Photoelectron interference fringes by super intense x-ray laser pulses

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Abstract. The photoelectron spectra of H\textsuperscript{−} produced by circularly polarized strong high-frequency laser pulses are theoretically studied. An oscillating substructure in the above-threshold ionization (ATI) peaks is observed, which extends the validity of the earlier findings in the 1D calculations [K. Toyota et al., Phys. Rev. A 76, 043418 (2007)] and 3D calculations for linear polarization [O. I. Tolstikhin, Phys. Rev. A 77, 032712 (2008)]. Its origin is due to an interference between a pair of photoelectron wave packets created in the rising and falling part of the pulse, which appears clearly in the stabilization regime.

1. Introduction
Recent experimental developments in free-electron lasers [1] provide us with coherent light sources in the X-ray range. Such new light sources experimentally opened up the so-called high-frequency regime, and revealed interesting dynamics of atoms [2, 3]. The experimentalists may further aspire to develop an ultra intense laser pulse to reach the stabilization regime in future. The stabilization is a phenomenon in which the total ionization yield decreases once the laser intensity exceeds a certain critical value. It was first predicted by theory (see [4, 5] for the history and detailed discussion of the stabilization).

In this paper, we study the photoelectron spectra of H\textsuperscript{−} in the stabilization regime, where oscillating substructures appear in the ATI peaks, an interest feature first found in a 1D case [6]. It is shown that this is due to the interference of a pair of photoelectron wave packets produced at different moments in time, and that the stabilization plays a key role. Subsequently, the effect was confirmed by 3D calculations for linear polarization [7]. Here, we follow these preceding papers but consider circular polarization. We interpret the effect in terms of an adiabatic version of the high-frequency Floquet theory (HFFT) [8]. Although this analysis is similar to that in [6], the generalization to the 3D case is not straightforward, and it is not evident a priori that such a simple approximation applies to the 3D case as well.

2. Theoretical approach
We consider a negative hydrogen ion H\textsuperscript{−} interacting with a laser pulse. The ion is treated in the single-active-electron approximation. The time-dependent Schrödinger equation (TDSE) in
the Kramers-Henneberger (KH) frame reads (the atomic units are used in this paper),

\[ i \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left( -\frac{1}{2} \Delta + V(|\vec{r} + \alpha(t)|) \right) \psi(\vec{r}, t), \tag{1} \]

where \( V(r) \) is the atomic potential and \( \alpha(t) \) is the classical trajectory of the free-electron in a laser electric field \( F(t) \). The potential is modeled by \[ V(r) = -V_0 \exp \left( -r^2/r_0^2 \right) \]
with \( V_0 = 0.3831087 \) and \( r_0 = 2.5026 \). This potential supports only one bound state with energy \( E_0 = -0.0277510 \). The field \( F(t) \) is assumed to vanish beyond the time interval \( 0 \leq t \leq T \).

The classical trajectories satisfies \( \ddot{\alpha}(t) = -F(t) \) with initial conditions \( \dot{\alpha}(0) = \alpha(0) = 0 \). In the KH frame, the effect of the laser field is combined into the atomic potential. This transformed potential is called the KH potential. The interaction between the electron and the laser field is thus described by a quiver motion of the KH potential along the classical trajectory. We solve Eq. (1) using the procedure described in [7].

3. Photoelectron spectra in the stabilization regime

3.1. Laser pulse

For circularly polarized pulse, we assume that the polarization vector lies in the \( xz \) plane. The components of the electric field \( F(t) \) are represented by \( (0 \leq t \leq T) \)

\[ F(t) = (\varepsilon F_0 f(t) \sin \omega t, 0, F_0 f(t) \cos \omega t) \tag{2} \]

where \( \varepsilon, F_0, \omega, \) and \( T \) are the ellipticity, amplitude, frequency, and duration of the pulse, respectively. The pulse envelope \( f(t) \) is defined so that the classical trajectory satisfies \( \alpha(T) = \dot{\alpha}(T) = 0 \).

3.2. Numerical results

Figure 1. The photoelectron spectrum \( P(E) \) of \( \text{H}^- \) produced by the high-frequency strong laser pulse with the parameters \( \varepsilon = 1, F_0 = 1.2, \omega = \pi/5, \) and \( T = 2000 \). (a) The overall view of the spectrum. The multiphoton absorption energies \( E_0 + n\omega (n = 1, 2) \) are shown by arrows. (b) The one-photon absorption peak at \( E \approx 0.601 \) on a magnified scale. The solid and broken lines represent the exact TDSE result and the reconstruction by the high-frequency Floquet theory (HFFT), respectively.

The photoelectron spectrum in the stabilization regime is illustrated in Fig. 1(a). The laser parameters are \( F_0 = 1.2, T = 2000, \omega = \pi/5 \). An oscillatory substructure in the ATI peaks is clearly seen in Fig. 1(b). In the rest of the paper, we discuss this substructure and clarify the underlying interference mechanism focusing on the first ATI peak. In doing so, we follow a train of thought similar to that in [6, 7], but deal with circular polarizations.
3.3. Analysis in terms of the high-frequency Floquet theory

Here we develop an approximate picture of the dynamics and reconstruct the first ATI peak using an adiabatic version of the HFFT [8]. The present analysis generalizes that of [6] to the 3D case. It is convenient to rotate the coordinate axes in such a way that the polarization plane coincides with the $xy$ plane, thus the laser pulse propagates along the $z$ axis.

Let us consider a monochromatic laser field, i.e., temporarily omit the envelope factor $f(t)$ in Eq. (2). The classical trajectory in this case is given by $\alpha(t) = (\alpha \cos \omega t, \alpha \sin \omega t, 0)$, where $\alpha = F_0 / \omega^2$ is the excursion amplitude. The KH potential can be expanded into a Fourier series,

$$V(|r + \alpha(t)|) = \sum_{n=-\infty}^{\infty} V_n(r, \theta; \alpha) e^{in(\varphi - \omega t)}, \quad (3)$$

where $\theta$ and $\varphi$ are the polar angles defining the direction of $r$. In the zeroth order of the HFFT [8], the system is described by the stationary ‘dressed’ Hamiltonian

$$H_{\text{HFFT}}(\alpha) = -\frac{1}{2} \Delta + V_0(r, \theta; \alpha). \quad (4)$$

The eigenfunctions of $H_{\text{HFFT}}(\alpha)$ will be called the dressed states. Let $\psi_0(r, \theta; \alpha)$ and $E_0(\alpha)$ denote the eigenfunction and eigenvalue, respectively, of the initial bound dressed state which coincides with the ground state of the unperturbed atom for $\alpha = 0$. Let $\psi(r, k; \alpha)$ be the scattering dressed state corresponding to the momentum $k = (k, \Omega)$ and energy $k^2/2$, normalized to unit amplitude of the incoming plane wave. Then, in the first order of the HFFT [8], the partial width of the initial state associated with the absorption of one photon is given by

$$\Gamma(\alpha) = \frac{k(\alpha)}{(2\pi)^2} \int |A(k(\alpha), \Omega; \alpha)|^2 d\Omega, \quad (5)$$

where $A(k, \Omega; \alpha)$ is the transition amplitude, $A(k, \Omega; \alpha) = \int \psi^*(r, k; \alpha) V_1(r, \theta; \alpha) e^{i\varphi} \psi_0(r, \theta; \alpha) d\mathbf{r}$, and $k(\alpha)$ is the momentum of the photoelectron, $k(\alpha) = \sqrt{2(E_0(\alpha) + \omega)}$. The width $\Gamma(\alpha)$ calculated for $\omega = \pi/5$ is shown in Fig. 2(a). It first grows with $\alpha$, but then decays after $\alpha$ passes the critical value $\alpha_c \approx 1.5$. Such a behavior of $\Gamma(\alpha)$, which is a signature of stabilization, is the key to understand the ionization dynamics.

The remaining part of the analysis parallels that in [6]. A part of the photoelectron spectrum near the first ATI peak $(E_0 + \omega \approx 0.601)$ calculated for this pulse is shown in Fig. 1(b). This pulse is not monochromatic. However, its envelope varies slowly, the pulse contains $n_{oc} = 200$ optical
cycles. So, one could expect that the picture suggested by the HFFT is followed adiabatically. The adiabatic approximation is implemented by the substitution \( \alpha \rightarrow \alpha(t) = \frac{E_0}{\omega^2} f(t) \). The maximum value of \( \alpha(t) \) for the present parameters is \( F_0/\omega^2 = 3.04 \); it is shown by the vertical dotted line in Fig. 2(a). The behavior of \( E_0(t) \) and \( \Gamma(t) \), now as functions of \( t \) recalculated using the adiabatic approximation, is shown in Fig. 2(b). The decay rate \( \Gamma(t) \) indeed has two humps. The probability to stay in the initial state until the moment \( t \) is, in this approximation, \( P_0(t) \approx \exp \left[ -\int_0^t \Gamma(t') \, dt' \right] \). This gives \( P_0(T) \approx 0.063 \), which is not very far from the survival probability 0.055 obtained in our accurate calculations. Within the adiabatic approximation, the energy \( E \) of a photoelectron is a function of time \( t \), \( E = E_0(t) + \omega \rightarrow t = t(E) \), where \( t(E) \) is the inverse function. The electrons ionized in the interval from \( t \) to \( t + dt \) have energies between \( E \) and \( E + dE \), where \( dE = (dE_0(t)/dt) \, dt \). Equating the total ionization probability in this interval \( P_0(t) \Gamma(t) \, dE \) to \( C^2(E) \, dE \), where \( C(E) \) is the amplitude of the photoelectron wave packet created, one finds

\[
C(E) = \sqrt{P_0(t) \Gamma(t) \left| \frac{dE}{dt} \right| \bigg|_{t=t(E)}}.
\]

As can be seen from Fig. 2(b), for the present pulse \( t(E) \) is a double valued function. Let \( t_1(E) \) and \( t_2(E) \) denote its two branches, and \( C_1(E) \) and \( C_2(E) \) denote the corresponding amplitudes defined by Eq. (6). There are two different paths for the photoelectron with the energy \( E \) to evolve from \( t = t_1(E) \) to \( t = t_2(E) \). The first one is to be ionized at \( t_1(E) \) and then propagate until \( t_2(E) \) in the scattering state. The second one is to propagate between \( t_1(E) \) and \( t_2(E) \) in the bound state and then to be ionized. These paths lead to the same final state, but with different phases. Summing up their contributions, the photoelectron spectrum is given by

\[
P_{\text{HFFT}}(E) = \left| C_1(E) + C_2(E)e^{i\Phi(E)} \right|^2,
\]

where \( \Phi(E) \) is the phase difference for the two paths, \( \Phi(E) = E \, [t_2(E) - t_1(E)] - \int_{t_1(E)}^{t_2(E)} [E_0(t) + \omega] \, dt \). The results obtained using these formulas are shown in Fig. 1(b). This approximate theory yields the spectrum only in a limited energy interval from \( \min[E_0(t) + \omega] \) to \( \max[E_0(t) + \omega] \) shown in the figure by vertical dotted lines. Equation (7) diverges at the upper boundary of this interval because of the factor \( dt(E)/dE \) in Eq. (6). It reproduces the phase of the interference substructure nicely, but the amplitude is somewhat overestimated, especially in the lower part of the spectrum. However, in spite of these limitations, it is clear that the theory correctly accounts for the mechanism responsible for the appearance of the interference substructure. This analysis confirms our qualitative interpretation of the dynamics.

4. Conclusion
In this paper we studied the photoelectron spectrum of \(^-\) generated by high-frequency strong laser filed. The oscillating substructures are found in the ATI peaks. We employed the HFFT and showed that this is due to the interference between photoelectron wave packets produced in the rising and falling parts of the pulse.

References
[1] V. Ayvazyan et al., Euro. Phys. J. D 37, 297 (2006).
[2] R. Moshammer et al., Phys. Rev. Lett. 98, 203001 (2007).
[3] M. Nagasono et al., Phys. Rev. A 75, 051406(R) (2007).
[4] J. H. Eberly and K. C. Kulander, Science 262, 1229 (1993).
[5] N. B. Delone and V. P. Krainov, Usp. Fiz. Nauk 165, 1295 (1995) [Sov. Phys. Usp. 38, 1247 (1995)].
[6] K. Toyota, O. I. Tolstikhin, T. Morishita, and S. Watanabe, Phys. Rev. A 76, 043418 (2007).
[7] O. I. Tolstikhin, Phys. Rev. A 77, 032712 (2008).
[8] M. Gavrila and J. Z. Kaminski, Phys. Rev. Lett. 52, 613 (1984).