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Single Photoionization of Xenon

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Abstract: *Our main intention to find the photonionization cross section (σ) and asymmetry parameter (β) for photoelectron in the reaction hν + Xe($1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$ $4s^2$ $4p^6$ $4d^{10}$ $5s^2$ $5p^6$) →Xe^+($1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$ $4s^2$ $4p^6$ $4d^{10}$ $5s^2$ $5p^5$) + e^- employing the Russell-Saunders (R-S)coupling and j-j coupling schemes under Hartree-Fock (HF) wave function in the non-relativistic R-matrix and relativistic R-matrix (RR-matrix) methods for length and velocity forms for experimental observations. Computation is done in the range of experimental observations and compared with other predictions. Present result shows that that the independent particle model (IPM) completely fails.*

Keywords : *Atoms, Photons, Photoionization, cross section, asymmetry parameter.*

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Introduction:

Interaction of photons with matter produces ionization of electrons is photoionization. It is the most basic fundamental phenomenon of nature that help to perception of the orbital, in general, atomic structure, molecules and solids[2]. Now a days, photoionization is successful tool, that operated several applications in condense matter, atomic, ionic, Laser and molecular. Collision of radiations with atoms and molecules are categorized into absorption, scattering and pair production. In this manuscript, low and intermediate energy range radiations (photons) are used and so that only the absorption process is studied [1], [3]. Atoms absorb photons causes photoionization, given by reaction

(photon) h + (atom)A → (ion atom)A^+ + (photoelectron) e^-

Authentic computation of photo ionization cross-sections of ions, molecules, crystals, clusters, atoms beneficial for analysis in the astrophysics, space physics, laser physics, plasma physics, etc. this is very useful for x-ray laser flash lamp photo pumping schemes. Independent particle approximation methods are used for the present computations to obtain photo ionization cross sections. The IPMcomputed energy-level employing Hartree-Fockmathod for the atoms wave function. Photon and atom collision can be successfully explained by first order perturbation theory.

Many computer codes and approximation methods on photo ionization previously published works[1-27]. Many body perturbation (MBPT), time-dependent local density approximation (TDLDA), multi-channel quantum defect theory (MQDT), random phase approximation (RPA) have been employed.

Close-coupling (CC), quantum defect theory (QDT), multi-channel quantum defect theory (MQDT), density function method (DFM), R-matrix, local density random phase approximation (LDRPA),Dirac atomic R-matrix code (DARC), random phase approximation (RPA), time dependent local density approximation (TDLDA), many body perturbation theory (MBPT), employed for photoionization of the non-relativistic. To obtain relativistic photoionization cross-section relativistic R-matrix (RR-matrix), Relativistic random phase approximation with exchange (RRPAE), and relativistic many body perturbation theory (RMBPT) are mostly employed.

CIV3, SMART, superstructure (SS) Cowan, multi configuration Hartee-Fock (MCHF), GRSP, and multi configuration Dirc-Fock (MCDF) computer codes have been extensively employed for both relativistic and non-relativistic.

We[15-17] have intended investigation work for noble gas Ne, Ar and Kr. During continuity, we have achieved computation for the photo ionization cross-section (σ) and photoelectron asymmetry parameter (β) for the reaction h + Xe($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^2\ 5p^6$)$\rightarrow$Xe$^+$($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^2\ 5p^5$) + e^- in for heavier noble gas atoms precisely.

Approximation method :

Photoionization cross-section for unpolarized light is given by

$$\sigma = \frac{4\pi}{3}\omega\left|D_{if}\right|^2\delta\left(E_i - E_f - E\right) \quad (1)$$

Where, electric dipole matrix element (D) in terms of initial and final wave function as row and column matrix

$$D_{if} = \langle\Psi_f|D|\Psi_i\rangle \quad (2)$$

In the electric dipole approximation, the angular distribution is given by

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi}\left[1 + \beta\ P_2\left(\cos\ \theta\right)\right] \quad (3)$$

photoelectron asymmetry parameter is β.

In the R-matrix method,

R-matrix method for Photoionization cross-sections are computed, the wave function given as

$$\Psi = A\sum_i \psi_i\,\theta_i + \sum_j \phi_j\,c_j \quad (4)$$

where $\psi_i\rightarrow$ the wave function for an N-electron system,

$\theta i\rightarrow$ a function for an added electron,

$A\rightarrow$ an operator for vector coupling and anti-symmetrization,

$\phi_j\rightarrow$ a wave function for the (N+1)-electron system and

$c_j\rightarrow$ are coefficients to be determined.

The wave functions Ψ_i and function ϕ_j gives constraint. The R-matrix method optimized orbitals θ_i and coefficients c_j.

Z is the atomic number which represents charge on nucleus, which affect relativity in the target wave function showing the scattered electron also significant in low energy. For electron with kinetic energies far below the rest energy mc^2= 511 keV the B.P. Hamiltonian employed by Bethe and Salpeter

$$H_{BP}^{N+1} = H_{NR}^{N+1} + H_{R}^{N+1} \quad (5)$$

Equation of motion for one-electron and two-electron given by Bathe and Salpeter. The non-relativistic Hamiltonian for H_R^{N+1} and perturbative contributions H_R^{N+1} gives rise to the relative magnitudes are lower powers of α. [9]

In the present code, we specifically retain only the one-electron terms resulting from the reduction of the Dirac equation to Breit-Pauli form up to order $\alpha^2 Z^4$.

The low-Z Breit-Pauli Hamiltonian for an (N+1)-electron is given as

$$H_R^{N+1} = H_{mass}^{N+1} + H_{D_1}^{N+1} + H_{SO}^{N+1} \quad (6)$$

$$H_{BP}^{N+1} = H_{NR}^{N+1} + H_{mass}^{N+1} + H_{D_1}^{N+1} + H_{SO}^{N+1} \quad (7)$$

Every of the one-electron Breit-Pauli terms can electively be contained:

$$H_{mass}^{N+1} = \frac{\alpha^2}{8} \sum_{n=1}^{N+1} V_n^4 \quad \text{(Mass-correction)} \quad (8)$$

$$H_{D_1}^{N+1} = -\frac{\alpha^2 Z}{8} \sum_{n=1}^{N+1} V_n^4 \left(\frac{1}{r_n}\right) \quad \text{(Darwin)} \quad (9)$$

$$H_{SO}^{N+1} = -\frac{\alpha^2 Z}{8} \sum_{n=1}^{N+1} \frac{l_n . S_n}{r_n^3} \quad \text{(Spin-orbit)} \quad (10)$$

Hamiltonian non-fine structure part

$$H_{nfs}^{N+1} = H_{NR}^{N+1} + H_{mass}^{N+1} + H_{D_1}^{N+1} \quad (11)$$

commutes with L^2, S^2, L_z, S_z and parity, whereas H_{SO}^{N+1} H_{BP}^{N+1} and only commute with J2, Jz and parity.

Results and Discussion:

In this paper, the photoionization cross-section (σ) and asymmetry parameter (β) for the reaction hν + Xe $(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^2\ 5p^6) \rightarrow Xe^+(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^2\ 5p^5) + e^-$ have been computed the Russell-Saunders (R-S) coupling and j-j coupling schemes under Hartree-Fock (HF) wave function in the non-relativistic R-matrix[23] as well as RR-matrix[24]approximation for velocity and length forms for experimental observation. Computation is done in the range of experimental measured value and compared with other predictions result.

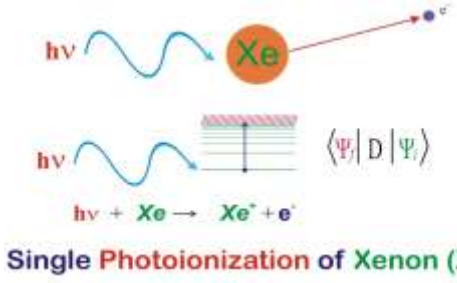

Figure Caption

Figure 1: Photoionization cross section (σ) for the 5p-subshell of xenon (Xe).

Present R-matrix results (Length form)
Present R-matrix results (Velocity form)
Present RR-matrix results (Length form)
Present RR-matrix results (Velocity form)
Becker (Ref.22)
Fahlmann (Ref.22)
Adam (Ref.22)
Berkowitz (Ref.22)
Kutzner (Ref.22)

Figure 2: Photoelectron asymmetry parameter (β) for xenon.

Present R-matrix results
Present RR-matrix results
Southworth (Ref.22)
Southworth (Ref.22)
Krause (Ref.22)
Torop (Ref.22)
Dahmer (Ref.22)

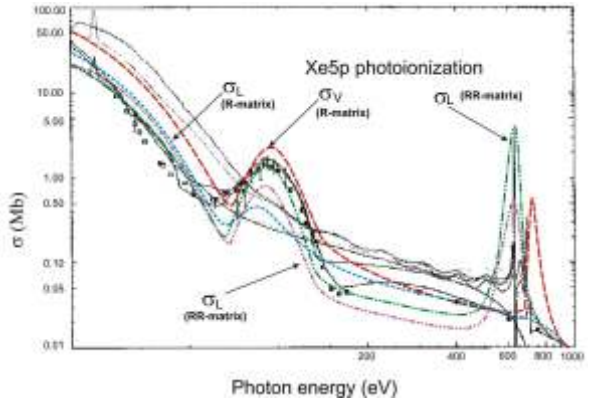

Fig.1.

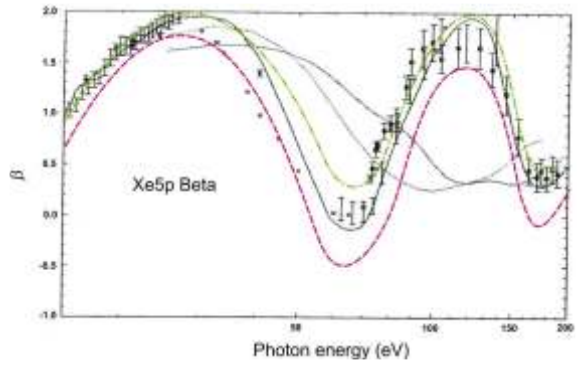

Fig.2.

Fig. 1 shows that current results of R-matrix and RR-matrix integral photoionization cross sections of xenon (Xe) compared with other available theoretical predictions and observations. In low energy region length form (σL) and velocity form (σV) close to experimental observations but slightly far from other theorical predictions [20]. In the intermediate energy range our computed results and experimental observations slightly discrepancy, which display significance of correlation as well as relativity. Fig. 2 displays photoelectron asymmetry parameter (β) for 5p photoionization of xenon (Xe). It display computed present result and experimental data valid in low energy range and considerable discrepancy in intermediate energy range.

Conclusion:

We have computed photoionization cross-section (σ) and photoelectron asymmetry parameter (β) for Xenon (Xe) using Hartree-Fock (HF) wave function under dependable R-matrix and R. R-matrix methods. Our current results reveals that in the case of heavier noble gas atoms (Xe), thus independent particle model completely fails which display the significance of relativity as well as correlation. HF cross sections are both qualitatively and quantitatively invalid in the entire energy range which display that the multi electron correlation as well as relativity are both significant but inter-channel interactions are more essential than the relativity and intra-channel interaction for accomplishing more validity theoretical prediction.

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