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Photoionization of noble gas atoms

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Abstract : Photon impact ionization cross sections for the noble gas atoms (Ne and Ar) have been calculated in the *L–S* and *j–j* coupling schemes employing the reliable non-relativistic *R*-matrix and relativistic *R*-matrix methods in both the length and velocity gauges in the energy range of experimental data available. Comparison is made with all available experimental data as well as other theoretical results. Our present theoretical investigation clearly demonstrates that there is a good agreement between our present results and other results in the case of neon which reflects the correlation and relativity are not important in this case. In the case of Ar, the independent particle approximation breaks down. It exhibits that the multielectron correlation as well as relativity are important but interchannel interactions are more important than the intrachannel interaction for obtaining high precision results.

Keywords : Atoms, photons, photoionization.

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Introduction

Interaction between matter and radiation corresponding to photoionization is a fundamental process of nature and of major importance that occurs everywhere in the Universe. Photoionization of matter was the first in a series of experimental discoveries followed by a corresponding theoretical explanation which led to the foundation of quantum physics. It was infact Einstein's interpretation of the photoelectric effect that proved the concept of energy quantization by Plank to be generally valid. Despite this early success it took more than 40 years until photoelectron spectroscopy became a growing field of scientific research and finally, an analytical tool for industrial research. This was because the early efforts to record line spectra in measurements of the photoelectric effect were hampered by experimental difficulties such as insufficient energy resolution.

after the pioneer work of the Uppsala group did photoelectron spectroscopy become a powerful tool for studying the electronic structure of matter and its chemical composition.

Accurate calculations of photoionization cross sections f atoms, molecules, clusters, solids and ions are useful in a variety of investigations in laser physics, plasma physics, astrophysics, space physics, fusion research, *etc.* It is particularly useful in the context of flash lamp photopumping schemes for X-ray lasers. Most of the existing calculations of the photoionization cross sections are performed employing independent particle model (IPM). In this model, the energy-level and wavefunction of the target are first calculated using the Hartree-Fock method. The interaction of the incident electromagnetic radiation with the target is treated *via* the first order perturbation theory. There are several theoretical methods as well as computer codes for photoionization processes in atoms, molecules and ions available in the literature [1–21]. For the non-relativistic photoionization cross sections, close coupling (CC), quantum defect theory (QDT), multi-channel quantum defect theory (MQDT), density function method (DFM), local density random phase approximation (LDPRA), time dependent local density approximation (TDLDA), many body perturbation theory (MBPT), random phase approximation (RPA) and *R*-matrix have been used extensively. For relativistic photoionization cross sections, relativistic *R*-matrix (*RR*-matrix), relativistic many body perturbation theory (RMBPT),

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Dirac atomic R-matrix code (DARC) and relativistic random phase approximation with exchange (RRPAE) have been employed in many cases. For the non-relativistic as well as relativistic structure calculations, CIV3, superstructure (SS), multiconfiguration Hartree-Fock (MCHF), Cowan, Bates, SMART, multiconfiguration Dirac Fock (MCDF), GRASP, RRPAE and RPA computer codes have been used widely. In our present work photon impact ionization cross sections (σ) for the reaction $h\nu + \text{Ne}(1s^22s^22p^6) \rightarrow \text{Ne}^+(1s^22s^22p^5) + e$ and $h\nu + \text{Ar}(1s^22s^22p^63s^23p^6) \rightarrow \text{Ar}^+(1s^22s^22p^63s^23p^5) + e$ have been calculated in the L–S and j–j coupling schemes using Hartree-Fock wavefunctions [22] within the reliable non-relativistic R-matrix as well as relativistic R-matrix (RR-matrix) methods in both the length and velocity gauges in the energy range of experimental data available.

2. Theory

Photoionization cross section is given by

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

for non-polarized isotropic radiation, where

$$D_{if} = \left\langle \Psi_f \left| D \right| \Psi_i \right\rangle \tag{2}$$

is the matrix element of dipole operator D.

In the dipole approximation, the angular distribution is given by

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

where β is the photoelectron asymmetry parameter.

In the R-matrix method, photoionizaton cross sections are calculated by using wavefunction expansions of the form as follows :

$$\Psi = A\sum \psi_i \theta_i + \sum \phi_j c_j \tag{4}$$

where ψ_i is the wavefunction for an N-electron system, θ_i a function for an added electron, A an operator for anti-symmetrization and vector coupling, ϕ_j a wave function for the (N + 1)-electron system and c_j are coefficients to be determined. The functions ψ_i are referred to as target states. The orbitals θ_i are taken to be orthogonal to all orbits in the ψ_i, and this constraint provides and main reason for including the functions ϕ_j. The orbitals θ_i and coefficients c_j are optimized using the R-matrix method.

As the charge Z on the nucleus increases, relativistic effects both in the target wavefunction and in the wavefunction representing the scattered electron become important even for low energy electron scattering. For electrons with kinetic energies far below the rest energy $mc^2 = 511$ keV the Breit-Pauli Hamiltonian

$$H_{BP}^{N+1} = H^{N+1} + H_{REL}^{N+1} \tag{5}$$

discussed by Bethe and Salpeter for the case of one- and two-electron suffices as an equation of motion. H is the non-relativistic Hamiltonian. H_{REL} gives rise to perturbative contributions whose relative magnitudes are lower powers of α.

The non-relativistic R-matrix method has been extended to include relativistic terms from the Breit-Pauli Hamiltonian by Scott and Burke. In the current code we explicitly retain only the one electron terms resulting from the reduction of the Dirac equation to Breit-Pauli form up to order α^2Z^4, i.e. the mass-correction term, the one-electron Darwin term and the spin-orbit term; implicitly accounted for the fine-structure two-electron contributions from closed subshells.

The low-Z Breit-Pauli Hamiltonian for an (N + 1)-electron is taken to be

$$H_{BP}^{N+1} = H^{N+1} + H_{\text{mass}}^{N+1} + H_{D_1}^{N+1} + H_{SO}^{N+1} \tag{6}$$

Each of the one-electron Breit-Pauli terms can optionally be included :

$$H_{\text{mass}}^{N+1} = -\frac{\alpha^2}{8}\sum_{n=1}^{N+1} \nabla_n^4 \quad \text{(mass-correction)} \tag{7}$$

$$H_{D1}^{N+1} = -\frac{\alpha^2 Z}{8}\sum_{n=1}^{N+1} \nabla_n^2\left(\frac{1}{r_n}\right) \quad \text{(Darwin)} \tag{8}$$

$$H_{SO}^{N+1} = \frac{\alpha^2 Z}{2}\sum_{n=1}^{N+1} \frac{l_n.S_n}{r_n^3} \quad \text{(spin orbit)} \tag{9}$$

Note that the non-fine structure part of the Hamiltonian

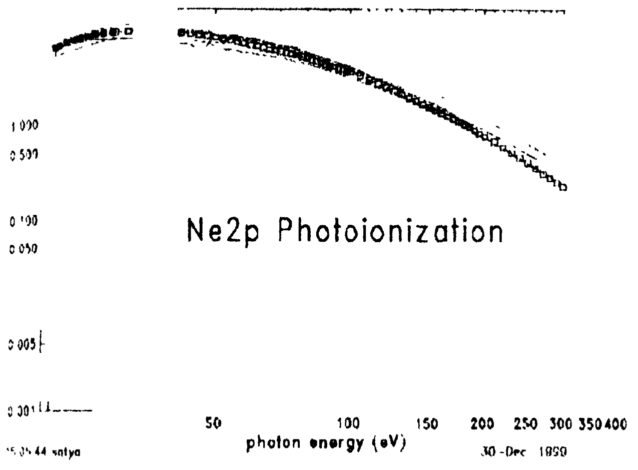
$$H_{nfs}^{N+1} = H^{N+1} + H_{\text{mass}}^{N+1} + H_{D_1}^{N+1} \tag{10}$$

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

3. Results and discussion

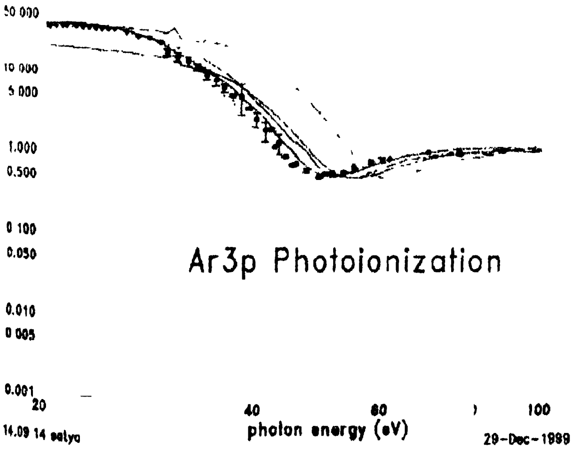
In the present work, the photon impact integral ionizatio cross sections (σ) for the reaction $h\nu + \text{Ne}(1s^22s^22p^6)$ - $\text{Ne}^+(1s^22s^22p^5) + e$ and $h\nu + \text{Ar}(1s^22s^22p^63s^23p^6)$ $\text{Ar}^+(1s^22s^22p^63s^23p^5) + e$ have been calculated in the L- and j–j coupling schemes using Hartree-Fock wavefunc within the reliable non-relativistic R-matrix as well relativistic R-matrix (RR-matrix) methods in both the leng and velocity gauges in the energy range of experiment data available. Comparison is made with all available experimental data as well as other theoretical results.

Figure 1 exhibits our present R-matrix total photoionization oss sections of neon atomic system along with other perimental as well as theoretical results from the threshold about 400 eV energy range. It is clear from this figure that r R-matrix results in both length and velocity gauges are good agreement with other theoretical predictions and perimental observations which show that the effect of lativity and correlation is negligible in this case.



gure 1. Total photon impact ionization cross section for the subshell of neon —— present R-matrix results in the length form present R-matrix results in the velocity form, ☐ Wulleumier ef 4), Δ Saito (Ref. 4), ■ Marr (Ref. 4), χ Wulleumier (Ref 4), Berkowitz (Ref 4), -- Yeh (Ref. 4), — — Johnson (Ref. 4), — nnedv (Ref 4)

Figure 2 displays our R-matrix integral photoionization oss sections of argon (Ar) atomic system along with other ailable theoretical and experimental results. It is seen from this figure that in the low energy range, the length form is better than the velocity form of cross sections which indicates that the length gauge is valid in the lower energy region and the velocity form is good in the intermediate energy range. However, there is considerable disagreement between our results and the experimental data which shows the importance of correlation and relativity.



gure 2. Total photon impact ionization cross section for the subshell of argon : —— present R-matrix results in the length m : .... present R-matrix results in the velocity form, ■ Langer ef 4), ∇ Chan (Ref. 4), ● Adam (Ref. 4), □ Berkowitz (Ref. 4), Tulkki (Ref. 4), -— Wijesundera (Ref. 4), ---Huang (Ref 4).

4. Conclusion and future direction

Our present theoretical investigation clearly demonstrates that the effect of correlation and relativity in the case of lighter noble gas atom neon is negligible. These effects increase with the increase of the atomic number (Z). In case of the rare gas atom argon, there is a breakdown of independent particle approximation which demonstrates the importance of correlation and relativity. HF cross sections are both qualitatively as well as quantitatively incorrect which exhibit that the multielectron correlation as well as relativity are important but interchannel interactions are more important than the intrachannel interactions for obtaining reliable results. Our present results suggest that full configuration interaction wave functions must be used in the R-matrix as well as RR-matrix in order to obtain high precision results. The output of CIV3, SS, MCHF, Cowan, and MCDF may be input to the R-matrix and RR-matrix for accurate predictions.

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