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Spatial position scaling on harmonic generation from He atom in bowtie-shaped nanostructure

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ABSTRACT

Spatial position scaling on the harmonic generation from He in the bowtie-shaped nanostructure has been theoretically investigated. It shows that (i) due to the surface plasmon polaritons in the nanostructure, the laser intensity can be enhanced and presents the nonhomogeneous effect in space. As a result, the extension of the harmonic cutoff can be achieved when He is away from the gap center of the nanostructure. However, due to the limit of the gap size, there is a maximum harmonic cutoff extension for a given nanostructure. (ii) Due to the asymmetric enhancement of the laser intensity in space, the extended harmonics are mainly from $E(t) > 0$ a.u. and $E(t) < 0$ a.u. when He is injected into the positive and the negative positions, respectively. Moreover, the intensities and the cutoffs of the extended harmonics can be controlled by changing the pulse duration or by adding the second controlling pulse. Finally, by properly superposing the harmonics from the two-color field, four single attosecond pulses with the durations of 30 as can be produced.

1. Introduction

Attosecond science has become an important research area of ultrafast phenomena within the past two decades [1–3]. High-order harmonic generation (HHG) from noble gas as the most important tool to produce the single attosecond pulse (SAP) in the XUV or the X-ray region has been widely investigated [4–6]. Currently, HHG in the tunneling regime can be explained through the semi-classical three-step model (STM) with the processes of ionization-acceleration-recombination [7]. Further, the harmonics with the cutoff energy of $E_{cutoff}=I_p+3.17U_p$, where I_P is the ionization potential and $U_p = I/4\omega^2$ can be obtained. Based on the STM, the harmonic cutoff is related to the pulse intensity and the laser frequency. Thus, many methods have been proposed to extend the harmonic cutoff and to produce the SAP in the XUV or the X-ray region. For instance, the polarization gating or the double optical gating methods [8–11]; the few-cycle driven pulse scheme [12]; the lighthouse method using a space-time coupled fundamental beam [13], the mix-color field scheme [14–17] and the non-collinear harmonic generation [18] etc.

In 2008, with the assistance of the bowtie-shaped gold nanostructure, Kim et al. [19] first reported that the harmonics can be emitted in the nonhomogeneous field. Further, the physical mechanism of the HHG from the nonhomogeneous field has been explained through the quantum and the classical methods [20–22]. Recent 5 years, the investigations of the HHG and the SAP driven by the nonhomogeneous field receive much more attention [23–34]. For instance, by using the atomic model, Yavuz et al. [23] obtained a 130 as pulse by using the single-color nonhomogeneous field. Cao et al. [24] obtained a 10 as pulse with the combination of the two-color nonhomogeneous field. Xue et al. [25] obtained a 35 as pulse by using the three-color nonhomogeneous field. Feng et al. [26] produced a 50 as pulse by using the nonhomogeneous polarization gating scheme. Fetić et al. [27] investigated the effects of the carrier-envelope phase (CEP) and the pulse duration on the HHG in the nonhomogeneous field. Recently, by using the molecular model, Yavuz et al. [28], Feng et al. [29] and Yu et al. [30] found that the extension of the HHG can also be achieved in molecular systems.

Although the HHG from the nonhomogeneous field has been investigated, the spatial positions of the noble gas are all injected into the gap center. As we know due to the nonhomogeneous effect, the laser intensity can be enhanced as the spatial positions of the laser field are away from the gap center [19], as shown in Fig. 1(a) for the case of

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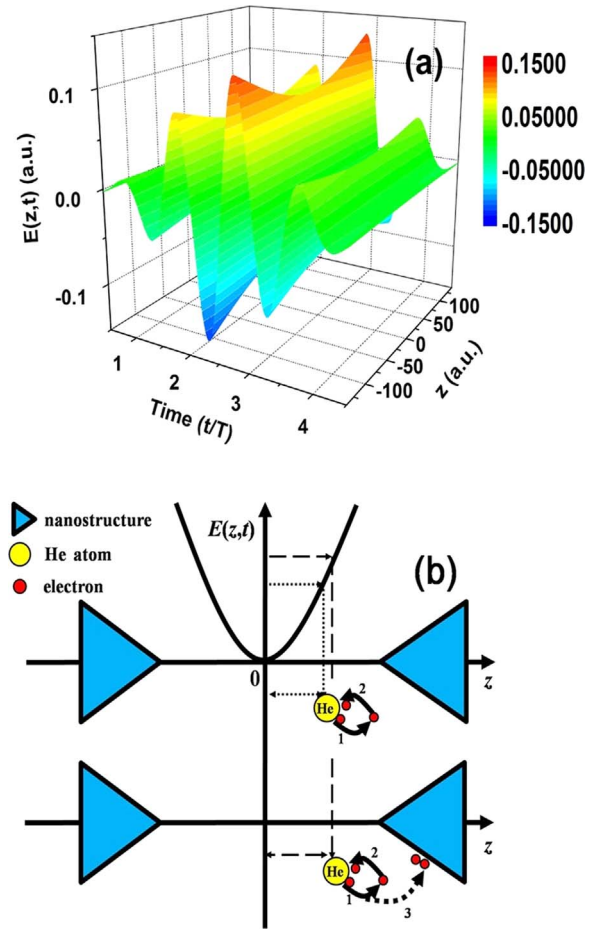

Fig. 1. (a) 5 fs/800 nm nonhomogeneous field with the variation in time and space. The pulse intensity is I =3.0×10^{14} W/cm^2. T is the optical cycle of 800 nm field. (b) Sketch of the electron motion in the bowtie-shaped nanostructure when He is injected in to different positions.

the 5 fs/800 nm nonhomogeneous field with the pulse intensity of I =3.0×10^{14} W/cm^2. Here, the quoted laser intensity is the plasmonic-enhanced value near the gap center. Thus, if the spatial positions of the noble gas are away from the gap center, the electron should obtain the additional energy in its acceleration, thus leading to the extension of the HHG, as shown in Fig. 1(b) (up row). For instance, Luo et al. [35] found that the HHG is very sensitive to the atomic spatial positions and much broader harmonic plateaus can be found when the positive atomic spatial positions are chosen. However, whether the harmonic cutoff can be persistently extended as the spatial positions of the noble gas keep increasing. The answer is negative. This is attributed to the limit of the gap size, the accelerated electron with the higher energy and the larger electron motion will be absorbed by the nanostructure, as shown in Fig. 1(b) (down row). For instance, Yavuz [36] found that the absorption of the higher energy electron could lead to the suppressions in both the harmonic yield and the harmonic cutoff. Moreover, the wavelength scaling of harmonic efficiency in the nanostructure has also been investigated by Yavuz [36].

As can be seen, the spatial positions of the atoms play an important role in the HHG. However, in Ref. [35] (by Luo et al.), the calculations are from the 1 dimensional (1D) model and only one gap size of g =18 nm is considered. While in Ref. [36] (by Yavuz), although the 3D calculations are performed, the nonhomogeneous effect of the laser field is chosen to be the first-order approximation. Moreover, the detail harmonic emission process for a given atomic position is unclearly.

Thus, in this paper, we further investigate the spatial position scaling on the HHG from He in the bowtie-shaped nanostructure through solving the 3D time-dependent Schrödinger equation (TDSE). Moreover, the fourth-order polynomial functions are used to describe the nonhomogeneous effect, which can be obtained by fitting the real electric field that results from the finite-domain time-difference simulation considering the real geometry of the bowtie-shaped nanostructure [25]. We found that the harmonic cutoff can be extended when He is injected away from the gap center of the nanostructure and a maximum harmonic cutoff extension can be obtained for a given nanostructure. Also, due to the asymmetric enhancement of the laser intensity in space, when He is injected into the positive or the negative positions, the contributions of the extended harmonics come from $E(t)$ > 0 a.u. or $E(t)$ < 0 a.u., respectively. Finally, with the introduction of the second controlling pulse, a 344 eV super-continuum and four single 30 as pulses can be obtained. Atomic units (a.u.) are used throughout this paper unless stated otherwise.

2. Method

HHG from He can be investigated through solving the 3D-TDSE [23,36–42],

$$i\frac{\partial\phi(r,t)}{\partial t} = H(t)\phi(r,t) = [-\frac{1}{2}\nabla^2 + V(r) - zE(z,t)]\phi(r,t). \quad (1)$$

$V(r) = -1.353/r$ is the Coulomb potential of He atom. Here, we assume that the laser field is linearly polarized along the z axis. Thus the electron motion and the harmonic emission are mainly along the z axis.

The laser field can be expressed as,

$$E(z,t) = E(1 + sg(z + z_0))\exp[-4\ln(2)t^2/\tau^2]\cos(\omega_1 t), \quad (2)$$

where E, ω_1, and τ are the amplitude, the frequency, and the full width at half maximum (FWHM) of the laser field. z_0 is the position of He atom. $g(z) = \sum_{i=1}^{N}\beta_i z^i$ means the nonhomogeneous form of the laser field produced by the bowtie-shaped nanostructure. s is the switch function with the values of s=0 (homogeneous field) and s=1 (nonhomogeneous field). Here three gap bandwidths of g =18 nm, g =16 nm and g =14 nm are chosen in this paper and the nonhomogeneous forms are given by [25],

$$g(z)_{18nm} = -5.2\times10^{-8}z + 3.0\times10^{-5}z^2 - 2.5\times10^{-12}z^3 - 3.4\times10^{-10}z^4, \quad (3)$$

$$g(z)_{16nm} = -2.0\times10^{-18}z + 3.1\times10^{-5}z^2 + 3.1\times10^{-22}z^3 - 5.3\times10^{-10}z^4, \quad (4)$$

$$g(z)_{14nm} = -2.5\times10^{-8}z + 3.2\times10^{-5}z^2 + 4.7\times10^{-12}z^3 - 8.0\times10^{-10}z^4. \quad (5)$$

The time-dependent wave function $\varphi(r,t)$ can be expanded as $\varphi(r,t) = \sum_{l=0}^{l_{max}=50}\frac{1}{r}\chi_l(r,t)Y_l^0(\theta)$, where $\chi_l(r,t)$ and $Y_l^0(\theta)$ are the radial and the spherical harmonics functions. In the present calculations, the maximum radius of 200 a.u. with the grid spacing of 0.1 a.u., and maximum number of partial waves of l_{max} =50 is sufficient to obtain converged results. The time step is chosen to be 0.05 a.u. Moreover, to guarantee the absorption of the wave packet near the surface of the nanostructure, which does not contribute to the HHG, the absorbed function with the form of $\cos^{1/8}$ has been used starting from 170 a.u (gap boundary for g =18 nm), 150 a.u. (gap boundary for g =16 nm) and 130 a.u. (gap boundary for g =14 nm) for the cases of g =18 nm, g =16 nm and g =14 nm, respectively.

The HHG spectra are given by,

$$S(\omega) = \left|\frac{1}{\sqrt{2\pi}}\int_0^{T_{total}} d_A(t)e^{-i\omega_1 t}dt\right|^2, \quad (6)$$

where $d_A(t) = -\langle\phi(r,t)|[H(t),[H(t),z]]|\phi(r,t)\rangle$[43].

The SAP can be given by,