Numerical Simulation of an Intense Isolated Attosecond Pulse by a Chirped Two-Color Laser Field

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Abstract—We investigate theoretically the high-order harmonic spectrum extension and numerical generation of an intense isolated attosecond pulse from He⁺ ion irradiated by a two-color laser field. Our simulation results show that the chirp of the fundamental field can control HHG cutoff position. Also, these results show that the envelope forms of two fields are important factors for controlling the resultant attosecond pulses. Besides, the effects of relative intensity are investigated. As a result, by using the optimized conditions an intense isolated 126-as (attosecond) pulse can be observed.

KEYWORDS: Attosecond pulse (as), High order harmonic generation (HHG), Two-color laser field.

I. INTRODUCTION

The generation of extreme ultraviolet attosecond (as) pulses has opened new fields of time-resolved studies with high precision [1-3]. The as pulses are important tools for detecting and controlling the electronic dynamics inside atoms and molecules, such as inner-shell electronic relaxation and ionization by optical tunneling [4]. Attosecond pulses have been generated, by using the process of high-order harmonic generation in noble gases, in the form of trains of pulses separated by half optical cycle and in the form of isolated pulses [5]. However, for practical application, an isolated as pulse is preferable to a chain of as pulses [6], thus much effort has been paid out to obtain an isolated as pulse [7]. So far, several schemes have been proposed for generation of isolated as pulses [8-11]. One of the most important methods of generating the isolated as pulses is to apply a two-color scheme. It is demonstrated that a two-color laser pulse can extend the harmonic plateau to higher energy [12-14]. However, in these methods, the efficiency of the continuous harmonics is low, which directly affects the intensity of the generated as pulse and its applications [15]. Hence, the optimization of the two-color scheme for practical applications is important [16-18]. Therefore, in this paper we try to produce an intense and clean isolated as pulse with the shortest duration.

II. THEORY

Our theory is based on solving the one-dimensional time-dependent Schrödinger equation (TDSE). This equation describes the motion of the electron in the presence of the combined field and expresses as (atomic units are used throughout this paper)

$$i \frac{\partial}{\partial t} \psi(x,t) = \left( -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x) - E(t)x \right) \psi(x,t) \quad (1)$$

where $V(x) = -z/\sqrt{x^2 + a}$ is the soft coulomb potential [19] with $z=2$ and $a=0.5$ to match the ionization potential $I_p=-2.0$ a.u. of a real He⁺ ion [16]. In this study, a 7 fs/800 nm pulse and its second harmonic pulse are combined to serve as the driving pulse. Time duration of the controlling laser field is equal to 10 fs. Besides, the peak intensity of the fundamental laser pulse and the controlling laser pulse is chosen to be $10^{15} W/cm^2$ and $10^{14} W/cm^2$. 
respectively. The time-varying electric field of the driving laser can be expressed as

\[ E(t) = E_1(t)\cos(\omega t + \delta(t)) + E_2(t)\cos(\omega t) \]  

(2)

In this equation, \( \omega_1 = 0.057 \) (wavelength is 800nm) is the frequency of the fundamental laser field and \( \omega_2 = 2\omega_1 \) is the frequency of the controlling laser field.

\( E_i \) and \( f_i(t) = \exp(-4\ln(2)t^2/\tau_i^2) \) with \( i=1,2 \) are the amplitudes and envelopes of the laser fields, respectively. Also, \( \tau_i \) is the pulse duration at full width of half maximum \( (i=1,2) \). \( \delta(t) \) is the carrier envelope phase (CEP) and it is set to be \( [17] \),

\[ \delta(t) = -\beta \tanh\left(\frac{t}{\sigma}\right) \]  

(3)

Therefore, the instantaneous frequency of the pulse has the following form:

\[ \omega(t) = \omega + \frac{d\delta(t)}{dt} = \omega - \frac{\beta}{\sigma} \cosh^{-1}\left(\frac{t}{\sigma}\right) \]  

(4)

\( \beta \) and \( \sigma \) are important constants for controlling the chirp form.

\( \beta \) controls the frequency sweeping range and \( \sigma \) controls the steepness of the chirping function.

The time-dependent Schrödinger equation can be solved with the splitting-operator fast Fourier transform algorithm \([20]\) and finally the wave function \( \psi(x,t) \) can be obtained.

According to the Ehrenfest theorem, the time-dependent dipole acceleration \( d(t) \) is given by

\[ d(t) = \langle \psi(x,t) \left| \frac{d^2V(x)}{dx^2} + V(x)\psi(x,t) \right| \rangle \]  

(5)

The harmonic spectrum can be obtained, which is proportional to the modulus squared of the Fourier transform of \( d(t) \),

\[ P_q(\omega) = \left| \int_0^{\infty} d(t) e^{-i\omega t} dt \right|^2 \]  

(6)

By superposing several orders of the harmonics, an ultra-short pulse can be obtained with the temporal profile

\[ I(t) = \sum_q d_q e^{i\omega_q t} \]  

(7)

In this equation \( d_q = \int d(t)e^{-i\omega_q t} dt \) and \( q \) is the harmonic order.

### III. RESULTS AND DISCUSSION

In order to demonstrate our scheme, we first investigate the HHG spectrum in the chirp-free two-color laser field.

For this purpose, we set \( \beta = 0 \) in Eq. (2). Figure 1 shows the harmonic spectrum for this case. One can see that the intensity of the harmonics is very low in this structure. We also investigated the effect of the fundamental field chirp on the cutoff position. So, we consider to the HHG power spectrum under the condition that adding a slight amount of chirp to the fundamental field with changing the \( \beta \) values \([21]\), while keeping the second harmonic field unchanged. First, we fix \( \sigma = 200 \text{a.u.} \), while varying the \( \beta \) parameter. After investigation, we found out that the \( \beta = 6.25 \) is the best chirping parameter for the cutoff extension, as shown in Fig. 2. The cutoff position for the \( \beta = 6.25 \) is markedly

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**Fig. 1.** Harmonic spectra from He\(^+\) exposed to chirp-free two-color laser field.
extended, compared with the $\beta = 0$ (chirp-free) case. If the $\beta$ parameter is further increased, the cutoff extension is not as far reaching as in the case of $\beta = 6.25$.

**Fig. 2.** Dependence of the harmonic spectrum cutoff order on sweeping parameters $\beta$ in rad with fixed $\sigma = 200 \text{a.u.}$.

Second, we fix $\beta = 6.25$, while varying the $\sigma$ parameter. Figures 3-6, show the harmonic spectrum for $\sigma$ parameters for 400, 300, 200 and 100, respectively.

**Fig. 3.** HHG spectra from chirped two-color laser pulse with $\sigma = 400 \text{a.u.}$ and $\beta = 6.25 \text{rad}$.

After investigation, we found out that the $\sigma = 200$ is the best chirping parameter for the cutoff extension, as shown in Fig. 5.

**Fig. 4.** HHG spectra from chirped two-color laser pulse with $\sigma = 300 \text{a.u.}$ and $\beta = 6.25 \text{rad}$.

**Fig. 5.** HHG spectra from chirped two-color laser pulse with $\sigma = 200 \text{a.u.}$ and $\beta = 6.25 \text{rad}$.

**Fig. 6.** HHG spectra from chirped two-color laser pulse with $\sigma = 100 \text{a.u.}$ and $\beta = 6.25 \text{rad}$.
We can see that the cutoff position is expanded with the decreasing of the intensity of the harmonic laser the \( \sigma \) parameter. But we select the \( \sigma = 200 \), this is because the harmonic intensity for the \( \sigma = 200 \) case is effectively enhanced by 1–3 orders of magnitude compared with the \( \sigma = 100 \) case.

Thus, according above discussion, the intense HHG with extended cutoff position can be realized by using the optimal values of the \( \beta = 6.25 \) and \( \sigma = 200 \) parameters.

In this case (Fig. 5), the harmonic spectrum has a double plateau structure similar to that of Fig. 1.

In order to better understand the two-plateau structure of HHG in the chirped two-color pulse with the \( \beta = 6.25 \), we give a clear physics picture in terms of the semiclassic three-step model [22].

Fig. 7 shows the dependence of the kinetic energy \( E_k \) of electron at the recombination instant on the ionization time. As shown in this figure, the electron is ionized at \( t_a = -1.08T \) (\( T = 2\pi / \omega \) is an optical period of the few-cycle pulse) with a maximum kinetic energy of 552 eV (marked as A), emitting harmonic photon with the maximum energy of \( I_p + 552 \) eV (398th order) which \( I_p \) is the ionization potential, the second-highest kinetic energy at the ionization time \( t_B = -1.84T \) approaches 245 eV (marked as B), corresponding to the harmonic photon with energy of \( I_p + 321 \) eV (207th order), the third-highest kinetic energy at the ionization time \( t_C = 0.21T \) reaches 245 eV (marked as C). On based this classical model, we have a three-plateau structure with three cutoffs at 398th-, 207th-, and 198th-order harmonics, while one can clearly see that the harmonic spectrum in Fig. 5 presents a two-plateau structure with two cutoffs at 398th-, and 198th-order.

The reason resulting in this feature can be understood from the laser field by the solid black line in Fig. 8:

The electrons contributing to the harmonics of the third, the second, and the first plateaus are ionized near \( t_A, t_B, \) and \( t_C \), which are marked in a two-color electric field. The electric field strength near \( t_B \) is much smaller than the one near \( t_C \), and its contribution to the HHG in low harmonics below 198th can be ignored.

Therefore, there are two major emission events taking place due to the electrons which ionize near the peaks labeled A and C. This is an important factor leading to the two-plateau structure.

A plausible explanation regarding the cutoff extension mechanism has to do with the excess
energy acquired by the electron in the laser field. This is a direct consequence of breaking the oscillatory periodicity of the laser field, i.e., the oscillatory periodicity of the laser field for the fundamental pulse alone (the dashed red line) and chirp-free two-color pulse (the dotted blue line) have no change, but for chirped two-color pulse varies, as shown in Fig. 8. On the other hand, as the chirping becomes more salient close to the center of the laser pulse (the frequency variation), when time grows the instantaneous frequency becomes increasingly smaller until reaching a minimum value (in the center of the pulse), then, the instantaneous frequency increases again, as shown in Fig. 9. Since the ponderomotive energy \[ U_p = \frac{E^2}{4\omega^2} \] acquired by the electron is inversely proportional to the instantaneous frequency, the energy attained by the electron will achieve the maximum value near the instantaneous frequency minimum. In this manner, the electron has substantial more returning energy at the recollision event with the core, leading to the observed extension of the cutoff.

Fig. 9. Instantaneous frequency of the hyperbolic tangent form of the CEP.

Next, the time profiles of the generated attosecond pulses by superposing the harmonics in the cutoff region from the harmonics spectra of the Figs. 1 (the chirp-free case) and 5 (the optimized case) are shown in Figs. 10 and 11.

Fig. 10. Time profile of the generated attosecond pulse corresponding to Fig. 1.

Fig. 11. Temporal profile of generated attosecond pulse from the HHG spectrum corresponding to Figs. 5.

In the case of Fig. 1, we can obtain one attosecond burst per laser pulse. The duration of this isolated attosecond pulse is 178 as. It is notable that the intensity of this pulse is very low. From Figs. 10 and 11, it is obvious that the low intensity attosecond pulses are generated by superposing the low intensity harmonics.

In the case of Fig. 5, by superposing the harmonics near the second cutoff region, an intense isolated attosecond pulse with duration (FWHM) of 139 as is produced, as shown in Fig. 11.
Compared to Fig. 10, the intensity of the attosecond pulse in Fig. 11 is approximately 5 times higher.

\[ f_i(t) = \sin^2 \left( \frac{\pi t}{\tau_s} + \frac{\pi}{2} \right) \]  

(8)

These isolated attosecond pulses are achieved by restricting the number of driver laser cycles by means of the synthesizing of two pulses that allow for the ejection of electrons in combination with either spectral selection. These two color laser fields behave similar to extremely short, so-called few-cycle laser pulses [23-24], in which the electric field amplitude differs considerably from one half-cycle to the next. For these suitable waveforms of the pulses, the highest-energy XUV photons are produced only during the most intense half-cycle of the driver laser, as example, the ionized electron at \( t_s \) (the peak labeled as A in Fig. 7) oscillates in the most intense half-cycle of the driver laser, i.e., the center of the laser pulse field. Selection of these highest energy XUV photons (the cutoff harmonics) consequently allows for the generation of an isolated attosecond pulse [25].

In the next step, we consider to the results of using various envelope forms for both of fundamental and controlling laser fields. First we use sin envelope form for both of two fields. The sin envelope form is characterized with below equation,

Fig. 12. HHG spectra in main chirped two color laser field with different (Gaussian and sin) envelope forms.

Fig. 13. Time profile of the generated attosecond pulse corresponding to Fig. 12.

Fig. 14. HHG spectra in chirped two color laser field with two sin envelope forms.

Other parameters are the same as those in Eq. (2). As shown in Fig. 12, the harmonic spectrum for this case presents a double plateau structure. Harmonic spectrum whose orders are from 190th to 258th (i.e., 68 orders) forms the second plateau and the second cutoff is positioned at the 258th order harmonic. From Fig. 13, it can be seen that an irregular attosecond burst is generated by superposing the harmonics near the second cutoff region and the intensity of this burst is low. Then we use Gaussian and sin envelope forms for the fundamental and the controlling pulses,
respectively. Compared to the intensity of the harmonics generated from fields with the same envelope forms the intensity of the harmonics shows a reduction, as shown in Fig. 14. From Fig. 15, it can be seen that two attosecond bursts are generated, and the durations of the strong one and weak one are 230 as and 154.4 as, respectively. Finally, from Figs. 10, 11, 13 and 15, it is obvious applying the same envelope forms for both of fields with optimized chirp is a good condition for producing an intense isolated attosecond pulse.

In the final step, we study the relative intensity variation effects on harmonic spectrum’s cutoff order. All parameters are the same as Eq. (2). Also, we use optimum values for chirping parameters, i.e., \( \beta = 6.25 \) and \( \sigma = 200 \).

In Figs. 16-19, the effects of this variation on cutoff order position are shown. The peak intensity of the chirped fundamental pulse is \( I_1 = 10^{15} \text{W/cm}^2 \).

By fixing this value for fundamental pulse, we set these values for controlling laser pulse:

\[
I_2 = 10^{15} \text{W/cm}^2, \quad 5 \times 10^{13} \text{W/cm}^2, \quad 10^{13} \text{W/cm}^2, \quad 8 \times 10^{12} \text{W/cm}^2
\]

Our numerical results show that by increasing the intensity of the controlling laser pulse, broadband continuous high-order harmonics are observed.

As shown in Figs. 16-19 and Fig. 5 the maximum harmonic’s cutoff order appearing at the intensity ratio \( I_2/I_1 = 1 \). On the other hand, when the intensity of controlling pulse is more than the intensity of fundamental pulse, the cutoff position shows a reduction in his order. As we know, in the quasi-classical approximation the electron after the ionization has zero velocity if the ionization takes place in the tunneling regime and non-zero one if it occurs in the barrier-suppression regime [26]. Calculations of the classical motion of a free electron in laser field show that the presence of the initial velocity reduces the maximal energy of the recombining electron [27]. We believe
that this can explain the reduction in the harmonic’s spectrum cutoff order.

Next, the time profile of the generated attosecond pulse by superposing the harmonics in the cutoff region from the optimum harmonics spectra (Fig. 18) is shown in Fig. 20. It can be seen that an isolated 126 as pulse is generated from these optimum conditions.

**Fig. 18.** HHG spectra from chirped two-color laser pulse with $I_1 = 10^{14} W/cm^2$ and $I_2 = 10^{15} W/cm^2$.

**Fig. 19.** HHG spectra from chirped two-color laser pulse with $I_1 = 10^{14} W/cm^2$ and $I_2 = 8 \times 10^{14} W/cm^2$.

**IV. CONCLUSION**

We investigated theoretically the HHG and attosecond pulses generation from He$^+$ exposed to chirp-free two-color laser field and various chirped two-color laser fields. We also showed that the HHG enhancement could be realized by using a chirped fundamental pulse. Particularly, by optimizing chirp of the fundamental pulse, we show that the plateau of the HHG are extended up to $522$ eV and the intensity of HHG plateau is enhanced by seven order of magnitude compared to the chirp-free two-color laser.

Among our calculations, it can be seen in a chirped two color laser field the proper selection of the envelope forms of fields and the relative intensity of two fields have salient effects on formation of HHG and the time profile of generated as pulse.

As a result, an isolated attosecond pulse with duration of 126 as can be obtained for the optimized chirp parameters and the Gaussian envelope forms of fields. In these optimum conditions the relative intensity is $I_2/I_1 = 1$.

**REFERENCES**


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