

Multiphoton ionization through the triplet states of Mg by linearly and circularly polarized laser pulses

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We theoretically study multiphoton ionization through the triplet states of Mg by linearly polarized and circularly polarized fs laser pulses. After the construction of the atomic basis using the frozen-core Hartree-Fock potential as well as the model potential approaches for both singlet and triplet series which show rather good agreements with the existing data in terms of state energies and dipole matrix elements, we solve time-dependent Schrödinger equations with $3s3p\ ^3P_1$ as an initial state, and calculate the total ionization yield and photoelectron energy spectra.

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I. INTRODUCTION

During the last 30 years many theoretical and experimental investigations have been performed for Mg to obtain the atomic data and to understand its interaction with radiation through *single-photon processes*. The first extensive theoretical studies for the triplet states of Mg were performed by Fischer [1] with a multiconfiguration Hartree-Fock method which included correlations between the valence electrons, and by Victor and co-workers [2] with a semiempirical model potential which included core-polarization and dielectronic terms to calculate the oscillator strengths (OSs) for bound-bound transitions with $1,^3S$, $1,^3P$, and $1,^3D$ symmetries. Using a frozen-core Hartree-Fock potential (FCHFP) with core-polarization and dielectronic terms Chang [3] calculated the OSs between $3snl\ ^{1,3}L$ ($L=S, P, D$, etc.) states of Mg. Mendoza and Zeippen [4] studied photoionization from the excited triplet state $3s3p\ ^3P$ of Mg using a FCHFP with core-polarization and dielectronic terms in the close coupling approximation. Moccia and co-workers [5] developed a non-empirical description of the core-polarization effects of Mg employing a basis set of modified Slater-type orbitals to study the transitions between the $3snl\ ^{1,3}L$ ($L=S, P, D$, and F) states of Mg. Luc-Koenig and co-workers [6] used an eigenchannel R -matrix and multichannel quantum defect theory (MQDT) to investigate two-photon ionization of the Mg atom. Lately, Fang and Chang [7] studied single-photon ionization from the excited singlet and triplet states of Mg below the Mg^{2+} threshold using an approach based on the B -spline functions and Kim [8] studied single-photon ionization from the $3s3p\ ^{1,3}P$ states with a R -matrix method combined with MQDT. Most recently Fang and Chang has developed a B -spline-based complex rotation method with spin-dependent interaction to calculate atomic photoionization of Mg with singlet-triplet mixing [9].

As for the *multiphoton processes* of Mg interacting with a laser pulse there are several experimental and theoretical

works, all of which involve only *singlet states*: Kim and co-workers [10] studied single and double ionization of Mg by 10 ns Nd:YAG laser pulses at both 532 and 1064 nm in the intensity range of 10^{12} – 10^{13} W/cm². Druten and co-workers [11] measured photoelectron energy spectra (PES) associated with single and double ionization of Mg using 1 ps laser pulses in the wavelength of 580–595 nm and 10^{12} – 10^{13} W/cm² intensity range, respectively. Xenakis and co-workers [12] investigated multiphoton ionization of Mg using 150 fs laser pulses at the wavelength of 400 nm for the peak laser intensities of up to 6×10^{13} W/cm². Gillen and co-workers [13,14] measured the ionization yield for single and double ionization of Mg exposed to the 800 nm, 120 fs Ti:sapphire laser pulses for the peak intensities of 10^{12} – 10^{13} W/cm², which was followed by the theoretical analysis [15]. Lontos and co-workers [16] investigated single and double ionization of Mg by Nd:YAG laser pulses with a ns duration for peak intensities up to 10^{12} W/cm². Zhang and Lambropoulos [17] performed time-dependent calculations of Mg for the case in which ions are left in excited states. Recently we have studied the ionization yield and PES of Mg and clarified the origin of the subpeaks in the PES by the second and third harmonics of the fs Ti:sapphire laser pulse [18]. Note that all the previous studies have focused on multiphoton ionization from the *singlet states* of Mg.

The purpose of this paper is to perform the theoretical study for the multiphoton ionization processes through the *triplet states* of Mg by linearly polarized (LP) and circularly polarized (CP) fs laser pulses. Specifically we choose $3s3p\ ^3P_1$ as an initial state and perform time-dependent calculations after the construction of the atomic basis for both singlet and triplet series. This paper is organized as follows. In Secs. II and III we present the theoretical model: The time-dependent Schrödinger equation (TDSE), which describes the time-dependent interaction dynamics of the Mg atom with a laser pulse, is solved on the atomic basis states of Mg with two-active-valence electrons. Atomic units (a.u.) are used throughout this paper unless otherwise mentioned. In Sec. IV we present representative numerical results for the

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state energies and the J -independent and -dependent OSs between the triplet states. Our results are compared with the existing data to confirm the accuracy of our atomic basis. Using those atomic basis states, we solve the TDSE to calculate the total ionization yield and PES from the $3s3p\ ^3P_1$ initial state of Mg by LP and CP fs laser pulses. Similar to the PES from the singlet ground state $3s^2\ ^1S_1$ of Mg [18], the PES from the triplet $3s3p\ ^3P_1$ state also exhibits subpeak structure. Finally, concluding remarks are given in Sec. V.

II. ATOMIC BASIS STATES

To start with, in order to study the interaction of the Mg atom with a laser pulse we have to construct the atomic basis of the Mg atom. The Mg atom is a two-valence-electron atom; it consists of a closed core (the nucleus and the ten inner-shell electrons $1s^22s^22p^6$) and the two valence electrons. As it is already mentioned in the literature [19] there are several approaches to solve the Schrödinger equation for one- and two-valence-electron atoms in a laser field. Since the general computational procedure has already been presented in Refs. [20–22] to construct the atomic basis states and the specific details about the atomic structure calculation of Mg have been reported in recent works [23,24], we only briefly describe the method we employ. The field-free one-electron Hamiltonian of Mg^+ , $h_a(r)$, is expressed as

$$h_a(r) = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{Z}{r} + \frac{l(l+1)}{2r^2} + V_{eff}(r), \quad (1)$$

where r represents the position vector of the valence electron, Z is the core charge, l is the orbital quantum number, and $V_{eff}(r)$ is the effective potential acting on the valence electron of Mg^+ . Since the spin-orbit interaction is very weak for a light alkaline-earth-metal atom such as Mg [25,26], it might be safely neglected in the atomic Hamiltonian for our specific purpose. Similar to our recent study [24] in which we have presented detailed comparisons between the frozen-core Hartree-Fock (FCHF) and model potential (MP) calculations for the singlet states of Mg, we employ two different approaches in this paper to describe the effective potential, V_{eff} , in Eq. (1). Namely (i) a FCHF potential and (ii) a MP.

A. One-electron orbitals: Frozen-core Hartree-Fock approach

In the last years the most widely used method to describe the ionic core is the FCHF approach. In the FCHF approach the effective potential is given by

$$V_{eff}(r) = V_l^{HF}(r) + V_l^p(r), \quad (2)$$

where V_l^{HF} represents the FCHF potential and V_l^p is the core-polarization potential which effectively accounts for the interaction between the closed core and the valence electrons [21]. Specifically we employ the following form for the core-polarization term:

$$V_l^p(r) = -\frac{\alpha_s}{2r^4} [1 - \exp^{-(r/r_l)^6}], \quad (3)$$

in which $\alpha_s=0.491$ is the static dipole polarizability of Mg^{2+} [4] and r_l ($l=0, 1, 2, \dots$) are the cutoff radii for the different

orbital angular momenta: $r_0=1.241$, $r_1=1.383$, $r_2=1.250$, $r_3=1.300$, and $r_4=1.100$ [27].

B. One-electron orbitals: Model potential approach

Another simpler way to describe the ionic core is to use a MP, V_l^{MP} [2,24,25,28] instead of the FCHF, V_l^{HF} . The advantage of the MP approach is that we can obtain the one-electron orbitals without self-consistent iterations, since the interactions of the valence electrons with the Mg^{2+} core are replaced by pseudopotentials for each angular momentum. Thus the complexity of the problem is greatly reduced. That is, instead of the FCHF, i.e., $V_l^{HF}(r)$, we employ the pseudopotential we have obtained in our previous work [24] to describe the interaction of the valence electron with the Mg^{2+} core:

$$V_l^{MP}(r) = V_l^p(r) - \frac{A}{r} \exp(-\alpha r^2) + B_l \exp(-\beta_l r^2), \quad (4)$$

where the values of the parameters introduced above, after the least-squares fitting, are $A=0.541$, $\alpha=0.561$, $B_0=11.086$, $B_1=5.206$, $B_{l \geq 2}=0$, $\beta_0=1.387$, $\beta_1=1.002$, and $\beta_{l \geq 2}=0$ [24]. We note that this form of V_l^{MP} is different from the one used in Refs. [2,25,28]. In Sec. IV, we will compare the results obtained by FCHF, MP, and the experimental data.

In either approach described above to obtain the one-electron orbitals, we employ a set of B -spline functions to expand them. Thus solving the Schrödinger equation for the nonrelativistic one-electron Hamiltonian given in Eq. (1) is now reduced to an eigenvalue problem.

C. Two-electron states

Once the one-electron orbitals have been obtained using either the FCHF or MP, we can construct two-electron states with the configuration interaction (CI) approach as we describe below. The field-free two-electron Hamiltonian, $H_a(\mathbf{r}_1, \mathbf{r}_2)$, can be expressed as

$$H_a(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i=1}^2 h_a(r_i) + V(\mathbf{r}_1, \mathbf{r}_2), \quad (5)$$

where $h_a(r_i)$ represents the one-electron Hamiltonian for the i th electron as shown in Eq. (1), and $V(\mathbf{r}_1, \mathbf{r}_2)$ is a two-electron interaction operator, which includes the static Coulomb interaction $1/|\mathbf{r}_1 - \mathbf{r}_2|$ and the effective dielectronic interaction potential [5,21]. \mathbf{r}_1 and \mathbf{r}_2 are the position vectors of the two valence electrons. By solving the two-electron Schrödinger equation for the Hamiltonian given in Eq. (5), the two-electron states are constructed with the CI approach [20–22]. For Mg, which is a light alkaline-earth-metal atom, the LS coupling is known to give a good description and hence it is sufficient to label a two-electron state by the following set of quantum numbers: the principal, orbital, and spin quantum numbers for each electron, $n_i l_i s_i$ ($i=1, 2$), total orbital momentum L , total spin S , total angular momentum J , and its projection M on the quantization axis. After the CI procedure, two-electron states may be most generally labeled by the state energy and the quantum numbers (L, S, J, M) .

For singlet states ($S=0$), the above state labeling can be simplified to (L, M) , since J is automatically equal to L . This is not the case, however, for the triplet states ($S=1$) since $\mathbf{J}=\mathbf{L}+\mathbf{S}$ due to the presence of spin-orbit interaction. Physically, introduction of spin-orbit interactions influences the wave functions in two aspects: The dynamical (radial) part and the geometric (angular) part. As for the dynamical part we neglect its influence in this paper, since the spin-orbit interaction in the Mg atom is small [25], anyway, as one can easily see from the very small fine structure splittings, and hence the radial wave function may be assumed to be J independent as a lowest-order approximation. As for the geometric part, we can fully include it by introducing the additional quantum numbers J and its projection M to specify the state. Thus it is necessary and sufficient that the triplet state is labeled by (L, S, J, M) .

Now, once we have obtained the two-electron wave functions we are able to calculate the dipole matrix elements as well as OSs for both LP and CP fields. In the following two subsections we present two useful conversion relations between the J -dependent and J -independent dipole matrix elements and OSs, respectively.

D. Calculation of the J -dependent dipole matrix elements

By applying the well-known Wigner-Eckart theorem the following conversion relation exists between the J -dependent and J -independent dipole matrix elements if we define the initial and final states, i and f , by a set of quantum numbers $\gamma_i=(n_i, L_i, S_i, J_i, M_i)$ and $\gamma_f=(n_f, L_f, S_f, J_f, M_f)$, respectively:

$$D_{n_i J_i M_i n_f J_f M_f} = (-1)^{J_f - M_f + L_f + S_f + J_i + 1 + q} \delta_{S_i S_f} \sqrt{(2J_i + 1)(2J_f + 1)} \\ \times \begin{pmatrix} J_f & 1 & J_i \\ -M_f & q & M_i \end{pmatrix} \\ \times \begin{Bmatrix} L_f & J_f & S_i \\ J_i & L_i & 1 \end{Bmatrix} D_{n_i L_i M_i n_f L_f M_f}, \quad (6)$$

in which $D_{n_i J_i M_i n_f J_f M_f}$ and $D_{n_i L_i M_i n_f L_f M_f}$ represent the J -dependent and J -independent dipole matrix elements, respectively. q is associated with laser polarization, i.e., $q=0$ for LP and $q=\pm 1$ for right or left circular polarization (RCP or LCP), respectively. Recall that the allowed transitions take place between states accordingly to the dipole selection rules, which are generally written as $J_f - J_i = 0, \pm 1$ ($J_f - J_i = 0$ is forbidden if $J_i = 0$) and $M_f - M_i = q$ ($M_f = M_i = 0$ is forbidden if $J_f - J_i = 0$). In addition the following dipole selection rules are satisfied since L and S are good quantum numbers: $L_f - L_i = \pm 1$, $M_{L_f} - M_{L_i} = q$, and $S_f - S_i = 0$, where $M_{L_f(i)}$ represents the projection on the quantization axis of the orbital quantum momentum.

E. Calculation of the J -dependent oscillator strengths

Similarly, the OSs for multiplet transitions between two states, i and f , could be related to the J -dependent OSs [29]:

$$f(n_i J_i, n_f J_f) = (2L_i + 1)(2J_f + 1) \left\{ \begin{matrix} S_i & L_i & J_i \\ 1 & J_f & L_f \end{matrix} \right\}^2 f(n_i L_i, n_f L_f), \quad (7)$$

where $f(n_i L_i, n_f L_f)$ is the J -independent absorption OS, while $f(n_i J_i, n_f J_f)$ represents the J -dependent absorption OS.

III. TIME-DEPENDENT SCHRÖDINGER EQUATION

Having obtained the two-electron states constructed in a spherical box, we can now solve the TDSE. The TDSE for the two-electron atom interacting with a laser pulse reads

$$i \frac{d}{dt} \Psi(\mathbf{r}_1, \mathbf{r}_2; t) = [H_a(\mathbf{r}_1, \mathbf{r}_2) + D(t)] \Psi(\mathbf{r}_1, \mathbf{r}_2; t), \quad (8)$$

where $\Psi(\mathbf{r}_1, \mathbf{r}_2; t)$ are the total (two-electron) wave function at positions \mathbf{r}_1 and \mathbf{r}_2 for each electron at time t , and $H_a(\mathbf{r}_1, \mathbf{r}_2)$ is the field-free atomic Hamiltonian as shown in Eq. (5). The time-dependent interaction operator $D(t)$ between the atom and the laser pulse is written in the velocity gauge as

$$D(t) = -\mathbf{A}(t) \cdot (\mathbf{p}_1 + \mathbf{p}_2), \quad (9)$$

where the dipole approximation has been employed, and \mathbf{p}_1 and \mathbf{p}_2 are the momenta of the two electrons with $\mathbf{A}(t)$ being the vector potential given by

$$\mathbf{A}(t) = \mathbf{A}_0 f(t) \cos(\omega t). \quad (10)$$

Here $\mathbf{A}_0 = A_0 \mathbf{e}_q$ represents the amplitude of the vector potential and \mathbf{e}_q is the unit polarization vector of the laser pulse, expressed in the spherical coordinates. ω and $f(t)$ represent the photon energy and the temporal envelope of the laser field. In this paper we have assumed an envelope with a cosine-squared function, i.e., $f(t) = \cos^2(\pi t / 2\tau)$ where τ is the full width at half maximum (FWHM) of the vector potential $\mathbf{A}(t)$. The integration time of Eq. (8) is taken from $-\tau$ to τ .

In order to solve Eq. (8), the time-dependent wave function, $\Psi(\mathbf{r}_1, \mathbf{r}_2; t)$, is expanded on the atomic basis as a linear combination of two-electron states $\Psi(\mathbf{r}_1, \mathbf{r}_2; E_n)$:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2; t) = \sum_{nJM} C_{E_n JM}(t) \Psi(\mathbf{r}_1, \mathbf{r}_2; E_n), \quad (11)$$

where $C_{E_n JM}(t)$ is the time-dependent coefficient for a state with an energy E_n , total two-electron angular momentum J , and its projection on the quantization axis M . Now, by replacing Eq. (11) into Eq. (8) we obtain a set of first-order differential equations for the time-dependent coefficients $C_{E_n JM}(t)$:

$$i \frac{d}{dt} C_{E_n JM}(t) = \sum_{n'J'M'} [E_n \delta_{nn'} \delta_{JJ'} \delta_{MM'} \\ - D_{nJMn'J'M'}(t)] C_{E_n'J'M'}(t), \quad (12)$$

where $D_{nJMn'J'M'}(t)$ represents the J -dependent dipole matrix element calculated in Sec. II D between two *triplet* states defined by the quantum numbers (nJM) and $(n'J'M')$. This

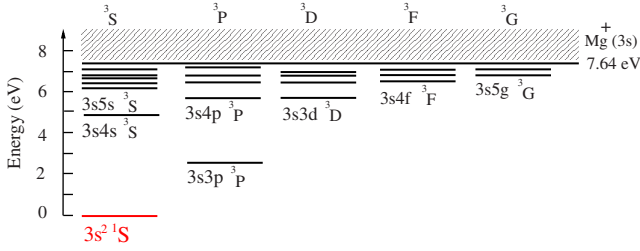


FIG. 1. (Color online) Energies of the triplet states of Mg. In order to show the relative positions with respect to the singlet ground state, $3s^2 1S$ is also shown in this energy diagram.

means that we have neglected the spin-forbidden transitions between triplet and singlet states, which is reasonable for a light atom such as Mg. Specifically in what follows, we assume that the Mg atom is initially in the triplet state of the lowest electronic configuration, $3s3p 3P_1(M=0)$, i.e.,

$$|C_{E_n JM}(t = -\tau)|^2 = \delta_{n3} \delta_{J1} \delta_{M0}. \quad (13)$$

The relevant energies of triplet states, averaged over the multiplet components, are presented in Fig. 1. Note that $3s3p 3P_J$ is the lowest triplet state located at approximately 2.71 eV from the ground state, $3s^2 1S$. Our specific choice for the initial state results in the great simplification of the time-dependent problem to deal with, since the allowed transition paths by the LP or CP field become very simple as shown in Figs. 2(a) and 2(b), respectively. If we chose a different initial state, for instance, $3s4s 3S_1$, the transition paths for the LP field would be far more complicated than those shown in Fig. 2(a), and accordingly Eq. (12) would become much more difficult to solve due to the enormous complexity of the transition paths. In contrast, this kind of complexity does not happen for the transitions between the singlet states [18].

Once we have obtained the time-dependent coefficients $C_{E_n JM}$ by solving Eq. (12), the ionization yield Y and PES dP/dE can be calculated at the end of the pulse:

$$Y = 1 - \sum_{n,J,M(E_n < 0)} |C_{E_n JM}(t = +\tau)|^2, \quad (14)$$

and

$$\left. \frac{dP}{dE} \right|_{E_n = E_e} = \sum_{J,M(E_n = E_e)} |C_{E_n JM}(t = +\tau)|^2, \quad (15)$$

where E_e represents the photoelectron energy.

IV. NUMERICAL RESULTS

Before solving the TDSE we must perform several checks regarding the accuracy of the atomic basis for the *triplet states* of Mg. Related to this, we have already obtained accurate atomic basis for the *singlet states* in our previous work [24] using FCHFP as well as MP approaches. The atomic basis states we need to solve the TDSE is constructed in a box size of 300 a.u. for the total angular momentum up to $J=9$ with 1000 states for each total angular momentum. A number of 302 B -spline polynomials of order 9 with a sine-

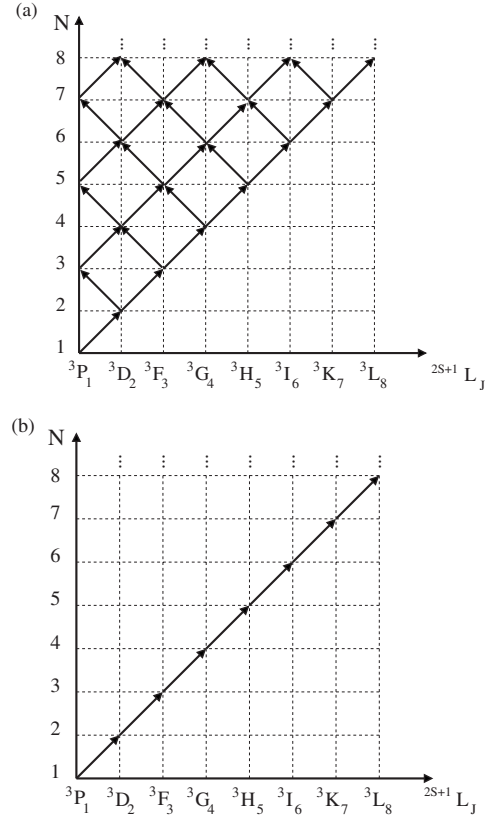


FIG. 2. Allowed ionization paths in multiphoton ionization from an $3P_1(M=0)$ initial state by (a) a linearly polarized field and (b) a right circularly polarized field.

like knot grid is employed. To check the numerical convergence we have increased the box size up to 1000 a.u. together with an increased number of total angular momentum up to $J=14$ for each given intensity. It turned out that the basis states constructed in a box of 300 a.u. with the total angular momentum up to $J=9$ with 800 states for each angular momentum are sufficient to obtain a reasonable convergence in terms of the total ionization yield as well as PES. In Table I we present the two-electron angular configurations of type $(n_1 l_1, n_2 l_2)$ included in the construction of the two-electron wave functions. The principal quantum numbers are taken values in the range $n_1=(3-7)$ and $n_2=(1-290)$ (with $n_1 \neq n_2$ if $l_1=l_2$), respectively for each symmetry. The number of the two-electron configurations varies between 1100 and 1300 for the total angular momentum up to $J=9$.

To start with, we have compared the OSs for the *triplet states* obtained by the length and velocity gauges with the FCHFP approach, and confirmed that the agreement is quite good. This is a good indication that our wave functions are accurate. As for the MP approach, however, it is well known that the physically correct dipole matrix elements can be calculated only in the length gauge [30], since the Hamiltonian becomes nonlocal due to the l dependence of the MP (see Ref. [24]), and we cannot perform a similar comparison between the two gauges.

As a more direct comparison, we have calculated the state energies, OSs, and dipole matrix elements by both FCHFP and MP approaches and compared them with the existing

TABLE I. Types of two-electron angular configurations used for the construction of two-electron wave functions.

${}^3S^e$	${}^3P^o$	${}^3D^e$	${}^3F^o$	${}^3G^e$	${}^3H^o$	${}^3I^e$	${}^3K^o$	${}^3L^e$	${}^3M^o$
<i>ss</i>	<i>sp</i>	<i>sd</i>	<i>sf</i>	<i>sg</i>	<i>sh</i>	<i>si</i>	<i>sk</i>	<i>sl</i>	<i>sm</i>
<i>pp</i>	<i>pd</i>	<i>pf</i>	<i>pd</i>	<i>pf</i>	<i>pg</i>	<i>ph</i>	<i>pi</i>	<i>pk</i>	<i>pl</i>
<i>dd</i>	<i>df</i>	<i>dg</i>	<i>pg</i>	<i>dg</i>	<i>df</i>	<i>dg</i>	<i>dh</i>	<i>di</i>	<i>dk</i>
<i>ff</i>	<i>fg</i>	<i>fh</i>	<i>df</i>	<i>fg</i>	<i>pi</i>	<i>ff</i>	<i>fg</i>	<i>gg</i>	<i>gh</i>
<i>gg</i>	<i>gh</i>	<i>pp</i>	<i>fg</i>	<i>dd</i>	<i>fg</i>	<i>gg</i>	<i>gh</i>		
		<i>dd</i>		<i>ff</i>					
		<i>gg</i>		<i>gg</i>					

theoretical and experimental data. In Table II we show the comparison of the calculated energies for the first ionization threshold and the first few triplet states $3snl\ {}^3L$ with the corresponding experimental values, where $n=(3-6)$ or $(4-7)$ for each total orbital momentum $L=S, P, D,$ and F . The energies (in units of eV) are taken with respect to the second ionization threshold Mg^{2+} and the triplet states energies are averaged over the multiplet components. The theoretical data are taken from Ref. [7] and the experimental data are taken from the database of the National Institute of Standards and Technology (NIST) [31]. There is an overall good agreement between the calculated energies and the experimental values, and in addition our MP approach provides more accurate energies than our FCHFP approach. Of course, the accuracy of the energies do not guarantee the accuracy of the wave functions, and we must further check the accuracy of the

TABLE II. Comparison of the energies for the first ionization threshold and the first few triplet states of Mg. The energies (in units of eV) are taken with respect to the second ionization threshold Mg^{2+} and the triplet state energies are averaged over the multiplet components.

	FCHFP	MP	Theory [7]	Expt. (NIST)
E_{Mg^+}	-15.000	-15.042		-15.035
$E_{3s4s}\ {}^3S^e$	-17.532	-17.581	-17.578	-17.574
$E_{3s5s}\ {}^3S^e$	-16.212	-16.257	-16.246	-16.250
$E_{3s6s}\ {}^3S^e$	-15.715	-15.759	-15.752	-15.752
$E_{3s7s}\ {}^3S^e$	-15.472	-15.515		-15.508
$E_{3s3p}\ {}^3P^o$	-19.904	-19.979	-20.027	-19.969
$E_{3s4p}\ {}^3P^o$	-16.708	-16.756	-16.756	-16.749
$E_{3s5p}\ {}^3P^o$	-15.917	-15.962	-15.957	-15.955
$E_{3s6p}\ {}^3P^o$	-15.575	-15.619	-15.613	-15.612
$E_{3s3d}\ {}^3D^e$	-16.698	-16.740	-16.740	-16.736
$E_{3s4d}\ {}^3D^e$	-15.926	-15.969	-15.963	-15.963
$E_{3s5d}\ {}^3D^e$	-15.582	-15.625	-15.619	-15.618
$E_{3s6d}\ {}^3D^e$	-15.400	-15.442	-15.436	-15.436
$E_{3s4f}\ {}^3F^o$	-15.867	-15.909		-15.903
$E_{3s5f}\ {}^3F^o$	-15.553	-15.596		-15.589
$E_{3s6f}\ {}^3F^o$	-15.383	-15.426		-15.415
$E_{3s7f}\ {}^3F^o$	-15.281	-15.323		-15.317

wave function in terms of the J -independent and -dependent OSs.

Table III presents the comparison of the J -independent OSs for single-photon transitions calculated by the FCHFP and MP approaches with other theoretical works [1,3,5] and the experimental data taken from NIST. The OSs in the length gauge are shown for single-photon transitions among the first few triplet states: $3s4s\ {}^3S \rightarrow 3s(4-7)p\ {}^3P$, $3s3p\ {}^3P \rightarrow 3s(4-7)s\ {}^3S$, $3s3p\ {}^3P \rightarrow 3s(3-6)d\ {}^3D$, $3s3d\ {}^3D \rightarrow 3s(3-6)p\ {}^3P$, and $3s3d\ {}^3D \rightarrow 3s(4-7)f\ {}^3F$. From Table III it is clear that both FCHF and MP approaches provide an accurate atomic basis for the triplet states of Mg, and the overall agreement is quite well with other accurate calcula-

TABLE III. Comparison of the J -independent single-photon oscillator strengths (in a.u. and length gauge) between the first few triplet states with ${}^3S^e$, ${}^3P^o$, ${}^3D^e$, and ${}^3F^e$ symmetry. Numbers in square brackets indicate powers of 10.

$3s4s\ {}^3S^e \rightarrow$	$3s4p\ {}^3P^o$	$3s5p\ {}^3P^o$	$3s6p\ {}^3P^o$	$3s7p\ {}^3P^o$
FCHFP	1.320	3.434[-2]	6.963[-3]	2.524[-3]
MP	1.315	3.344[-2]	6.692[-3]	2.403[-3]
Theory [5]	1.308	2.97[-2]	5.60[-3]	1.90[-3]
Theory [1]	1.314	3.13[-2]	6.3[-3]	2.2[-3]
$3s3p\ {}^3P^o \rightarrow$	$3s4s\ {}^3S^e$	$3s5s\ {}^3S^e$	$3s6s\ {}^3S^e$	$3s7s\ {}^3S^e$
FCHFP	1.369[-1]	1.546[-2]	5.227[-3]	2.468[-3]
MP	1.355[-1]	1.533[-2]	5.178[-3]	2.442[-3]
Theory [1]	1.360[-1]	1.57[-2]	5.3[-3]	
$3s3p\ {}^3P^o \rightarrow$	$3s3d\ {}^3D^e$	$3s4d\ {}^3D^e$	$3s5d\ {}^3D^e$	$3s6d\ {}^3D^e$
FCHFP	6.294[-1]	1.263[-1]	4.743[-2]	2.333[-2]
MP	6.243[-1]	1.266[-1]	4.772[-2]	2.352[-2]
Theory [1]	6.311[-1]	1.254[-1]	4.74[-2]	2.32[-2]
$3s3d\ {}^3D^e \rightarrow$	$3s3p\ {}^3P^o$	$3s4p\ {}^3P^o$	$3s5p\ {}^3P^o$	$3s6p\ {}^3P^o$
FCHFP	3.776[-1]	7.520[-3]	8.551[-3]	1.714[-3]
MP	3.745[-1]	1.014[-2]	9.073[-3]	1.814[-3]
Theory [5]	3.802[-1]	8.0[-3]	8.5[-3]	1.7[-3]
$3s3d\ {}^3D^e \rightarrow$	$3s4f\ {}^3F^o$	$3s5f\ {}^3F^o$	$3s6f\ {}^3F^o$	$3s7f\ {}^3F^o$
FCHFP	7.899[-1]	1.603[-1]	6.017[-2]	2.965[-2]
MP	7.893[-1]	1.604[-1]	6.023[-2]	2.969[-2]
Theory [3]	7.97[-1]	1.60[-1]	6.00[-2]	2.90[-2]
Theory [5]	7.852[-1]	1.587[-1]	5.93[-2]	2.91[-2]

TABLE IV. Comparison of the J -dependent single-photon absorption oscillator strengths (in a.u. and length gauge) between the first few triplet states with ${}^3S_J^e$, ${}^3P_J^o$, ${}^3D_J^e$, and ${}^3F_J^e$ symmetry. Numbers in square brackets indicate powers of 10.

	FCHFP	MP	Expt. (NIST)
$3s4s\ {}^3S_1^e \rightarrow 3s4p\ {}^3P_0^o$	1.47[-1]	1.46[-1]	1.52[-1]
$3s4s\ {}^3S_1^e \rightarrow 3s4p\ {}^3P_1^o$	4.40[-1]	4.38[-1]	4.55[-1]
$3s4s\ {}^3S_1^e \rightarrow 3s4p\ {}^3P_2^o$	7.33[-1]	7.31[-1]	7.59[-1]
$3s3p\ {}^3P_0^o \rightarrow 3s4s\ {}^3S_1^e$	1.37[-1]	1.36[-1]	1.35[-1]
$3s3p\ {}^3P_1^o \rightarrow 3s4s\ {}^3S_1^e$	1.37[-1]	1.36[-1]	1.35[-1]
$3s3p\ {}^3P_2^o \rightarrow 3s4s\ {}^3S_1^e$	1.37[-1]	1.36[-1]	1.36[-1]
$3s3p\ {}^3P_0^o \rightarrow 3s3d\ {}^3D_1^e$	6.29[-1]	6.24[-1]	5.93[-1]
$3s3p\ {}^3P_1^o \rightarrow 3s3d\ {}^3D_1^e$	1.57[-1]	1.56[-1]	1.48[-1]
$3s3p\ {}^3P_1^o \rightarrow 3s3d\ {}^3D_2^e$	4.72[-1]	4.68[-1]	4.45[-1]
$3s3p\ {}^3P_2^o \rightarrow 3s3d\ {}^3D_1^e$	6.29[-3]	6.24[-3]	5.94[-3]
$3s3p\ {}^3P_2^o \rightarrow 3s3d\ {}^3D_2^e$	9.44[-2]	9.36[-2]	8.91[-2]
$3s3p\ {}^3P_2^o \rightarrow 3s3d\ {}^3D_3^e$	5.28[-1]	5.24[-1]	4.99[-1]
$3s3d\ {}^3D_1^e \rightarrow 3s5p\ {}^3P_0^o$	4.75[-3]	5.04[-3]	4.47[-3]
$3s3d\ {}^3D_1^e \rightarrow 3s5p\ {}^3P_1^o$	3.56[-3]	3.78[-3]	3.35[-3]
$3s3d\ {}^3D_1^e \rightarrow 3s5p\ {}^3P_2^o$	2.38[-4]	2.52[-4]	2.23[-4]
$3s3d\ {}^3D_2^e \rightarrow 3s5p\ {}^3P_1^o$	6.41[-3]	6.80[-3]	6.03[-3]
$3s3d\ {}^3D_2^e \rightarrow 3s5p\ {}^3P_2^o$	2.14[-3]	2.26[-3]	2.01[-3]
$3s3d\ {}^3D_3^e \rightarrow 3s5p\ {}^3P_2^o$	8.55[-3]	9.07[-3]	8.04[-3]
$3s3d\ {}^3D_1^e \rightarrow 3s4f\ {}^3F_2^o$	7.90[-1]	7.89[-1]	7.76[-1]
$3s3d\ {}^3D_2^e \rightarrow 3s4f\ {}^3F_2^o$	8.78[-2]	8.77[-2]	8.64[-2]
$3s3d\ {}^3D_2^e \rightarrow 3s4f\ {}^3F_3^o$	7.02[-1]	7.02[-1]	6.89[-1]
$3s3d\ {}^3D_3^e \rightarrow 3s4f\ {}^3F_2^o$	1.79[-3]	1.79[-3]	1.74[-3]
$3s3d\ {}^3D_3^e \rightarrow 3s4f\ {}^3F_3^o$	6.26[-2]	6.26[-2]	6.17[-2]
$3s3d\ {}^3D_3^e \rightarrow 3s4f\ {}^3F_4^o$	7.26[-1]	7.25[-1]	7.12[-1]

tions and the experimental data. There are, however, relatively large differences in the OSs for the $3s4s\ {}^3P \rightarrow 3s6p\ {}^3P$ transition calculated by the FCHFP approach and $3s3d\ {}^3D \rightarrow 3s4p\ {}^3P$ transition calculated by the MP approach. Besides a small difference exists in the OS of the $3s3d\ {}^3D^e \rightarrow 3s4p\ {}^3P^o$ transition calculated by both FCHF and MP approaches. This might be due to the very small energy difference between these two bound states of 0.016 eV.

Finally, in Table IV we show the comparison of the J -dependent single-photon absorption OSs calculated by the FCHF and MP approaches with the experimental data taken from NIST. The calculated OSs are shown for the length gauge for the single-photon transitions among the first few triplet states: $3s4s\ {}^3S_1 \rightarrow 3s4p\ {}^3P_{0,1,2}$, $3s3p\ {}^3P_{0,1,2} \rightarrow 3s4s\ {}^3S_1$, $3s3p\ {}^3P_{0,1,2} \rightarrow 3s3d\ {}^3D_{1,2,3}$, $3s3d\ {}^3D_{1,2,3} \rightarrow 3s5p\ {}^3P_{0,1,2}$, and $3s3d\ {}^3D_{1,2,3} \rightarrow 3s4f\ {}^3F_{2,3,4}$. Again, the overall agreement is quite good between our results and the experimental values. Therefore in what follows we present numerical TDSE results using the atomic basis calculated by the FCHFP only.

Having checked the accuracy of the atomic basis for the triplet states, we are now ready to perform the time integra-

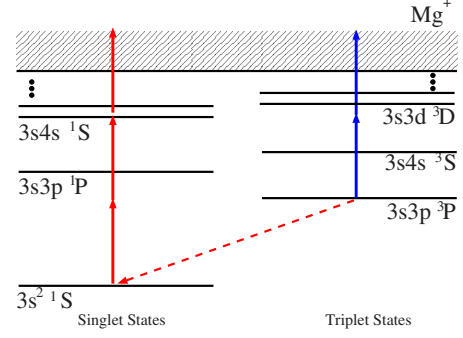


FIG. 3. (Color online) Ionization scheme for Mg, at the photon energy of 2.7 eV, which includes the atomic basis of both singlet and triplet states resonantly coupled through the $3s^2\ {}^1S \rightarrow 3s3p\ {}^3P$ transition.

tion of Eq. (12) under various intensities for both LP and CP laser pulses. Recall that a number of 800 two-electron states for each total angular momentum up to $J=9$ was used for the numerical integration of TDSE thus leading to a total number of 7200 coupled differential equation to be solved. Please note that the typical size of the dipole matrices is about 800×800 . The Runge-Kutta subroutines were used to perform the numerical integration of TDSE. As we have already mentioned, our initial state is $3s3p\ {}^3P_1$ ($M=0$) and the photon energy is 2.7 eV which can be obtained from the second harmonic of a Ti:sapphire laser. Since the energy difference from $3s3p\ {}^3P_1$ to the ionization threshold is about 4.93 eV, at least two photons are needed for ionization. The intensity range we have considered for the numerical calculations is from 10^{11} W/cm² up to 10^{14} W/cm². The Keldysh parameter γ is 1.1 at 10^{14} W/cm².

The last check we should perform is that we may neglect the entire singlet states when we solve the TDSE for the triplet states. This check is particularly important, since our photon energy (2.7 eV) is resonant with the spin-forbidden $3s^2\ {}^1S_0 - 3s3p\ {}^3P_1$ transition. Because we cannot calculate the dipole matrix elements for spin-forbidden transitions within the method we use, we have taken the experimental OS for the spin-forbidden $3s^2\ {}^1S_0 - 3s3p\ {}^3P_1$ transition, 2.38×10^{-6} a.u. from NIST, which is at least five and six orders of magnitude smaller than those for the (nearest) $3s3p\ {}^3P \rightarrow 3s3d\ {}^3D$ and $3s^2\ {}^1S \rightarrow 3s3p\ {}^1P$ transitions, respectively. By phenomenologically including this spin-forbidden $3s^2\ {}^1S_0 - 3s3p\ {}^3P_1$ transition as shown in Fig. 3, we now solve two sets of TDSEs for the singlet and triplet series which are coupled through the resonant but very weak spin-forbidden $3s^2\ {}^1S \rightarrow 3s3p\ {}^1P$ transition. After solving the two sets of TDSEs, we have ensured that, provided the $3s3p\ {}^3P_1$ initial state, the influence of the singlet states is extremely small as we expected, and we have safely neglected them in the following numerical calculations.

A. Ionization yield

The ionization yield is shown in Fig. 4(a) with a log-log scale as a function of peak intensity for the LP (solid) and RCP (dashed) pulses. For the photon energy 2.7 eV we have

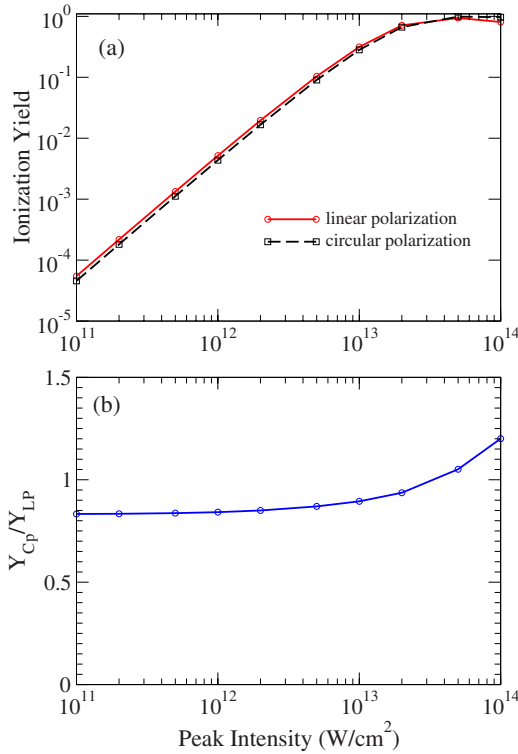


FIG. 4. (Color online) (a) Ionization yield as a function of the peak intensity for linearly (solid) and right circularly polarized (dashed) laser pulses at the photon energy of 2.7 eV. The initial state of Mg is the triplet state $3s3p\ ^3P_1$ ($M=0$) and the laser pulse duration is 20 fs (FWHM). (b) Ratio of the ionization yield by the right circularly polarized pulse Y_{CP} to that by the linearly polarized pulse Y_{LP} .

chosen, both curves have a linear dependence on the peak intensity, up to $10^{13} W/cm^2$, with a slope of 1.9, indicating that our results agree well with the prediction of lowest-order perturbation theory (LOPT). For peak intensities higher than $2 \times 10^{13} W/cm^2$, saturation starts to take place. Figure 4(b) presents the ratio between the ionization yield by the CP and LP pulses, Y_{CP}/Y_{LP} , as a function of peak intensity. For peak intensities up to $10^{13} W/cm^2$, the ionization yield by the RCP pulse is about 0.83 times smaller than that by the LP pulse. Figures 4(a) and 4(b) also suggest that ionization by the LP pulse is more efficient than the RCP pulse when ionization starts from the $3s3p\ ^3P_1$ initial state. This result is somehow different from our previous time-dependent calculations for multiphoton ionization of Mg [18]: It showed that, when less than four photons are needed for ionization, ionization from the singlet state with 1S symmetry by the CP field starts to become more efficient than that by the LP field for a wide range of photon energy. In the LOPT regime the main reason that the ionization yield by the CP pulse is larger or smaller than by the LP pulse, for a nonresonant photon energy, is determined by the particular values of the total angular momentum and its projection on the quantization axis.

B. Photoelectron energy spectra

In Fig. 5 we present representative results of the PES by the LP (solid) and RCP (dashed) pulses at the peak intensity

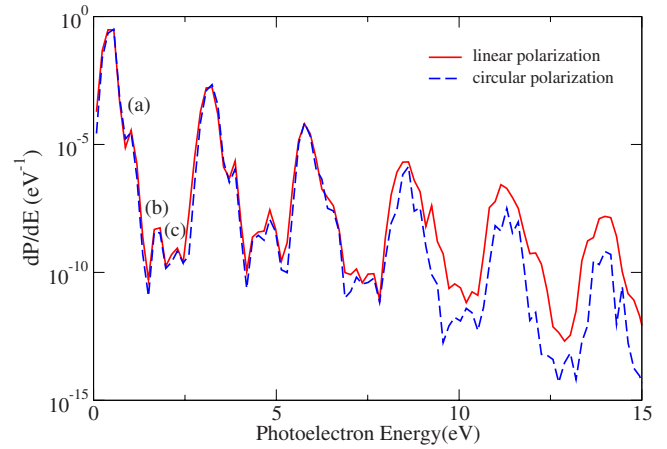


FIG. 5. (Color online) Photoelectron energy spectra by the linearly (solid) and right circularly polarized (dashed) laser pulses at the photon energy of 2.7 eV. The initial state of Mg is the triplet state $3s3p\ ^3P_1$ ($M=0$). The pulse duration and peak intensity are 20 fs (FWHM) and $5 \times 10^{12} W/cm^2$, respectively.

of $5 \times 10^{12} W/cm^2$. As it goes to the higher orders of above threshold ionization (ATI), the height of the ATI peaks by the LP pulse is more than one order of magnitude larger than that by the RCP pulse. Of course, this could be qualitatively understood that photoionization by the LP pulse has more chance to be near resonance with bound states than the CP pulse, and in addition there are more accessible continua for the LP pulse. It is interesting to note that subpeaks appear between the main ATI peaks, labeled as (b) and (c), for both LP and RCP pulses, and the height of the subpeaks is at least 5 orders of magnitude smaller than that of the main peaks. In addition there are small subpeaks, labeled as (a), on the right-side shoulders of the main peaks for both LP and RCP pulses. These results are reminiscent of the subpeaks studied in our recent paper for the singlet states of Mg [18], in which multiphoton ionization of Mg from the singlet ground state has been theoretically studied. In that paper the origin of the subpeaks is clearly attributed to the bound states $3snp\ ^1P$ ($n=3,4,5,\dots$) which are far off-resonantly excited by the spectral wing of the pulse. In the next subsection we will identify the origin of the subpeaks in PES in a similar manner.

Figures 6(a)–6(c) show the variation of the PES for three different pulse durations, (a) $\tau=80$ fs, (b) 40 fs, and (c) 20 fs (FWHM). The photon energy and peak intensity are 2.7 eV and $5 \times 10^{12} W/cm^2$, respectively. As the pulse duration decreases the ATI peaks are broadened and their heights are decreased. Besides, the subpeaks gradually disappear because of the broadening of the Fourier bandwidth of the shorter pulse.

C. Origin of the subpeaks in the photoelectron energy spectra

The method we have used to identify the origin of the subpeaks in the PES mentioned in the previous subsection is quite similar to the one employed in our previous work [18] for singlet states of Mg: If the subpeaks arise from some photoionization processes involving four or five photons to

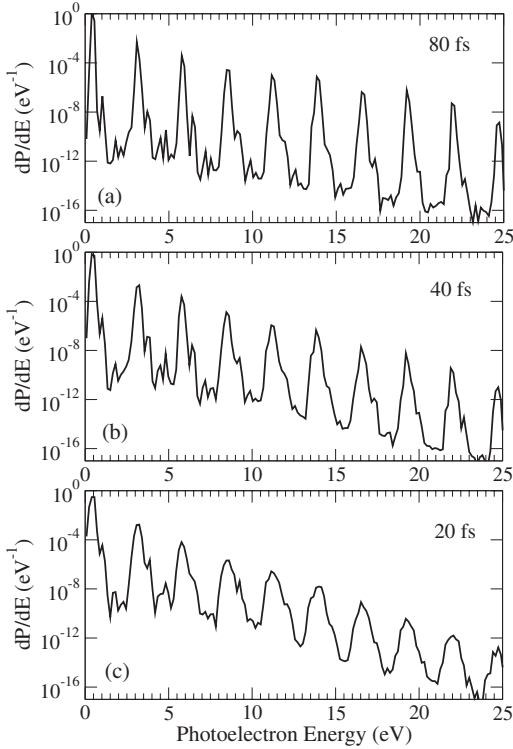


FIG. 6. Photoelectron energy spectra by the linearly laser pulses at the photon energy of 2.7 eV and the peak intensity 5×10^{12} W/cm² for three different values of the pulse duration (a) 80 fs, (b) 40 fs, and (c) 20 fs (FWHM). The initial state of Mg is the triplet state $3s3p\ ^3P_1$ ($M=0$).

leave the ionic core in some excited state, the height of the subpeaks with respect to the main peaks would be even much smaller than those in Fig. 5 at the peak intensity of 5×10^{12} W/cm², assuming the typical excitation or ionization efficiency with four or five photons. The subpeaks cannot be attributed to some intensity-dependent effects, either; the ponderomotive shift is as small as 0.098 eV at peak intensity 5×10^{12} W/cm², and there are no triplet states coming into resonance during the pulse duration for both LP and CP pulses. Perhaps the subpeaks originate from the *off-resonant excitations* of some bound states, which, however, must be confirmed by the numerical calculations. Since we propagate the TDSE on the atomic basis, we can easily check this by solving the TDSE after the removal of the particular bound state under suspect, and comparing the PES with the original one with all states included [18].

In Figs. 7(a)–7(c) we summarize the results for the PES calculated with the LP pulse at the peak intensity of 5×10^{12} W/cm². They are the results obtained after the removal of a particular bound state, namely (a) $3s3d\ ^3D_1$, (b) $3s4d\ ^3D_1$, and (c) $3s5d\ ^3D_1$, upon solving the TDSE, and compared with the result with the complete calculation of PES including all atomic triplet states of Mg. When the $3s3d\ ^3D_1$ state is removed [Fig. 7(a)], the spike on the right-side shoulders of each main peak disappears. In addition the height of the main peaks is reduced since the $3s3d\ ^3D_1$ state brings an important (but nonresonant) contribution to the ionization process. In this particular case the laser detuning

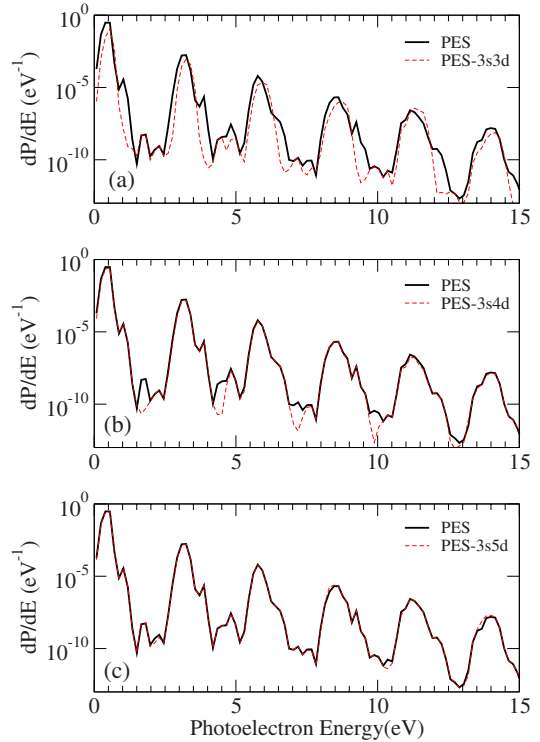


FIG. 7. (Color online) Comparison of the photoelectron spectra by a linearly polarized laser pulse at the photon energy of 2.7 eV when the (a) $3s3d\ ^3D_1$, (b) $3s4d\ ^3D_1$, and (c) $3s5d\ ^3D_1$ bound states of Mg are removed from the atomic basis when solving the time-dependent Schrödinger equation. The pulse duration and peak intensity are 20 fs (FWHM) and 5×10^{12} W/cm², respectively.

is 0.53 eV with respect to the $3s3p\ ^3P_1$ state. That is, the small spike, located at 1.02 eV, corresponds to the single-photon ionization process from the off-resonantly excited $3s3d\ ^3D_1$ state. Similarly, by removing the $3snd\ ^3D_1$ ($n=4$ and 5) states different subpeaks labeled as (b) and (c) in Fig. 5 disappear, as can be seen in Figs. 7(b) and 7(c). This indicates that the physical origin of the subpeaks (a), (b), and (c) in Fig. 5 for the triplet states of Mg is quite similar to that we have found for the singlet states of Mg [18]. Briefly, *off-resonant* bound states such as $3snd\ ^3D_1$ ($n=3,4,5,\dots$) are the origin of the subpeaks. Note that these states are located at 5.94, 6.71, and 7.06 eV, respectively, from the ground state $3s^2\ ^1S$, and accordingly the corresponding detunings are 0.53, 1.3, and 1.65 eV from the $3s3p\ ^3P_1$ state since the photon energy is 2.7 eV. As for Fig. 7(c) we note that, in addition to the $3s5d\ ^3D_1$ state, another not-identified state(s) might contribute to the subpeaks of interest labeled as (c).

V. CONCLUSIONS

In conclusion, we have theoretically studied multiphoton ionization of Mg from the triplet $3s3p\ ^3P_1$ state by linearly and circularly polarized fs pulses. For that purpose we have first constructed the atomic basis with J -dependent dipole matrix elements for two active electrons, and then solved time-dependent Schrödinger equations with them. Since the spin-orbit interaction is rather weak for the Mg atom,

J -dependent dipole matrix elements obtained by only taking into account the geometric (angular) part of the wave functions result in rather accurate values and compare well with the existing theoretical and experimental data. For the time-dependent calculations for multiphoton ionization from the triplet $3s3p\ ^3P_1$ state, the photon energy we have specifically chosen is 2.7 eV and corresponds to the $3s3p\ ^3P_1 \rightarrow 3s^2\ ^1S_0$ transition which is spin-forbidden and extremely weak. We have ensured that, even for the resonant photon energy, the

singlet states do not influence the photoionization process. The ionization yields have been found to be larger for the linearly polarized pulse than for the circularly polarized pulse. Since the Mg atom has a rather rich level structure, the photoelectron energy spectra exhibits subpeaks in addition to the ordinary main ATI peaks. We have clarified the source of those subpeaks as ATI originating from some triplet bound states which are far off-resonantly excited by the spectral wing of the pulse.

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