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Muhammed Sayraç

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Prof. Dr. Hikmet ESEN
IATS'21 CONFERENCE CHAIR

IATS'21 9th International Advanced Technologies Symposium

04 October 2021

Dear **M Sayrac**

It is a pleasure to inform you that your paper entitled **"Computation of Atomic Dipole Spectra for Different Atoms by Considering Short and Long Electron Trajectories under the Intense Laser Pulse"** has been accepted as face to face / online presentation to be presented in the 9th International Advanced Technologies Symposium, **IATS' 2021**.

We thank you for your fine contribution to the **IATS' 2021** and look forward to meeting you in the symposium soon.

Best wishes…

Prof. Dr. Hikmet ESEN
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Computation of Atomic Dipole Spectra for Different Atoms by Considering Short and Long Electron Trajectories under the Intense Laser Pulse

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Abstract

In this work, computation of the nonlinear dipole response of a single atom is performed by considering the ionization of the electron under the intense laser field. The dipole spectra for xenon (Xe) and argon (Ar) gases are obtained. Xe and Ar are the simples gas species having close ionization potentials. The interaction of these single atoms with the intense-short laser pulse leads to the laser-matter interaction. The short laser pulse is accepted as an ultra-short duration, i.e. the shorter time scale than the electron energy-lattice transfer process. The Keldysh parameter, which determines the ionization regime, is smaller than one because of the ionization potential of these gases. The harmonic spectra for Ar and Xe gas species are simulated by calculating the dipole spectrum considering the Lewenstein model by using a personal computer. After tunneling, the electron propagation in the short-trajectory and the combination of short and long trajectories are simulated. The effects of the short electron trajectory have noticeable effects on the dipole spectrum of a single electron.

Keywords: Lewenstein model, dipole moment, keldysh parameter, electron trajectories.

1. INTRODUCTION

Electron density oscillation influenced by the intense laser field is the fundamental of nonlinear phenomena. The laser-affected electron density can be controlled and allows to study of temporal electrons dynamics. Time evolution of the electric field of the laser pulse affects the nonlinear response of a single atom. The macroscopic field is determined by the coherent superposition of the single-atom response, which directly depends on the driving field features.

The laser-matter interaction results in the generation of coherent XUV pulses. This phenomena semi classically explained by Corkum et. al. [1], tunnel ionization, acceleration, and recombination. The semi-classical model explains the most important feature of the electron propagation under the effect of the intense laser field, the generation of coherent XUV pulses. The maximum emitted energy after the laser-matter interaction is determined by the cutoff frequency ω_c

$$\hbar\omega_c \approx 3.17U_p + I_p \tag{1}$$

here $U_p \sim I/\omega_0^2$ is the ponderomotive energy, which depends on the driving laser field intensity (I), and I_p is the ionization potential of the used atom.

On the other hand, Lewenstein et. al. [2] described a quantum mechanical explanation for laser-matter interaction. In this study, the Lewenstein model is calculated by an integral considering the electron excursion time by using MATLAB to obtain the dipole spectrum of a single atom response by using a personal computer. The novelty of this work is to obtain the dipole spectrum of a single atom for short electron

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trajectory and the combination of the short and long electron trajectories. Xe and Ar species are modeled since they are single atom molecules at standard temperature and pressure (noble gases) and are easy to ionize under the short laser pulse due to having low ionization potential.

2. THEORY

The derivation of the Lewenstein model is outlined [2]. The time-dependent Schrödinger equation (TDSE) for one electron is

$$i\frac{\partial}{\partial t}\left|\psi(t)\right\rangle=\left[-\frac{1}{2}\nabla^2+V(r)-ECos(t)x\right]\left|\psi(t)\right\rangle \quad (2)$$

here $V(r)$ is the atomic potential, and $ECos(t)x$ is the additional potential due to the electric field of the driving laser. The TDSE has been solved using three assumptions [2]: (i) the only bound state plays a role in the evolution of the system, (ii) the depletion of the ground state is neglected, i.e. driving field is weak or the short driving pulses, and (iii) there is no overlap of the continuum states with the ground state.

By considering the TDSE, the dipole moment element is derived by considering the electron trajectories start and end at the same position. The dipole moment is

$$d(t)=-er(t)=-\left\langle\psi(t)\right|\hat{r}\left|\psi(t)\right\rangle \quad (3)$$

and

$$d(t)=-ie_x\int_0^\infty d\tau\left(\frac{\pi}{\varepsilon+i\tau/2}\right)^{3/2}.E\cos(t-\tau).D_x(p_s(t,\tau)-A_x(t-\tau))\times\exp(-iS_s(t,\tau)).D_x^*(p_s(t,\tau)-A_x(t))+c.c. \quad (4)$$

where $E\cos(t-\tau).D_x(p_s(t,\tau)-A_x(t-\tau))$ is the probability amplitude that the driving field $E\cos(t-\tau)$ releases the electron to the continuum. $D_x(p_s(t,\tau)-A_x(t-\tau))$ gives a coupling the ground state to the vacuum continuum state. The second term $\exp(-iS_s(t,\tau))$ is the phase that the electron acquires during propagation, and S_s is the quasi-classical action corresponding to the electron trajectory.

The third term $D_x^*(p_s(t,\tau)-A_x(t))$ gives probability amplitude for recombination. The recombination means interference of the ground state wave function with the returning wave packet. By considering the above assumptions, the shape of the dipole spectra was obtained by solving the TDSE [2].

On the other hand, there are limitations when the above-mentioned approximations are considered. The first assumption is that the magnetic field is neglected for the intensities below 10^{16}W/cm^2, and wavelength below 2000nm is accepted [3]. Then, the electron should propagate freely without seeing the atomic Coulomb potential. This only happens if the kinetic energy of the free electron is sufficiently high, i.e. high driving field intensity. The Keldysh parameter, which is defined as the ratio between the frequency of the laser light and the frequency of an electron tunneling through the potential barrier formed by Coulomb potential checks whether the driving field intensity is high enough for the tunneling ionization [4]

$$\gamma\approx\sqrt{\frac{I_p}{2U_p}} \quad (5)$$

The Keldysh parameter should be smaller than one $\gamma<1$ that corresponds to the tunnel ionization is the dominant process while $\gamma>1$ indicates the multi-photon channels in the transition regime [5].

3. RESULTS

The simulation parameters are following: the wavelength is 1000nm (corresponding to 1.24eV photon energy), laser intensity 10^{14}W/cm^2. The Keldysh parameter is 0.914, which justifies the tunnel ionization regime. The ionization potential for the used atom is 12.12eV for Xe and 15.7eV for Ar gas [6]. The nonlinear dipole response of a single target atom is obtained by considering the Lewenstein model. The different atoms having different ionization potential produces different dipole responses.

Dipole spectra are obtained for the short electron trajectory and combination of short and long electron trajectories. In theory, the electron recombination mostly produces more signals at the short trajectory since the electron is less exposed to the ultrashort driving field. On the other hand, the combination of short and long trajectories results in electrons shifting from the propagation direction and ends up with a low signal under the short laser pulse.

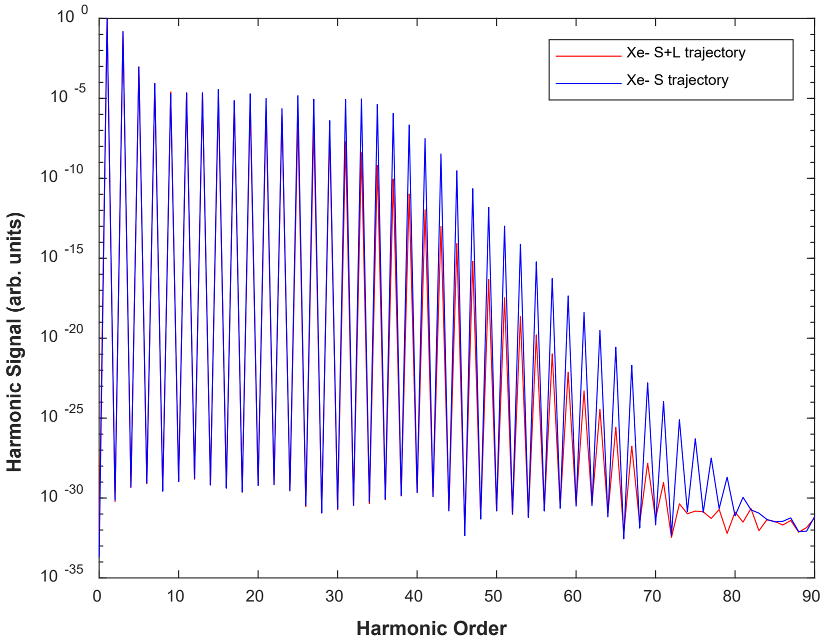

Fig. 1. Dipole spectra for Xe under the ultrashort laser pulse. S: short electron trajectory, L: long electron trajectory

Figure 1 presents the dipole spectrum for Xe atom. Electron propagates under the laser field at different electron trajectories. The red color is for the combination of short and long electron trajectories, and the blue color is for the short electron trajectory. The short trajectory produces a more dipole spectrum yield than the combined electron trajectories because the electron is less affected by the oscillating laser field. This allows for more signals compared to the combination of short and long electron trajectories. In addition, the extensions of the dipole spectra to higher photon energies are observed when the short electron trajectories are considered. ($\left(1240/\lambda_{driving}\right) \times HO$, $\lambda_{driving}$: driving laser wavelength, and *HO*: harmonic order).

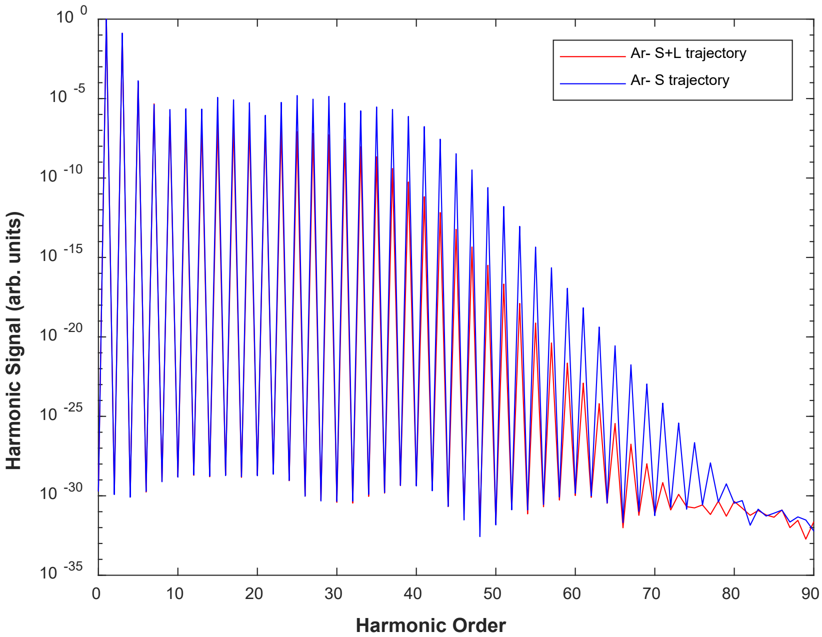

Fig. 2. Dipole spectra for the Ar gas under the short laser pulse. S: short electron trajectory, L: long electron trajectory

Figure 2 is simulated for the Ar atom. Similar to the Xe atom, the dipole spectrum extends to more orders at short electron trajectories. The dipole spectrum reaches slightly higher-order for the Ar atom because of the higher ionization potential. Figures 1-2 give more signals at the short trajectory where electrons are less affected by the driving laser field, i.e. most likely the interference of the ionized electron wave-function with the ground state wave function.

4. CONCLUSION

In conclusion, the ionization of atomic Xe and Ar in intense laser fields is theoretically studied. The calculation is performed applying a quantum mechanical approach. The computation of nonlinear dipole response for a single atom under the external short laser field is obtained by solving the Lewenstein model by considering the time-dependent Schrödinger equation for one electron system. Laser-mater interaction is considered, and the tunnel ionization regime is justified from the Keldysh parameter ($\gamma < 1$). For the computation parameters, the short electron trajectory and the combination of short and long electron trajectories are taken into account, respectively. The short electron trajectories produce a strong dipole spectrum than the combination of short and long trajectories as well as the extension to higher photon energies. The results of this study show that the ionization potential of electrons and the external driving fields directly control the ionization rate of an electron. Major differences between short and long electron trajectories under the ultrashort laser field are that the electron recombination probability decreases under the combination of short and long trajectories because the electron exposed the driving field longer time and could miss the recombination. The obtained simulation results could help for pre-experimental studies to estimate the simulation parameters that play a role in how laser-matter interaction response to the application of the generation of coherent optical pulses.

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