Molecular Attosecond Photoionization with Few Cycle XUV Laser Pulses

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Abstract. We present molecular attosecond ionization with few cycle XUV laser pulses from numerical solutions of time dependent Schrödinger equations. Simulations performed on aligned \( \text{H}_2^+ \) exhibit a signature of red-shifts in photoelectron energy spectra. This is shown to be critically sensitive to the pulse duration and wavelength and is attributed to the broad spectral width of the ionizing pulses and diminishing electronic Franck-Condon factors with short pulses. We analyze the laser parameter dependence of the energy spectra by a perturbative model.

1. Introduction
Investigation of electron dynamics in atoms, molecules and solids on its nature time scale of the attosecond (1 asec=10\(^{-18}\)s) nowadays has become a topical subject with the rapid developments of the generation and characterization of such ultrashort laser pulses [1, 2, 3]. In particular, the generation of attosecond laser pulses has led to imaging pump-probe techniques from laser Coulomb explosion imaging [4] of nuclear motion to laser induced electron diffraction (LIED) [5, 6] of coupled electron-nuclear motion. To date the shortest single pulse width of 67 asec duration has been achieved from high-order harmonic generation (HHG) [7], thus offering a new tool to watch pure electronic quantum effects without interference from nuclear motion [8], and allowing in particular through attosecond imaging the creation of electron movies [9]. Attosecond pulses therefore allow one to separate electronic and nuclear effects due to the different time scales of attosecond for electron motion and femtosecond for nuclear motion.

Using extreme ultraviolet (XUV) light from high-order harmonics (HHG) [10] or free electron lasers (FEL) [11], coherent electron wave packets (CEWPs) can be created inside atoms and molecules on the attosecond time scale and sub-nanometer dimension [12, 13, 14, 15]. Thus electron dynamics in CEWPs can be monitored by measuring ultrafast photoelectron angular and energy distributions. Many studies have focused on determining atomic and molecular orbital configurations [16, 17], multi-pathway quantum interference [18, 19, 20, 21, 22] and electron correlations [23, 24, 25] by XUV source or combined with ultrashort intense infrared (IR) laser pulses. An alternative efficient tool has been recently proposed to observe attosecond electron motion by measuring the generated radiation, molecular high-order harmonic generation (MHOHG), as a function of the pump-probe delay in a dissociating molecule [26]. XUV-pump-probe experiments have been adopted in tracing atomic coherences [27] and molecular nuclear wave packet dynamics [28]. Few cycle attosecond XUV pulses have recently been used also to control electronic motion [29, 30]. It has been shown that the symmetry of electron wave packet...
momentum and energy spectra is critically sensitive to the pulse carrier-envelope phase (CEP) and intensities [29]. Such sensitivity in the vicinity of two-electron doubly excited (autoionizing) states has also been examined [30]. We also have shown that intense attosecond magnetic field pulses and circular electronic currents can be induced [31] by means of few cycle circularly polarized attosecond XUV pulses which can be produced from circularly polarized MHOHG [32, 33].

In the present report, we investigate ultrafast molecular photoionization distributions in intense few cycle laser pulses from numerical solutions of the three dimensional (3D) time dependent Schrödinger equation (TDSE) for aligned $\text{H}_2^+$. It is found that an energy red shift occurs in the molecular photoelectron energy spectra relative to the classical above threshold ionization (ATI) kinetic energy $n\hbar\omega - I_p$, where $I_p$ is the molecular ionization potential. The shift is shown to be sensitive to the pulse duration and is a function of ATI photoelectron kinetic energies. We adopt a perturbative theory model to describe such sensitivity. A fixed nuclei approach (Born-Oppenheimer approximation) is appropriate for the simulation due to the longer femtosecond (fs) time scale of nuclear motions. Throughout this paper, atomic units (a.u.) $\hbar = m_e = 1$ are used unless otherwise stated.

The paper is arranged as follows: In section 2, we briefly describe the computational methods for time-dependent quantum electron wave packet calculations from the corresponding TDSEs. Numerical results for intense ultrashort linearly polarized XUV laser pulses interacting with an aligned $\text{H}_2^+$ are shown in section 3. Effects of pulse duration and wavelength and photoelectron kinetic energies are reported. Finally, we summarize our findings in section 4.

2. Numerical methods

We here briefly describe the method for numerically solving the TDSE for an aligned molecular ion $\text{H}_2^+$ interacting with a linearly polarized laser pulse. The corresponding 3D TDSE with static nuclei in cylindrical coordinates $(\rho, \theta, z)$ is expressed as

$$i\frac{\partial}{\partial t} \Psi(t, r) = H(r, t)\Psi(r, t), \quad (1)$$

where the field-mater Hamiltonian $H(r, t) = T(r) + V(r) + \mathbf{r} \cdot \mathbf{E}(t)$, $r = (\rho, \theta, z)$ with $x = \rho \cos \theta$ and $y = \rho \sin \theta$. $(x, y)$ defines the molecular plane. The molecular kinetic energy (Laplacian) term is given by

$$T(\rho, \theta, z) = -\frac{1}{2\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) - \frac{1}{2\rho^2} \frac{\partial^2}{\partial \theta^2} - \frac{1}{2\rho^2} \frac{\partial^2}{\partial z^2}. \quad (2)$$

$V(r)$ is the two center Coulomb repulsion for protons separated by internuclear distance $R$. The field-molecule interaction is treated in the length gauge with a laser pulse of the form

$$E(t) = E_0 \sin^2(\pi t/T) \cos(\omega t + \phi), \quad (3)$$

propagating along the $z$ axis with polarization in the molecular $(x, y)$ plane. $T = n\tau$ is the pulse duration where one optical cycle $1\tau = 2\pi/\omega$ and $n$ is the number of cycles.

We solve numerically the 3D $\text{H}_2^+$ TDSE by a five-point finite difference method and fast Fourier transform technique combined with high-order split-operator methods [34, 35]. The time step is fixed at $\Delta t = 0.01$ a.u. (1 a.u.$=24$ asec) and the spatial discretization is $\Delta \rho = \Delta z = 0.25$ a.u. (1 a.u.$=1$ a$_0$, Bohr radius), ensuring a maximin momentum spread $\Delta p = \pi/\Delta \rho = 4\pi$ a.u., for radial grid sizes $0 \leq \rho \leq 128$ a.u., $|z| \leq 64$ a.u., and the angle grid size $\Delta \theta = 0.01$ radian. To prevent unphysical effects due to the reflection of the wave packet from the boundary, a “mask function” with the form $\cos^{1/8}[\pi(\rho - \rho_a)/2\rho_{\text{abs}}]$ [17] is used at $\rho_{\text{abs}} = \rho_{\text{max}} - \rho_a = 24$ a.u. with $\rho_{\text{max}} = 128$ a.u.
For an intense laser pulse, a quite large grid range must be used to obtain via Fourier transform the high energy of the ejected electron in the ionization spectra. In the present work we use an efficient method by calculating a radial flux (electron current density) \( S_e(t) \) to describe the ionization spectra, where high kinetic energy of ionized electron can be accurately calculated. The electron wave function \( \psi(p, \theta, t) \) generates the radial flux \( S_e(t) \) at an asymptotic point \( \rho_f = 100 \text{ a.u.} \) along the radial direction in the molecular \((x, y)\) plane before the wave packet is absorbed. Then the electron angular distributions are given by \[ S_e(\theta, t) = \frac{1}{2i} \left[ \psi^*(t) \frac{\partial \psi(t)}{\partial \rho} - \frac{\partial \psi^*(t)}{\partial \rho} \psi(t) \right]_{\rho=\rho_f}. \] (4)

The corresponding energy-resolved angular differential yield (ionization spectra) is then obtained by a Fourier transform after integrating out \( z \) perpendicular to the \((x, y)\) molecular plane, i.e., averaged over \( z \):

\[ S_e(\theta, E_e) \sim \int dz \int e^{-iE_e t} S_e(\theta, t) dt, \] (5)

where \( E_e = p_e^2/2 \) is the kinetic energy of an ejected electron with electron wavelength \( \lambda_e = 2\pi/p_e \) (in a.u.), and \( p_e = (p_x^2 + p_y^2)^{1/2} \) is the total momentum of a photoelectron. With the transformation \( p_x = p_e \cos \theta \) and \( p_y = p_e \sin \theta \), we then obtain the 2D momentum distributions in the molecular \((x, y)\) plane of photoelectrons from equation (5).

### 3. Numerical Results and Discussions

We first consider single photon ionization processes by XUV laser pulses with frequency \( \omega > I_p \). For higher order ionization, their spectral intensity decrease rapidly as the photoelectron kinetic energy increases \[22\]. Figure 1 shows molecular photoelectron momentum \((p_x, p_y)\) distributions for the \( x \) aligned \( \text{H}_2^+ \) initial ground \( 1s\sigma_g \) electronic state at equilibrium \( R_e = 2 \text{ a.u.} \) by intense linearly polarized few cycle attosecond XUV laser pulses with intensity \( I_0 = 5 \times 10^{15} \text{ W/cm}^2 \) (\( E_0 = 0.38 \text{ a.u.} \)), wavelength \( \lambda = 10 \text{ nm} \) (\( \omega = 4.56 \text{ a.u.} \)), and phase \( \phi = 0 \). Four pulse durations \( T = n\pi \) are used with numbers of cycles \( n = 6, 4, 3, \) and \( 2 \), respectively. The laser pulses are polarized along the \( x \) axis (the molecular internuclear axis \( R \)). Since the Keldysh parameter \( \gamma = \sqrt{I_p/2U_p} = 18 \gg 1 \), where \( U_p = E_0^3/4\omega^2 \) is the ponderomotive energy and \( I_p = 1.1 \text{ a.u.} \), a multi-photon ionization regime defines the processes. Furthermore, since the wavelength of the continuum electron \( \lambda_e = 2.36 \text{ a.u.} \) \( > R_e \), no electron diffraction occurs \[5\].

**Table 1.** Photoelectron momenta \( p_e \) (kinetic energies \( E_e \)) and the corresponding momentum (energy) shift \( \Delta p_e = |p_e - p_e| \) (\( \Delta E_e = |E_e - E_e| \)) relative to the classic values \( p_e = \pm \sqrt{2(\omega - I_p)} \) (\( E_e = \omega - I_p \)) for the \( x \)-aligned equilibrium molecular ion \( \text{H}_2^+ \) with intensity \( I_0 = 5 \times 10^{15} \text{ W/cm}^2 \), wavelengths \( \lambda = 10 \text{ nm} \) (angular frequency \( \omega = 4.56 \text{ a.u.} \)) and \( \lambda = 20 \text{ nm} \) (\( \omega = 2.28 \text{ a.u.} \)) few cycle attosecond XUV laser pulses at different durations \( n\pi \). Atomic units (a.u.) are used for the momentum \( p_e \) and energy \( E_e \).

| \( n\pi \) | \( \lambda = 10 \text{ nm} \), \( p_e = \pm 2.63 \text{ a.u.} \) | \( \Delta p_e \) \((\Delta E_e)\) | \( \lambda = 20 \text{ nm} \), \( p_e = \pm 1.54 \text{ a.u.} \) | \( \Delta p_e \) \((\Delta E_e)\) |
|---|---|---|---|---|
| \( 6\pi \) | \( \pm 2.57 \) \((3.3)\) \| \(0.06 \) \((0.16)\) \| \( \pm 1.51 \) \((1.14)\) \| \(0.02 \) \((0.04)\) |
| \( 4\pi \) | \( \pm 2.5 \) \((3.13)\) \| \(0.13 \) \((0.33)\) \| \( \pm 1.49 \) \((1.11)\) \| \(0.04 \) \((0.07)\) |
| \( 3\pi \) | \( \pm 2.37 \) \((2.81)\) \| \(0.26 \) \((0.65)\) \| \( \pm 1.45 \) \((1.05)\) \| \(0.08 \) \((0.13)\) |
| \( 2\pi \) | \( \pm 2.0 \) \((2.0)\) \| \(0.63 \) \((1.46)\) \| \( \pm 1.38 \) \((0.95)\) \| \(0.15 \) \((0.23)\) |
From figure 1 we see that in the ultrashort few cycle attosecond XUV laser pulses the momentum distributions are critically sensitive to the pulse duration $n\tau$. Comparing to the classical momentum predicted by $p_c = \sqrt{2(\omega - I_p)}$ (dash circles), a red shift of the photoelectron distribution occurs. As the duration or number $n$ of pulse cycles decreases, the peak positions of the ionization distributions, i.e., the photoelectron energy, decreases as well. The corresponding photoelectron momenta and kinetic energies are listed in table 1. As shown in figure 1(a) for a duration of 6 cycles ($T = 200$ asec), the momenta of the photoelectron are $p_e = \pm 2.58$ a.u., which are nearly equal to the classical values $p_c = \pm \sqrt{2(\omega - I_p)} = \pm 2.63$ a.u. with a slight difference $\Delta p_e = 0.06$ a.u. ($\Delta E_e = 0.16$ a.u.). Decreasing the pulse duration $T = n\tau$ leads to an increase of the red shift of the photoelectron momentum $\Delta p$ and energy $\Delta E_e$. At $T = 2\tau = 66$ asec, the largest red shift of the ionization distributions is obtained, where $\Delta p_e = 0.63$ a.u. ($\Delta E_e = 1.46$ a.u.), approximate 10 times the results at $T = 6\tau$. Moreover, as the pulse duration $n\tau$ decreases, the pulse spectral width broadens correspondingly.

Similar results are obtained in figure 2 with $\lambda = 20$ nm ($\omega = 2.28$ a.u.) laser pulses at different durations. The other parameters are the same as those in figure 1. It is found that the photoelectron distributions shift to low energy region, i.e., a red shift, with decrease of the number $n$ of the pulse cycle as well. The values of the photoelectron momentum (kinetic energy) and corresponding energy shifts are also listed in table 1. Comparing with the ionization at shorter wavelength $\lambda = 10$ nm laser pulses, we note that these distributions exhibit smaller shifts $\Delta p_e$ ($\Delta E_e$).
Figure 2. (Color online) Photoelectron momentum distributions in $x$ aligned H$_2^+$ by a single color linearly $x$ polarized few cycle attosecond XUV laser pulse with intensity $I_0 = 5 \times 10^{15}$ W/cm$^2$, wavelength $\lambda = 20$ nm (angular frequency $\omega = 2.28$ a.u.), and phase $\phi = 0$ for four different durations: (a) $T = 6$ o.c. (400 asec), (b) $T = 4$ o.c. (266 asec), (c) $T = 3$ o.c. (200 asec), and (d) $T = 2$ o.c. (132 asec). The classical momenta $p_e$ corresponding to photoelectron energy $E_e = p_e^2/2 = \omega - I_p$ are shown as dash circles with radii $p_e = 1.54$ a.u. ($E_e = 1.18$ a.u.).

To understand the occurrence of momentum and energy shifts of the photoelectron in intense few cycle attosecond XUV pulses, we adopt a perturbation ionization model to describe the effect of the pulse duration $n\tau$ on the distributions. Considering a direct one photon electrical dipole transition from the initial ground $1s\sigma_g$ electronic state to the continuum, the probability amplitude is given by

$$\frac{dP}{d\Omega} \propto |\langle \psi_{Ec}^E | r | \psi_{1s\sigma_g} \rangle|^2 \tilde{E}^2(\omega)$$

(6)

where $\psi_{Ec}^E$ is the continuum electron wave function with energy $E_e$ and $\psi_{1s\sigma_g}$ is the initial state. The laser field $\tilde{E}(\omega)$ in the frequency domain obtained by a Fourier transform of the driving laser pulse, $E(t) = \int E(t)e^{-i\omega t}dt$, is a function of the pulse duration $n\tau$. Figure 3 illustrates the ionization amplitudes for the $\lambda = 10$ nm and 20 nm laser pulses with difference duration $n\tau$ obtained from equation (6) for a one dimensional (1D) model polarized along the molecular internuclear $R$ axis (the $x$ axis). We use a plane wave to describe the continuum wavefunction $\psi_{Ec}^E = A_0 \exp(ip_ex)$ and the initial $1s\sigma_g$ electronic state is a linear combination of the hydrogenic 1s orbitals $\psi_{1s\sigma_g} = (\psi_{1s}(-R/2) + \psi_{1s}(R/2))/\sqrt{2}$. From equation (6) one sees that the photoelectron distributions are a product of an electronic Franck-Condon factor $|\langle \psi_{Ec}^E | r | \psi_{1s\sigma_g} \rangle|$ and the pulse spectral width $\tilde{E}(\omega)$. The first depends on the photoelectron kinetic energy $E_e (p_e)$ and the second one is a function of the number $n$ of cycle. The higher the photoelectron kinetic energy the smaller the ionization probability due to decreasing Franck-Condon factor. Of note is that we only consider the case of the photoelectron distributions along
Figure 3. (Color online) Ionization yields obtained from the 1D perturbation model in equation (6) by \( \lambda = 10 \text{ nm} \) and \( \lambda = 20 \text{ nm} \) few cycle laser pulses with different durations. Green line denotes central photon energy of \( \omega - I_p \). Signal intensity units are arbitrary.

The laser polarization since no electron diffraction occurs.

For the ionizing \( \lambda = 10 \text{ nm} \) and \( 20 \text{ nm} \) laser pulses in figures 1 and 2, the spectral widths are limited. The ionization distribution is a resulting effect of \( |\langle \psi_{Ee}^{Ee} | r | \psi_{1s\sigma_g} \rangle| \) and \( \tilde{E}(\omega) \) in equation (6). As illustrated in figures 3(a) and 3(b), the photoelectron energy spectra are asymmetric with respect to the kinetic energy \( E_c = \omega - I_p \), corresponding to the central frequency \( \omega \) of the attosecond pulse. The ionization probability in the low energy region is slightly larger than that in the high energy region. As a result, a red shift occurs in photoelectron energy spectra in figures 3(a) and 3(b). Decreasing the pulse duration \( T \) leads to broadening of the pulse field \( \tilde{E}(\omega) \). The photoelectron energy spectra become broad as well. Then the asymmetry arising from the product of \( |\langle \psi_{Ee}^{Ee} | r | \psi_{1s\sigma_g} \rangle| \) and \( \tilde{E}(\omega) \) increases, i.e., the energy shift increases. Thus one gets in figures 1 and 2 the energy shifts in photoelectron energy spectra are sensitive to the pulse duration. For ionization with many cycle laser pulses the corresponding asymmetry and the energy shift in photoelectron energy spectra are very small and can be ignored due to narrow spectral widths. This can be seen in figure 3(b) for the \( 6\tau \) pulses. Moreover, for the cases with fixed \( n \), the pulse spectral width \( \tilde{E}(\omega) \) at \( \lambda = 10 \text{ nm} \) is broader than that at \( \lambda = 20 \text{ nm} \). Thus a larger momentum shift \( \Delta p_e (\Delta E_e) \) is obtained in figure 1 and table 1 by the \( \lambda = 10 \text{ nm} \) laser pulse.

We next show the energy shift of photoelectron energy spectra in higher order molecular ATI spectra. Figure 3 shows ATI spectra of \( x \)-aligned \( \text{H}_2^+ \) for \( \lambda = 20 \text{ nm} \) linearly polarized laser pulses at \( I_0 = 5 \times 10^{15} \text{ W/cm}^2 \) and \( \phi = 0 \). Three ionization processes with pulse durations...
Figure 4. (Color online) Molecular ATI spectra in $x$ aligned $\text{H}^+_2$ by a single color linearly $x$ polarized few cycle attosecond XUV laser pulse with intensity $I_0 = 5 \times 10^{15}$ W/cm$^2$, wavelength $\lambda = 20$ nm (angular frequency $\omega = 2.28$ a.u.), and phase $\phi = 0$ for different durations $T = 6$ o.c. (solid line) 4 o.c. (dash line), and 2 o.c. (dash-dot line). Green lines present the classical photoelectron energies $E_c = \omega - I_p = 1.18$ a.u. and $2\omega - I_p = 3.46$ a.u.

$T = 6\tau$, $4\tau$ and $2\tau$ are simulated. Form figure 4 one sees that the shift of photoelectron energy spectra is also sensitive to the photoelectron energy $E_e$. For both $6\tau$ and $4\tau$ pulses, small energy shifts $\Delta E_e$ are obtained in the first ATI at energy $E_e = \omega - I_p$, as listed in table 1. For the second ATI peak at $E_e = 2\omega - I_p$, the corresponding energy shift $\Delta E_e$ is larger. The higher the photoelectron energy $E_e$ the smaller the ionization probability. The amplitude of the Franck-Condon factor $|\langle \psi_{E_e}^E | r | \psi_{1s\sigma_g} \rangle |$ in equation (6) decreases for higher order ATI spectra, therefore resulting in large energy shifts with same pulse durations. Due to effects of the pulse spectral width, the energy shift with $T = 4\tau$ is also larger than that with $T = 6\tau$ at $E_e = 2\omega - I_p$. Similar processes occur for higher order ATI spectra at energies $E_e > 2\omega - I_p$, illustrated at the end of the spectrum (figure 4). Furthermore, as illustrated in figure 4 at $T = 2\tau$ the ATI spectra become nearly a continuum and the corresponding red shift can not read any more.

4. Conclusions
In summary, we present attosecond photoelectron distributions of aligned $\text{H}^+_2$ by few cycle XUV laser pulses. Numerical results show pulse duration dependent red energy shifts in the spectra. This coincides with predictions from a perturbative model. The red energy shift can be interpreted as diminishing electronic Franck-Condon factors with shorter pulses durations which increase spectral band widths of the attosecond pulses around a central frequency $\omega$. This is in contrast to high frequency, high intensity long pulses which induce ground state Stark shifts thus inducing blue shifts of ionized electron energies [36].

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6. References
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