Single Photon to Double Photoionization of Magnesium ($1s^2\ 2s^2\ 2p^6\ 3s^2$) $^1S_0^e$

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***Abstract*—We have calculated the double photoionization cross section [DPICS] of Magnesium [Mg] ($1s^2\ 2s^2\ 2p^6\ 3s^2$)] using configuration interaction (CI) wave function for the initial state and Brauner, Briggs and Klar (BBK) wave function for the final state involved in the electric dipole transition matrix element. In the double photoionization absorption of a single-photon by an atom [Mg] with the ejection of two electrons. One electron is photoelectron and other is correlated electron having less energy than photoelectron. Comparison is made with available experimental observations and other theoretical predictions. Our present result is encouraging**

***IndexTerms*— Photon, Atom, Photoionization, Cross section, wave function.**

INTRODUCTION

Alkali metal atom is a popular subject of theoretical and experimental investigations, because of abundant elements in the universe and their simple electronic structure, with two valence electron outside energetically separated from inner cores. In these atoms, the outer valence shell is well separated from the rest of the atom. Therefore, at relatively small photon energies, the inner core and subvalent electrons can be treated as "spectators," not taking direct part in photoionization of the outer valence shell. In this situation, double photoionization (DPI) process in alkaline-earth-metal atoms is similar to that in He($1s^2$) except for a different radial structure of the target *ns* orbital and the influence of the distorting potential on the departing photoelectrons.

Direct valence shell double photoionization (DPI) in heavier alkaline-earth-metal atoms Mg is studied. Ceraulo et. al. [1] within a theoretical scheme which took into account the final-state electron correlation by introducing a Coulomb hole factor. However, this approaches for He failed to provide even qualitative agreement with experimental data. Kazansky and Ostrovsky [2] calculated direct DPI in Be, Mg, Ca and Sr by employing an extended Wannier ridge model and mimicking the ground-state correlation by introducing a Coulomb hole in the initial state. The double photoionization cross section (DPICS) for He has been calculated by Byron and Joachain [3], Brown [4], Amusia *et al* [5], Yurev [6], Varnavshikh and Labzovskii [7], Carter and Kelly [8] and Tiwary [9], Becker and Shirley [10], Sonntag and Zimmermann [11] and Amusia [12], Tiwary and Kumar [13].

For the first time Tiwary [9] has used the Altick wavefunction to calculate DPICS of He. This investigation shows that the Altick wavefunction is not capable to yield encouraging results in the low-energy region. Brauner, Briggs and Klar (BBK) [14] have proposed a better double continuum wavefunction (DCWF). We [13] have employed BBK DCWF to calculate the DPICS of He. Result obtained is promising which reflects the adequacy of BBK DCWF. So that we have also used the BBK DCWF for Mg, because it behave as two valence electron system in outer most orbit.

Some experimental observations and theoretical predictions have been also made in heavier alkaline-earth-metals [1, 2]. Kheifets and Bray [15] have calculated the double photoionization cross sections of Magnesium atomic system (Mg) from the threshold to 45 eV. There is a reasonably agreement in mid energy region but large discrepancy exists in the lower region. Our earlier results of He [13] and of Ar [16] using BBK DCWF has encouraged to extend to calculate the double photoionization cross section of Mg. The primary purpose of the present work is to test the validity of the BBK DCWF in the case of double photoionization of Mg by single photon impact.

METHOD

The expression for the total double photoionization cross section can be written as

$$\sigma^{2+}\left(E_v\right) = \frac{4\pi^2 \alpha\, a_0^2}{E_v} \sum_l \int\int d\varepsilon\, d\varepsilon' \left| \left\langle \Psi_f \left| \sum_{j=1}^{2} \frac{\partial}{\partial z_j} \right| \Psi_i \right\rangle \right|^2 \delta\left(E_v - B_i - \varepsilon - \varepsilon'\right) \tag{1}$$

where $\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$ is the fine-structure constant and a_0 is the first Bohr radius. E_v is the incident energy, and Ψ_i and Ψ_f are the wavefunctions of the initial and final states involved in the transition.

We have employed the configuration interaction (CI) wavefunction for the initial state as given below

$$\Psi_i = \sum_{k=1}^{M} a_k \Phi_k\left(\alpha_k LS\right), \tag{2}$$

where $\{\alpha_k\}$ denote all the distinguishing features of Φ_k other than L and S.

We now turn to the problem of representing the final continuum state Ψ_f of Mg with two free electrons and Mg^{++}. We have employed the Brauner, Briggs and Klar double-continuum wavefunction (BBK DCWF) [14] as well as modified BBK DCWF which are given below:

$$\Psi_f^- = (2\pi)^{-3/2} e^{i(\boldsymbol{k}_1.\boldsymbol{r}_1+\boldsymbol{k}_2.\boldsymbol{r}_2)} \times {}_1F_1\left(-i\frac{Z}{k_1},1;-i(k_1r_1+\boldsymbol{k}_1.\boldsymbol{r}_1)\right) \times {}_1F_1\left(-i\frac{Z}{k_2},1;-i(k_2r_2+\boldsymbol{k}_2.\boldsymbol{r}_2)\right) \times {}_1F_1\left(i\frac{1}{2\kappa},1;-i(\kappa r_{12}+\boldsymbol{\kappa}.\boldsymbol{r}_{12})\right) \quad (3)$$

with $\boldsymbol{\kappa} = \frac{1}{2}(\boldsymbol{k}_1 - \boldsymbol{k}_2)$ and $\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. The essential property of this wave function is that it shows exact asymptotic behaviour in the Redmond [17] limit, i.e., for large particle separations.

An even better description of the double continuum state is achieved with help of local space dependent momenta. Actually Alt and Mukhamedzhanov [18] showed the necessity of modified momenta to correctly describe the asymptotic form of the wavefunction in the limiting case of one particle far away from the remaining 2-body subsystem. We present here a slightly different viewpoint and proceed as follows. First we separate off the plane wave factor for the electrons

$$\Psi_f^- = e^{i(\boldsymbol{k}_>.\boldsymbol{r}_>+\boldsymbol{k}_<.\boldsymbol{r}_<)}\,\overline{\Psi} \quad (4)$$

where $\overline{\Psi}$ describes the Coulomb modifications. $\boldsymbol{r}_{>(<)}$ stands for the larger (smaller) electron-ion separation and $\boldsymbol{k}_{>(<)}$ are the corresponding momenta. As in the BBK wavefunction, equation (4), we employ Coulomb waves for 2-body subsystems. For the outer electron located at $\boldsymbol{r}_>$ we use ordinary Coulomb waves for the 2-body subsystems as above,

$$\overline{\Psi} = A\,{}_1F_1\left(-i\frac{Z}{k_>},1;-i(k_>r_>+\boldsymbol{k}_>.\boldsymbol{r}_>)\right){}_1F_1\left(i\frac{1}{2\kappa},1;-i(\kappa r+\boldsymbol{\kappa}.\boldsymbol{r})\right) \propto Ae^{i\Phi} \quad (5)$$

where the phase Φ being chosen to produce correct asymptotic behaviour,

$$(\boldsymbol{k}_>.\nabla_> + \boldsymbol{k}_<.\nabla_<)\Phi = -\frac{Z}{r_>} + \frac{1}{r_{><}} \quad (6)$$

with the solution

$$\Phi = -\frac{Z}{k_>} ln(k_>r_> + \boldsymbol{k}_>.\boldsymbol{r}_>) + \frac{1}{2\kappa} ln(\kappa r_{><} + \boldsymbol{\kappa}(\boldsymbol{r}_> - \boldsymbol{r}_<)) \quad (7)$$

and $\boldsymbol{\kappa} = \frac{1}{2}(\boldsymbol{k}_> - \boldsymbol{k}_<)$. The amplitude in equation (5) describes the motion of the inner electron located at $\boldsymbol{r}_<$. For $r_> >> r_<$ the wave equation for $A = A(\boldsymbol{r}_<)$ reduces to

$$\left[\Delta_< + 2i\boldsymbol{\kappa}_{eff}.\nabla_< - \frac{2Z}{r_<}\right] A(\boldsymbol{r}_<) = 0 \quad (8)$$

with the solution

$$A = {}_1F_1\left(-i\frac{Z}{k_{<,eff}},1;-i(k_{<,eff}r_< + \boldsymbol{k}_{<,eff}.\boldsymbol{r}_<)\right) \quad (9)$$

where the effective momentum for the inner electron is given by

$$\boldsymbol{k}_{<,eff} = \boldsymbol{k}_< + \nabla_<\Phi \quad (10)$$

and Φ given by equation (7). This momentum modification (10) is identical to the result achieved by [14] to lowest order in $r_</r_>$. $\overline{\Psi}$ in equation (4) has correct asymptotic behaviour also if all three particle separations are large. This is easily seen because each of the confluent hypergeometric functions reduces then to a pure phase factor, and the effective momentum (10) approaches its static value in that limit. Equation (5) is still incorrect in the limit of two electrons close together but far away from the nucleus. We investigate therefore this limit now. To this end we introduce Jacobi coordinates $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_< + \boldsymbol{r}_>)$ and $\boldsymbol{r} = \boldsymbol{r}_> - \boldsymbol{r}_<$. For large values of $\boldsymbol{R}$ and finite values of r we expect a structure of the wavefunction like $\overline{\Psi} = B(\boldsymbol{r})e^{i\Lambda}$ where the phase Λ is now defined by the eikonal equation

$$(\boldsymbol{k}_>.\nabla + \boldsymbol{k}_<.\nabla) = -\frac{Z}{r_>} - \frac{Z}{r_<} \quad (11)$$

with the solution

$$\Lambda = -\frac{Z}{k_>}\ln(k_>r_> + \boldsymbol{k}_>.\boldsymbol{r}_>) - \frac{Z}{k_<}\ln(k_<r_< + \boldsymbol{k}_<.\boldsymbol{r}_<) \quad (12)$$

For the amplitude *B* we find then the wave equation (r << R)

$$\left[\Delta_r + 2i\boldsymbol{\kappa}_{eff}.\nabla_r - \frac{1}{r}\right]B(\boldsymbol{r}) = 0 \tag{13}$$

where $\boldsymbol{\kappa}_{eff}$ is given by

$$\boldsymbol{\kappa}_{eff} = \frac{1}{2}(\boldsymbol{k}_> - \boldsymbol{k}_<) + \frac{1}{2}(\nabla_> - \nabla_<)\Lambda \tag{14}$$

We conclude therefore that the wavefunction given by equation (5) should be an accurate solution of the Schrödinger equation provided the relative momentum $\boldsymbol{\kappa}$ is replaced by its effective value.

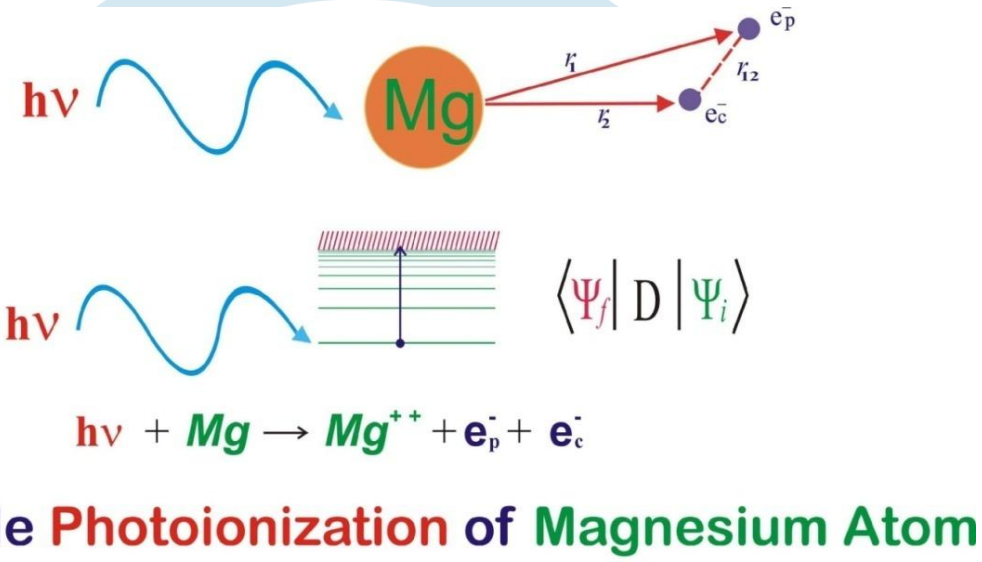


Fig.-1

RESULTS AND DISCUSSION

We have performed theoretical calculations for the double photoionization cross section (DPICS) of Mg by single photon impact employing the configuration interaction (CI) wave function for the ground state and BBK double continuum wave function of the electric dipole matrix elements in the incident energy range from threshold to 45 eV. Fig.2 displays our present calculated DPICS of along with other available relevant theoretical results of Kheifets and Bray [15] as well as experimental data of Nagata [19]. Fig.2 shows that our present result is very close to the experimental result in mid and higher energy range but there are discrepancies near threshold. The result of Kheifets and Bray [15] curve nature is similar to our present theoretical result. But the prediction of Kheifets and Bray [15] largely disagreed with experimental data of Nagata [19]. In present theoretical result disagreement near threshold suggest further investigation.

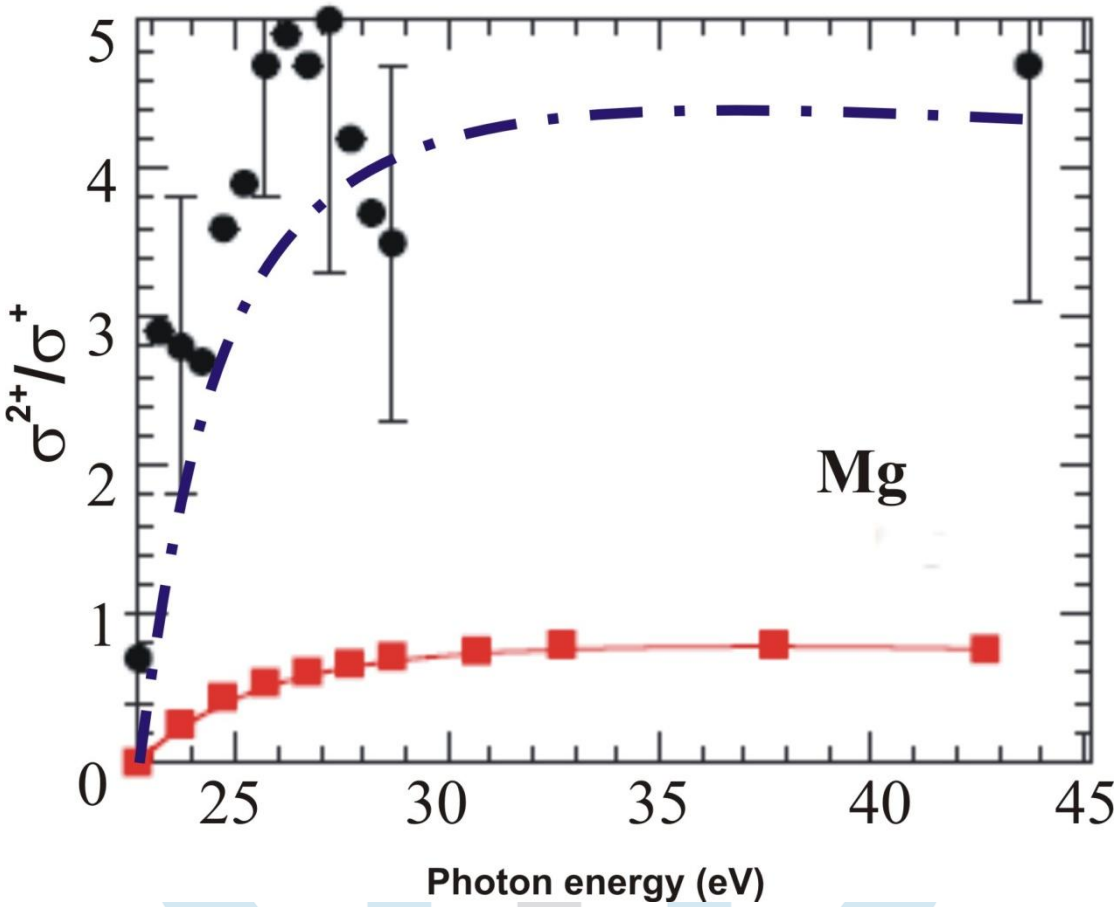
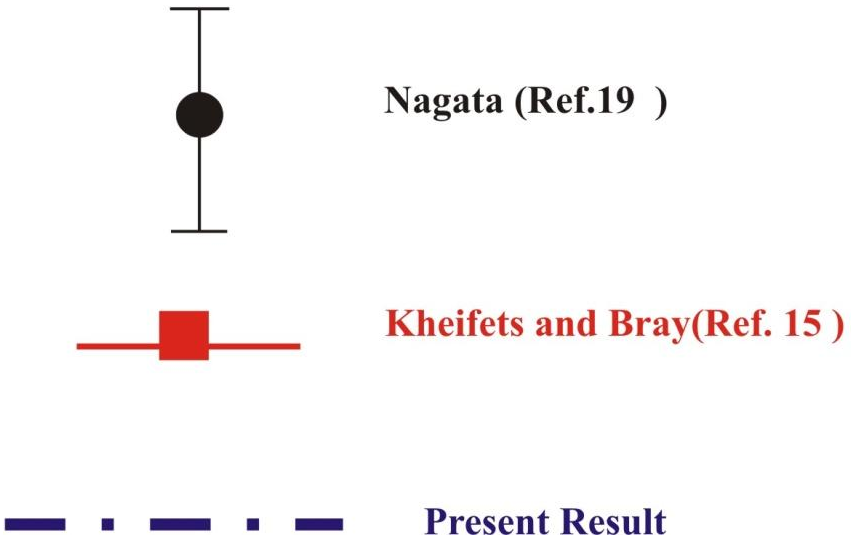


Fig.-2

Figure Caption

Fig.2 : Double Photoionization cross section (DPICS) for Mg.



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