IOCAT 2026 Conference
The 1st International Online Conference on Atoms
29–30 January 2026 | Online
atoms MDPI

IR-Assisted EUV Photoionization of Argon: Numerical Analysis of PADs and Fano's Propensity Rule

S. Chqondi [1, 2,*]
[1]Laboratory of Advanced Materials and Applications (LM2A), Faculty of Sciences Dhar El Mehraz, Sidi Mohamed Ben Abdellah University, Fez, Morocco
[2]Physics of Radiation and Laser-Matter Interactions, Faculty of Sciences, Moulay Ismail University, Meknes, Morocco
*Email: chqondi.s@ucd.ac.ma

Abstract

This work presents the results of a systematic study on the ionization of noble gas atoms, with a specific focus on the argon atom, under the effect of extreme ultraviolet radiation (XUV) in the presence of an intense, synchronized near-infrared (NIR) laser pulse. The theoretical study, carried out by solving the ab initio time-dependent Schrödinger equation in the one-active-electron (SAE) approximation, focuses solely on the response of the outermost valence electron of the argon atom to the laser field. The simulation results reveal an energy spectrum from two-color ionization, characterized by a harmonic peak surrounded by sideband peaks (SB±n). As the NIR field intensity increases, the amplitude of the harmonic peak decreases, while the sideband peaks broaden and shift to lower energies due to the Stark effect, reflecting the influence of the effective NIR field intensity. A deeper analysis of the angular distribution of the photoelectrons shows that interference between continuum states can occur as the infrared laser field intensity increases.

Objectives

The aim is to present the numerical results of the non-resonant two-color photoionization of argon, using femtosecond pulses of an infrared (IR) laser combined with its extreme-ultraviolet harmonics, with a particular focus on studying the influence of IR laser intensity on the photoelectron spectrum and its angular distribution.

Theoretical and Numerical Methods

➢**Laser Field Characteristics** : The interaction field we used results from the combination of an infrared laser field delivered by a Ti:Saphir laser (with a frequency ω_{IR}=0.057 a.u.≡1.55) eV) modulated by a trapezoidal envelope, and its 15th harmonic H15 of frequency ωH15=15×ωIR= 0.855 a.u..

$$\vec{E}_T(\vec{r},t)=\vec{E}_{H_q}(\vec{r},t)+\vec{E}_{IR}(\vec{r},t)$$

with

$$\vec{E}_{H_q}(\vec{r},t)=E_{0H_q}f(t,\omega_{IR})\sin(\omega_{H_q}t)\vec{e}_z$$

$$\vec{E}_{IR}(\vec{r},t)=E_{0IR}f(t,\omega_{IR})\sin(\omega_{IR}t)\vec{e}_z$$

and

$$f(t,\omega_0)=\begin{cases}\frac{t}{m.T_L} & \text{si } 0<t<m.T_L\\ 1 & \text{si } m.T_L<t<(n_{c.o}-m).T_L\\ -\frac{t}{m.T_L}+\frac{n_{c.o}}{m} & \text{si } (n_{c.o}-m).T_L<t<n_{c.o}.T_L\end{cases}$$

m=5 and $n_{o.c}$=30 in our case)

➢**The Time-Dependent Schrödinger Equation**: We performed the numerical resolution of the time-dependent Schrödinger equation (TDSE) using a potential model for argon and the single active electron approximation (SAE) [1]. Using the alternating direction implicit method [2]. We employed the semiclassical description of the laser-atom system, The time-dependent Schrödinger equation is written in a.u.

$$i\frac{\partial}{\partial t}\psi(\vec{r},t)=H(\vec{r},t)\psi(\vec{r},t),$$

$H=H_0+H_{int}(t)$. The total Hamiltonian of the system.

$H_0=-\frac{1}{2}\nabla^2+V(r)$ is the Hamiltonian of the atom and $H_{int}=\vec{E}(t).\vec{r}$ is the interaction Hamiltonian, In the length gauge

The model potential used takes the following Klapisch form [3] $V(r)=-\frac{1+(Z-1)e^{-c_1r}+c_2re^{-c_3r}}{r}$. The coefficients c1, c2 and c3 are adjusted in order to have energy values close to the experimental values.

➢**Angular distribution** : The chosen method to calculate the angular distributions of photoelectrons produced is based on the projection of the final wave function $\psi(\hat{r},t_{max})$ obtained by solving the TDSE at the end of the interaction, on the discretized continuum eigenstates ψck associated with the energy $E_k=\frac{k^2}{2}$ such that the differential ejection cross-section in the solid angle dΩ is

$$\left.\frac{d\sigma}{d\Omega}\right)_{E_k}=\left.\frac{d\sigma}{d\theta}\right)_{E_k}\propto\left|\langle\psi_{ck}((\hat{r})|\psi((\hat{r},t_{max}))\rangle\right|^2,$$

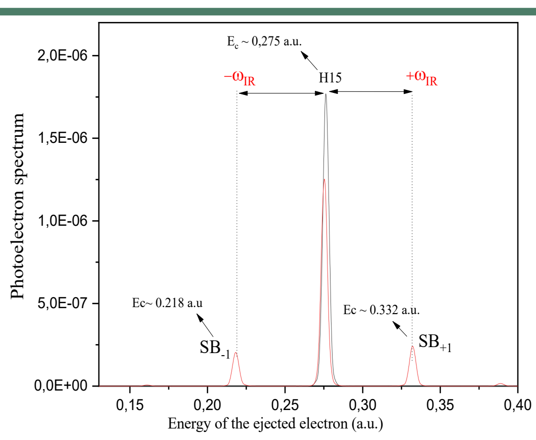


Figure 1: Photoelectron spectrum of two-color photoionization of argon (m=0). The EUV intensity is $I_{H15}=10^8 W/cm^2$ and the infrared intensity : $IIR = 0 W/cm^2$, $IIR = 5\times10^{11} W/cm^2$

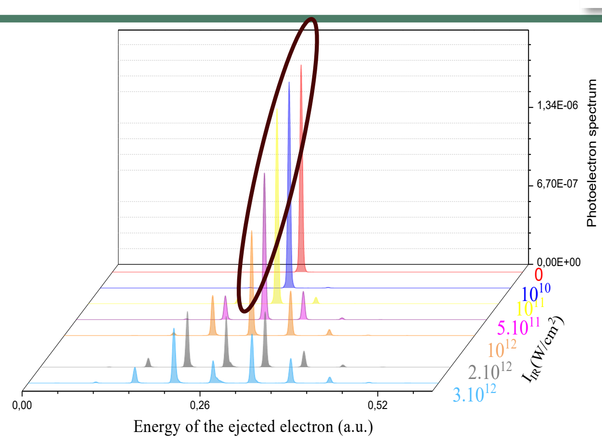
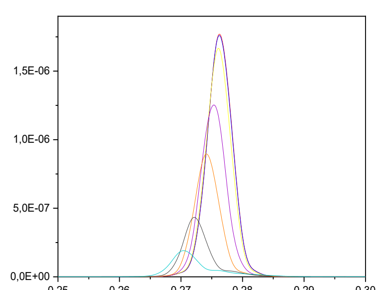
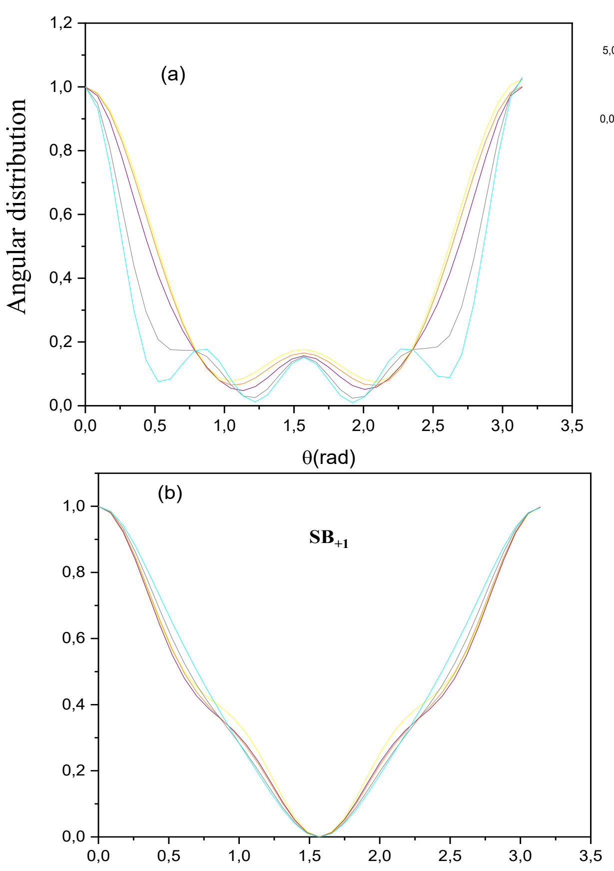


Figure 2 : Effect of Infrared Irradiation on the Photoelectron Spectrum





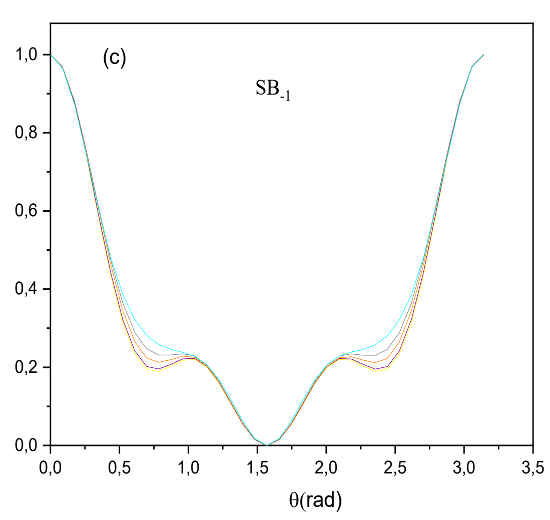


Figure 4 : Angular distribution of : (a) H15 peak (m=0) and (b) side peak (m=0)

Results and discussion

➢The energies of peaks (Fig.1) show a good agreement with the results calculated by energy conservation where $I_P(3p)$ =0,579 a.u.

➢The existence of satellite peaks is related to the harmonic peaks, and the increase in the intensity of the satellites is accompanied by a decrease in the harmonic peak. It appears as if the harmonic peak is partially transformed into satellite peaks (Fig.2). Moreover, the spectrum in this figure also shows a ponderomotive shift toward lower energies as the laser intensity increases (Fig.3).

➢shape of the angular distribution of Ar (3p) For different infrared laser intensities

❖H15 peak (m=0) is the interference between the partial waves s0and d0 with the dominance of **d0**, As the infrared intensity increases, the shape of the angular distributions broadens until a dip appears at its peak. This is actually due to the interference between the p and s waves (Fig.4-a).

❖SB+1 peak is the interference between the partial waves **p0** and **f0** with the dominance of orbital **f0** (Fig 4-b) and the orbital **p0** for SB+1(Fig 4-c). As the laser intensity increases, the angular distribution becomes progressively narrower, which results from the interference between the p and f waves. This phenomenon is necessarily related to the exchange of a large number of infrared photons above the ionization threshold.

❖The shape of the angular distributions confirms the dipole selection rule, Δl = ±1, as well as Fano's propensity rule, which states that, among the two possible transitions, the l → l + 1 channel is favored over l → l − 1 in the case of photon absorption, while the opposite tendency is observed for emission processes.

Conclusion and references

➢we have demonstrated that the IR illumination affects the harmonic peak by reducing its amplitude, while increasing the number and amplitude of the satellite peaks. Furthermore, the intensity of the IR laser field plays a crucial role in determining the shape of the angular distributions.

➢Our results confirm the generalization of selection rules and the Fano's propensity rule.

References

[1] A. K. Kazansky and N. M. Kabachnik, J. Phys. B: At. Mol. Opt. Phys.39,5173 (2006).

[2] R. S. Varga, Matrix Iterative Analysis (Englewood Cliffs, NJ : PrenticeHall), (1962)

[3] R. M. Potvliege Phys. Rev. A 81, 053402(2010)

[4] B. N. Parlett. The Symmetric Eigenvalue. No. 20, Classics in applied mathematics (1998)