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Single Photoionization of Beryllium [Be($1s^2$ $2s^2$)]

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Abstract: ***As Single photoionization cross section is very sensitive to the wave functions used in the matrix elements and hence provides an opportunity to test the accuracy of wave functions. So to test the accuracy of our configuration-interaction (CI) wave functions which have already produced reliable oscillator strengths , we have performed calculations for the single photoionization cross sections (SPICS) of alkali metal atom Beryllium [Be($1s^2$ $2s^2$)] employing configuration interaction (CI) wave function for the ground state and Coulomb wave function for the final state. Our present results length and velocity forms are closer than other theoretical results but there is discrepancy between experimental and present theoretical results near threshold to intermediate energy regions which suggests to do further investigation. 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.***

Keywords: Photoionization, Cross section, Wave function, Atom, Interaction

I. INTRODUCTION

Photoionization is constructive tool used for many purposes in atomic physics, molecular physics, solid-state physics, plasma physics, laser physics, astrophysics, space physics, cosmic physics, fusion research, etc. The interactions of photons (electromagnetic radiation) with atoms, ions and molecules are organized into absorption, scattering and pair-production. In this paper, low and intermediate energy region photons absorption is considered. Photoionization of atom can be represented by the reaction

$$h\nu + A \rightarrow A^+ + e^-$$

Accurate calculations of cross section (σ) of atoms are important parameters to study the process of photoionization. Most of the existing calculations of photoionization cross sections are performed applying independent particle model (IPM) [1]. In this model, the energy level and wave function of the target are first calculated using Hartree-Fock method [2-4]. The interaction of the photons or electromagnetic radiation with target as atom is dealt via the first order perturbation theory. There theoretical methods along with computer codes for photoionization processes in atoms, ions and molecules such as for the non-relativistic photoionization cross section, close-coupling (CC), convergent close-coupling (CCC).

Accuracy of the calculated collisional cross sections and oscillator strengths particularly for the neutral system is very sensitive to the target wave functions. Hence the choice of the target wave functions plays a very important for the reliable results. It is well known that the configuration interaction wave function is correlated functions. We have generated fully controlled wave functions for atoms using Tiwary approach [5-10]. We have calculated the photon impact ionization cross section (σ) for the atom (Be). The reaction is

$h\nu + Be(1s^2\ 2s^2) \rightarrow Be^+(1s^2\ 2s) + e^-$

II. THEORY : [METHOD OF CALCULATION]

Under the electric-dipole approximation, the differential cross section for the ejection of an electron with angular momentum l and energy ε in the energy range $d\varepsilon$ is

$$\frac{d\sigma}{d\varepsilon} = \frac{4\pi^2 \alpha a_0^2}{3} \sum \frac{df}{d\varepsilon} \qquad (1)$$

where $\frac{df}{d\varepsilon}$ is the differential oscillator strengths for the transition from the ground state ψ_i to the final state ψ_f. The quantity $\frac{df}{d\varepsilon}$ is conveniently expressed in the length and velocity forms as

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$$\frac{df_L}{d\varepsilon} = E\left|\left\langle \psi_f(\mathbf{r}) \middle| \mathbf{r} \middle| \psi_i(\mathbf{r}) \right\rangle\right|^2 \quad (2)$$

$$\frac{df_V}{d\varepsilon} = \frac{1}{E}\left|\left\langle \psi_f(\mathbf{r}) \middle| \nabla \middle| \psi_i(\mathbf{r}) \right\rangle\right|^2 \quad (3)$$

It is well known that equations (2 and 3) would provide the same results if ψ_i and ψ_f were exact.

Finally, the total cross section for the production of one continuum electron by single photon impact is

$$\sigma = \sum_l \int_0^E \frac{d\sigma}{d\varepsilon} d\varepsilon \quad (4)$$

In equation (4), summation over *l* corresponds to the contributions of all allowed final continuum configurations of the angular type $\varepsilon l \varepsilon' (l+1)$. Tiwary and his co-workers [11, 12, 13, 14, 15, 16] have extensively investigated the correlation in atoms and ions using the configuration-interaction (CI) wave functions. We have generated full CI wave functions for several atoms and tested the accuracy of wave functions calculating the length and velocity forms of the optical oscillator strengths. The wave function of the ground state of atom is represented by the full CI wave function which includes full correlations and generated exactly in the same way as in our earlier works and hence not reported in details here. Our CI wave function can be written as

$$\psi(\mathrm{LS}) = \sum_i a_i \, \phi_i \, (\alpha_i \mathrm{LS}) \quad (5)$$

The coefficients a_i are the eigenvectors components of the Hamiltonian matrix with the typical element

$$\mathrm{H}_{ij} = \left\langle \phi_j \middle| \mathrm{H} \middle| \phi_i \right\rangle \quad (6)$$

ϕ_i are single-configuration functions from one-electron functions, whose orbital and spin momenta are coupled to form the common total angular-momentum quantum numbers L and S according to a prescription denoted in (5)

by α_i .

We express the radial parts of the one-electron functions in analytical form as a sum of Slater-type orbitals, following Clementi and Roetti [17] :

$$P_{nl}(r) = \sum_{j=1}^{k} C_{jnl} \; r^{I_{jnl}} \; e^{-\xi_{jnl} r} \quad (7)$$

The parameters in (7) can be varied to optimize the energy of any state, subject to the orthonormality conditions.

$$\int_0^\infty P_{nl}(r) \, P_{n'l}(r) \, dr = \delta_{nn'} \quad (8)$$

The final state wave function is represented by a symmetrized one electron Coulomb wave function as follows :

$$\psi_f(\mathbf{r}) = \frac{1}{\sqrt{2}} \sum (l, m, | l, M) \phi(\varepsilon, l, m | r) \qquad (9)$$

where ε is kinetic energy of the escaping electron. In equation (9), $(l, m, | l, M)$ denotes the Clebsch-Gordan coefficients providing threshold final state and the one-electron spatial orbitals are given by

$$\phi(\varepsilon, l, m/r) = \left(\frac{2}{R\pi}\right)^{1/2} \frac{F_l(\eta, kr)}{r} Y_l^m(\hat{r}) \qquad (10)$$

where F_l is the regular spherical Coulomb wave function of order *l* with

$$R = \sqrt{2\varepsilon} \quad \text{and} \quad \eta = -Z/k \qquad (11)$$

The ϕ orbitals are normalized in the energy scale

$$\langle \phi(\varepsilon, l, m) | \phi(\varepsilon', l', m') \rangle = \delta(\varepsilon - \varepsilon') \delta_{l,l'} \delta_{m,m'} \qquad (12)$$

III. RESULTS

In this paper, the photon impact integral ionization cross section (σ) for Beryllium (Be) has been calculated for given energy range and compared with experimental data and many theoretical results.

As Single photoionization cross section is very sensitive to the wave functions used in the matrix elements and hence provides an opportunity to test the accuracy of wave functions. So to test the accuracy of our configuration-interaction (CI) wave functions which have already produced reliable oscillator strengths , we have performed calculations for the single photoionization cross sections (SPICS) of alkali metal atom Beryllium [Be($1s^2$ $2s^2$)] employing configuration interaction (CI) wave function for the ground state and Coulomb wave function for the final state.

Fig. shows the SPICS of beryllium (Be). It is seen from fig. that our both results length and velocity form are in better agreement with experimental results [18, 19] and other theoretical calculations [20, 21] in higher energy range but in disagreement near threshold to intermediate energy range.

Figures and Tables

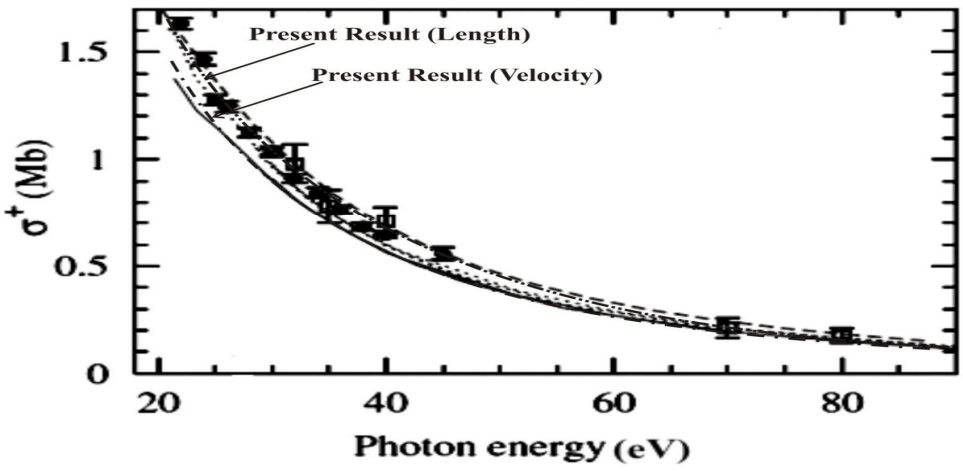

Fig.1. Single Photoionization (SPICS) cross section (Mb) of Beryllium (Be).

Figure Captions

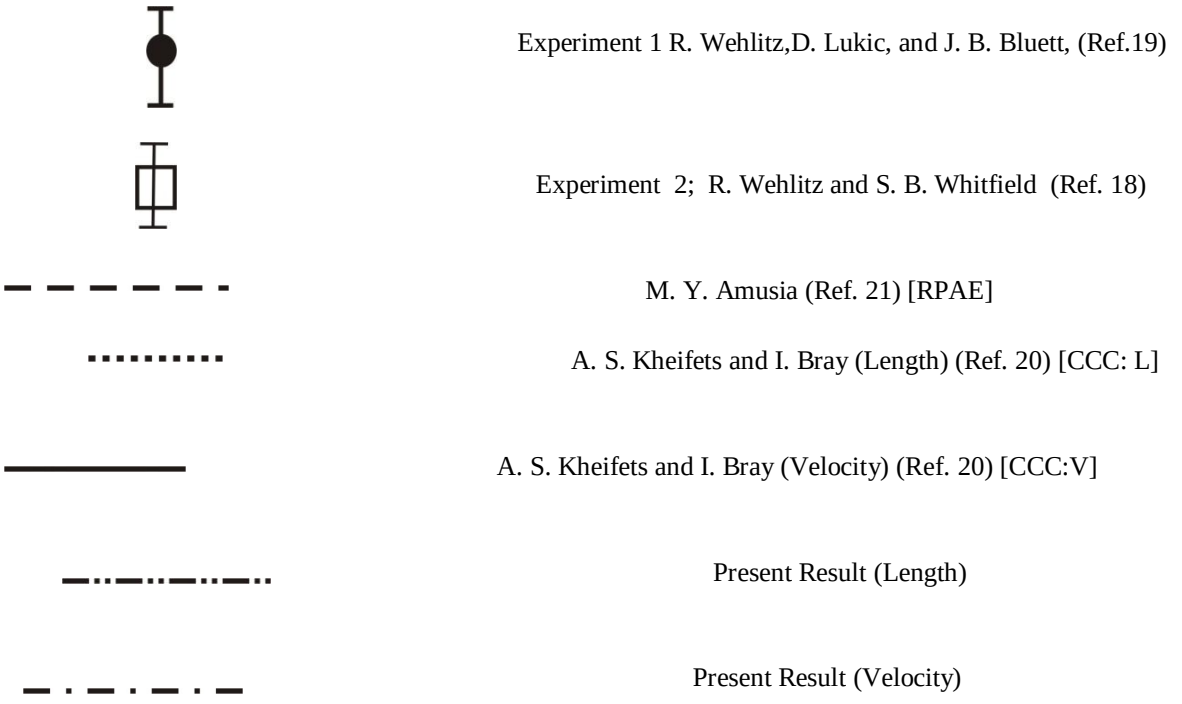

Fig. Single Photoionization (SPICS) cross section σ (Mb) of Beryllium (Be).

IV. CONCLUSIONS

In figure SPICS of Beryllium (Be) shows that our present results length and velocity forms are closer than other theoretical results [20,21] but there is discrepancy between experimental and present theoretical results near threshold to intermediate energy regions which suggests to do further investigation. 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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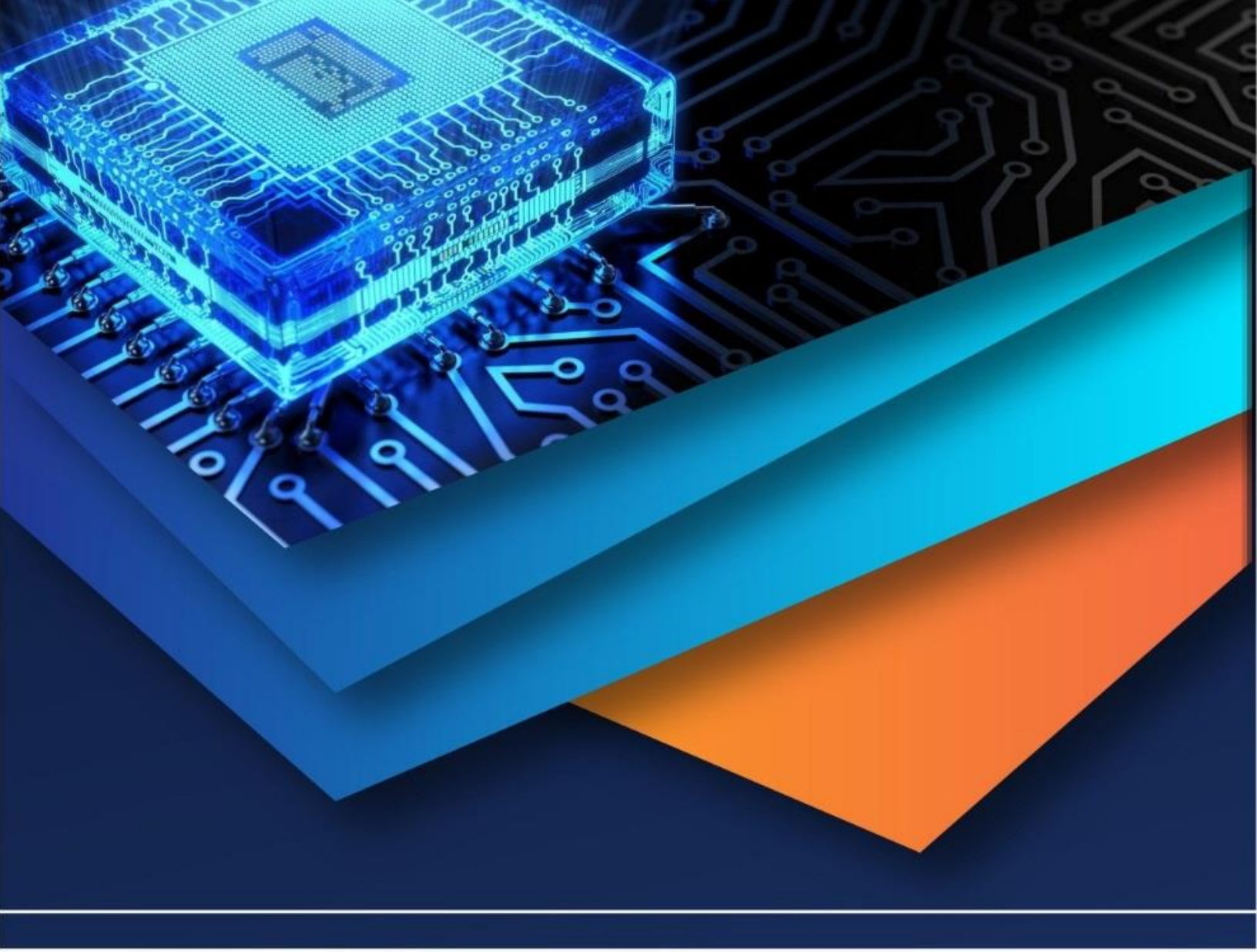

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