. This estimated accuracy also coincides with the value which is obtained through the generally accepted procedure for calculating the error of the numerical methods on a sequence of condensing grids, where the error is equal to the attained minimum deviation of the calculated value on two nearest most detailed grids. Indeed, in our case, for the deviation of the populations calculated on the most detailed grid from its closest number of nodes we get $\Delta P_{\text{ex}} = |P_{\text{ex}}(N_{ij} = 974) - P_{\text{ex}}(N_{ij} = 1202)| \approx 2 \times 10^{-5}$, $\Delta P_{\text{ion}} \approx 10^{-4}$. This method is also used in the next section to evaluate the accuracy of the calculations.

The above results were obtained on a radial grid with $r_m = 500$ and $\Delta \varepsilon = 0.0005$. To evaluate the error of the approximation over the radial variable we have performed calculations with increasing radial box size and decreasing steps of integration up to $r_m = 1000$ and $\Delta \varepsilon = 1/N_r = 0.00025$. The results given in table 5 demonstrate that the approximation error over the radial variable on the grid with $r_m = 500$ and $\Delta \varepsilon = 0.0005$ is less than that due to truncation of the 2D npDVR. Therefore, hereafter we choose this radial grid. The step of integration $\Delta \varepsilon = 0.05$ (1/2200 of one optical cycle) over time, which we use, also gives an error that is significantly less than the error introduced by truncating the 2D npDVR.

Although our results deviate from the results of [17] (the maximal deviation is for $P_{\text{ex}}$ values which differ from one another twice), our three DVR computational schemes...
converge to the same value in the frame of the reached accuracy. Moreover, the deviation of our results from the values obtained in [17] exceeds our accuracy by an order of magnitude.

In the next section we apply the 2D npDVRs for a hydrogen atom in elliptically polarized laser fields in the entire range of possible change in ellipticity.

3.2. Elliptically polarized laser field

The dynamics of a hydrogen atom in a laser field of three different polarizations $\varepsilon = 0.25, 0.5, 1.0$ has been investigated with the developed Popov and Lebedev 2D npDVRs. As mentioned above, the 1D Gaussian DVR is not applicable for a hydrogen atom in a laser field with $\varepsilon \neq 0$. The calculated ground state probabilities $P_g$ are presented in figure 6, which demonstrates the convergence of our 2D DVR computational schemes as $N_\Omega \to +\infty$. As in the linear polarization, the Popov and Lebedev 2D npDVRs schemes demonstrate more rapid convergence compared to the 2D Gaussian DVR for circular polarization as well. As in the linear polarization, all three computational schemes converge to the same values which, however, significantly deviate from the results obtained in [17]. This deviation decreases with increasing ellipticity and becomes minimal at $\varepsilon = 1$.

The distributions of the population ($P_n$ and $P_{nl}$) of excited states over the principal quantum number $n$ and angular momentum $l$ are presented in figure 7. While for the ellipticities $\varepsilon = 0.0, 0.25, 0.5$, a maximum is observed at the $n = 5$ bound state and a strong decrease in $P_n$ for higher excited states (in agreement with [34]), the $n$ distribution shows a different trend for the circularly polarized laser field. To calculate the probabilities of total excitation $P_{ex}$ and ionization $P_{ion}$ of the hydrogen atom, depending on the ellipticity of the laser field, we have used the Lebedev 2D npDVR scheme, which allowed us to carry out calculations with the largest number of basis DVR functions up to $N_\Omega = 1202$. Here, to approximate the infinite summation (32) when calculating the probability $P_{ex}$ of total excitation (31), we use the computational procedure (31) and (32), whose efficiency was demonstrated in section 3.1, for linear polarization of the laser field. Figure 8 illustrates this computational procedure for $\varepsilon = 0.5$ and $1.0$. The ground state population $P_g$ and thus calculated probabilities $P_{ex}$ and $P_{ion}$ are presented in tables 6–8. Figure 9 also depicts the obtained $P_{ex}$ and $P_{ion}$ values. The data presented in tables 6–8 and in figure 9 convincingly demonstrate the convergence of the Lebedev 2D npDVR scheme as $N_\Omega \to +\infty$ and give the estimate $\Delta P_{ex} \approx |P_{ex}(N_\Omega = 974) - P_{ex}(N_\Omega = 1202)|$ of the achieved absolute accuracy when calculating $P_g$, $P_{ex}$ and $P_{ion}$, which is improved from the values of the order $\sim 10^{-4}$ at $\varepsilon = 0$ to $10^{-6}$ at $\varepsilon = 1$. It should be noted that the errors due to the finiteness of the radial box size $r_m$ and the steps of integration over the radial and time variables do not exceed this achieved accuracy. Table 9 illustrates that the radial grid with $r_m = 500$ and $\Delta x = 1/N_r = 0.0005$ already meets this requirement when calculating $P_{ex}$ and $P_{ion}$. The difference between the calculated values $P_g$, $P_{ex}$ and $P_{ion}$ and most accurate values [17] calculated so far with alternative methods decreases with increasing ellipticity to $\varepsilon = 1$. However, in the entire range of $\varepsilon$ variation, this difference remains an order of magnitude greater than the achieved accuracy of our calculations. We explain this deviation by the fact that we managed to significantly improve, compared to [17], the approximation of the angular part of

![Figure 7](image_url)
Figure 8. An illustration of the $P_{\text{ex}}$ calculation by formulas (31) and (33) for the elliptically polarized laser fields with $\varepsilon = 0.5$ and 1.0. The calculations of $\text{ex}$ are performed using the Lebedev 2D npDVR scheme at $N_\Omega = 770$. All designations in the figure are similar to those in figure 4.

Table 6. The probabilities $P_g, P_{\text{ex}}$ and $P_{\text{ion}} = 1 - P_g - P_{\text{ex}}$ calculated using the Lebedev 2D npDVR scheme for the laser polarization $\varepsilon = 0.25$. The infinite summation in $P_{\text{ex}}$ is performed according to the procedure (31) and (32). In the last row, the results of [17] are presented.

| N   | $\sum_{n=1}^{7} P_n$ | $\sum_{n=8}^{+\infty} P_n$ | $P_{\text{ex}} = \sum_{n=1}^{+\infty} P_n$ | $P_g$     | $P_{\text{ion}}$ |
|-----|----------------------|-----------------------------|---------------------------------------------|-----------|-----------------|
| 170 | 4.066 x 10^{-04}     | 1.210 x 10^{-04}            | 5.276 x 10^{-04}                           | 0.987283  | 1.219 x 10^{-02}|
| 194 | 2.497 x 10^{-04}     | 4.597 x 10^{-05}            | 2.956 x 10^{-04}                           | 0.987878  | 1.183 x 10^{-02}|
| 302 | 3.286 x 10^{-04}     | 4.742 x 10^{-05}            | 3.760 x 10^{-04}                           | 0.987795  | 1.183 x 10^{-02}|
| 350 | 2.224 x 10^{-04}     | 5.688 x 10^{-05}            | 2.792 x 10^{-04}                           | 0.987915  | 1.181 x 10^{-02}|
| 434 | 4.101 x 10^{-04}     | 5.808 x 10^{-05}            | 4.682 x 10^{-04}                           | 0.987916  | 1.162 x 10^{-02}|
| 590 | 4.876 x 10^{-04}     | 7.656 x 10^{-05}            | 5.642 x 10^{-04}                           | 0.987969  | 1.147 x 10^{-02}|
| 770 | 5.705 x 10^{-04}     | 1.069 x 10^{-04}            | 6.774 x 10^{-04}                           | 0.988087  | 1.124 x 10^{-02}|
| 974 | 6.224 x 10^{-04}     | 1.233 x 10^{-04}            | 7.457 x 10^{-04}                           | 0.988130  | 1.112 x 10^{-02}|
| 1202| 6.763 x 10^{-04}     | 1.341 x 10^{-04}            | 8.104 x 10^{-04}                           | 0.988055  | 1.113 x 10^{-02}|

[17] – – 1.790 x 10^{-03} 0.987480 1.073 x 10^{-02}.

Table 7. The same as in table 6 for $\varepsilon = 0.5$.

| N   | $\sum_{n=1}^{7} P_n$ | $\sum_{n=8}^{+\infty} P_n$ | $P_{\text{ex}} = \sum_{n=1}^{+\infty} P_n$ | $P_g$     | $P_{\text{ion}}$ |
|-----|----------------------|-----------------------------|---------------------------------------------|-----------|-----------------|
| 170 | 5.284 x 10^{-05}     | 5.545 x 10^{-05}            | 1.083 x 10^{-04}                           | 0.994207  | 5.685 x 10^{-05}|
| 194 | 3.049 x 10^{-05}     | 1.622 x 10^{-05}            | 4.671 x 10^{-05}                           | 0.993874  | 6.079 x 10^{-05}|
| 302 | 1.790 x 10^{-05}     | 7.309 x 10^{-06}            | 2.521 x 10^{-05}                           | 0.994011  | 5.964 x 10^{-05}|
| 350 | 1.765 x 10^{-05}     | 1.187 x 10^{-05}            | 2.951 x 10^{-05}                           | 0.993992  | 5.978 x 10^{-05}|
| 434 | 1.438 x 10^{-05}     | 3.631 x 10^{-06}            | 1.801 x 10^{-05}                           | 0.993973  | 6.009 x 10^{-05}|
| 590 | 1.707 x 10^{-05}     | 4.900 x 10^{-06}            | 2.197 x 10^{-05}                           | 0.993978  | 6.000 x 10^{-05}|
| 770 | 2.232 x 10^{-05}     | 9.635 x 10^{-06}            | 3.195 x 10^{-05}                           | 0.993987  | 5.981 x 10^{-05}|
| 974 | 2.755 x 10^{-05}     | 1.637 x 10^{-05}            | 4.391 x 10^{-05}                           | 0.993994  | 5.962 x 10^{-05}|
| 1202| 3.354 x 10^{-05}     | 1.576 x 10^{-05}            | 4.930 x 10^{-05}                           | 0.993997  | 5.954 x 10^{-05}|

[17] – – 1.280 x 10^{-04} 0.993862 6.010 x 10^{-05}.

Table 8. The same as in table 6 for $\varepsilon = 1.0$.

| N   | $\sum_{n=1}^{7} P_n$ | $\sum_{n=8}^{+\infty} P_n$ | $P_{\text{ex}} = \sum_{n=1}^{+\infty} P_n$ | $P_g$     | $P_{\text{ion}}$ |
|-----|----------------------|-----------------------------|---------------------------------------------|-----------|-----------------|
| 170 | 2.161 x 10^{-07}     | 1.663 x 10^{-06}            | 1.879 x 10^{-06}                           | 0.9987628  | 1.235 x 10^{-03}|
| 194 | 4.424 x 10^{-07}     | 1.632 x 10^{-06}            | 2.075 x 10^{-06}                           | 0.9988135  | 1.184 x 10^{-03}|
| 302 | 1.352 x 10^{-07}     | 2.361 x 10^{-07}            | 3.713 x 10^{-07}                           | 0.9988226  | 1.177 x 10^{-03}|
| 350 | 4.387 x 10^{-08}     | 2.408 x 10^{-07}            | 2.847 x 10^{-07}                           | 0.9988253  | 1.174 x 10^{-03}|
| 434 | 7.752 x 10^{-08}     | 1.607 x 10^{-07}            | 2.382 x 10^{-07}                           | 0.9988216  | 1.178 x 10^{-03}|
| 590 | 8.459 x 10^{-08}     | 1.612 x 10^{-07}            | 2.457 x 10^{-07}                           | 0.9988227  | 1.177 x 10^{-03}|
| 770 | 6.134 x 10^{-08}     | 1.600 x 10^{-07}            | 2.213 x 10^{-07}                           | 0.9988201  | 1.180 x 10^{-03}|
| 974 | 5.407 x 10^{-08}     | 9.536 x 10^{-08}            | 1.494 x 10^{-07}                           | 0.9988219  | 1.178 x 10^{-03}|
| 1202| 3.359 x 10^{-08}     | 9.887 x 10^{-08}            | 1.325 x 10^{-07}                           | 0.9988216  | 1.178 x 10^{-03}|

[17] – – 2.390 x 10^{-08} 0.9987999 1.200 x 10^{-03}.
the 3D TDSE using our 2D npDVR, which ensured fast convergence and high computational efficiency of our algorithm, where the computational time is proportional to $N_r(2N_\Omega^2 + 200N_\Omega)$. Perhaps, this is also due to the fact that in the pseudospectral method of [17], instead of the unperturbed bound states of the hydrogen atom $R_{nl}(r)Y_{lm}(\theta, \phi)$, pseudostates are
used, starting from \( n > 16 \); although there is a fairly large set of them.

4. Conclusion

We have developed an efficient computational scheme for integrating the 3D TDSE and successfully applied it to calculate the probabilities of total excitation \( P_{\text{ex}} \) and ionization \( P_{\text{ion}} \) of a hydrogen atom in strong elliptically polarized laser fields. In our approach the nonseparable angular part of the 3D TDSE is approximated using 2D npDVRs based on the 2D Lebedev and Popov cubatures for the unit sphere. Using this approach, we have calculated the probabilities \( P_{g} \), \( P_{\text{ex}} \) and \( P_{\text{ion}} \) for a laser of \( I = 10^{14} \) W cm\(^{-2}\) and \( \lambda = 800 \) nm with absolute accuracy, which is improved by increasing the ellipticity of the laser field from the values of the order of \( \sim 10^{-4} \) for \( \varepsilon = 0 \) to \( \sim 10^{-6} \) for \( \varepsilon = 1 \). We associate such improvement with a more adequate approximation of the angular part of the 3D TDSE in 2D npDVR compared to the 2D DVR based on the direct product of 1D Gaussian DVRs, where clustering of the angular grid points is present near the poles \( x = y = 0 \). With an increase in ellipticity, our results approach the most accurate recent calculations [17]; however, the difference between them remains an order of magnitude greater than the achieved accuracy of our calculations. We believe that the record accuracy in our calculations of the probabilities of excitation and ionization of a hydrogen atom in a strong elliptically polarized laser field was achieved due to the high efficiency of approximation of the angular part of the 3D TDSE in 2D npDVR, which ensured a fast convergence of the method, and its high computational efficiency with the number of simulation operations \( \sim N_{r}(2N_{\Omega}^{2} + 200N_{\Omega}) \sim N_{r}N_{\Omega} \) compared to current best practices.

We have also proposed a novel simple procedure for infinite summation of the bound state populations of the hydrogen atom when calculating the total excitation probability \( P_{\text{ex}} \) and proved its accuracy by making a comparison with conventional methods.

The performed research demonstrates the potential prospects of the developed method for quantitative investigations of the phenomena stimulated by high-intensity lasers such as HHG, ATI and photoelectron momentum distribution, where the problem, even in the case of linear polarization of the laser field, becomes essentially 3D.

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