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K-Shell Double Photoionization Cross Section of (Be, Mg and Ca) Atoms

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Abstract:

Double photoionization cross sections has been calculated using Hartree-Dirac-Slater method for Be, Ca and Mg atoms, the result were compared with Colgan et.al and Kheifets et.al theoretical data. Experimental measurements of photoioniztion cross sections was not available in order to make a comparison with our calculations. In general our results of the photoionization cross sections gave a good match with the theoretical data that compared with for Be and Ca atoms specially at high energies, and the same behavior for Mg atom but with no matching.

1.Introduction:

The double K-Shell photoionization (or the so-called double K-Shell photoeffect) is a fundamental process, being persistently investigated for more than three decades[1]. The extended interest in the problem is due to the fact that the two-electron ejected is exclusively caused by the correlation interactions [1].

We has been done by [2], A work single cross sections of ionization by photon impact with atoms. In this research, we use the same line in double photoionization cross section for alkali earth atoms (Be, Mg and Ca).Accordingly, it serves as a testing ground for different theoretical approaches [3-5]. Most of the experimental measurements were about the energy behavior of the ratio of double-to-single photoionization cross sections in neutral helium [6-9]. The other atomic targets are investigated much less thoroughly [1]. Therefore, the theoretical study of the universal scaling is of particular importance, because it provides information about most generic features of the double-ionization process for a whole family of atomic systems [1].During the past decade, double photoionization of atoms has been under intensive investigation, both experimentally and theoretically [3-9]. Because photoelectric operator is a single-particle operator, the simultaneous detachment of two electrons by a single photon stems purely from electron correlation effects, which cannot be accounted for by the independent electron approximation. This makes from the double photoionization an ideal test case for our understanding of electron correlations and theories still exist, agreement has greatly improved over the years [3-5].The field of photoionization is very rich in phenomena of atomic and molecular physics which demonstrate the great importance of electron correlation interactions, and these phenomena are of great interest to both theorists and experimenters. The main research of atomic photoionization has been in the measurements and calculations of the cross sections [10].

However, beryllium (Be) is the most important close-shell atom which is simple enough to be calculated by *ab initio* methods. The double-photoionization process in other alkaline earths, such as calcium (Ca) has also attracted attention [10].

2.Theory:

An analytic fit to the photoionization cross section $\sigma(E)$ for alkali atoms using Hartree-Dirac-Slater method , may be written as[11]:

$$\sigma(E) = \sigma_\circ F(y) \quad Mb \qquad \ldots(1)$$

$$F(y) = [(x-1)^2 + y_w^2] y^{0.5p-5.5} (1+\sqrt{\frac{y}{y_a}})^{-p} \qquad \ldots(2)$$

$$x = \frac{E}{E_\circ} - y_\circ \qquad \ldots(3)$$

$$y = \sqrt{x^2 + y_1^2} \qquad \ldots(4)$$

where *(E)* is refers to the photon energy in (eV), and $\sigma_\circ, E_\circ, y_w, y_a, y_1, y_\circ$ and p are the fit parameters. All the fitting parameters taken from Verner et al.[11] as we present it in table(1).The Close-Coupling method was the method used by the groups which we will compare our data with it.

Table (1): Present the fitting parameters for atoms under investigation [11].

Element	$E_\circ(eV)$	$\sigma_\circ(Mb)$	y_a	P	y_w	$y_\circ$	y_1
Be	9.539	2.932+5	4.301-1	1.052+1	3.655-1	8.278-4	1.269-2
Mg	1.197+1	1.372+8	2.228-1	1.574+1	2.805-1	0.0	0.0
Ca	1.553+1	1.064+7	7.790-1	2.130+1	6.453-1	2.161-3	6.706-2

3.Results & Discussion:

In this research double photoionization (DPI) cross sections of $Be^4(2s^2)$ and $Mg^{12}(3s^2)$, $Ca^{20}(4s^2)$ has been calculated using equ. (1). Figure (1) show a comparison of the present results of (DPI) for Be-atom interact with photon for energy range from (200-400) eV with the calculations Colgan *et al*.(2005) [12]. Figure (2) shows the same comparison for energy range from (400-1000) eV compared with the calculations of Kheifets *et. al.* (2009) [13]. Figures (3) shows our results of (DPI) for Mg-atom which compared with the data of Kheifets *et. al.* (2009) [13] for the energy range from (2000-9000). Whereas figure (4) shows our results of (DPI) for Ca-atom compared with the calculations of Kheifets *et. al.* (2009) [13] for energy range (10000-30000) eV.

The calculated double photoionization cross sections were found to be in a reasonable agreement with the calculations for Be & Ca-atoms in figures (2) and (4) respectively. The results in figure (3) for Mg-atom were found very similar and reasonable. In figure (1) the results weren't in matching with data has compared with. It is important to mention that the (DPI) cross sections of (Ca & Mg)-atoms have been calculated with error about 10%. The beaks here are irregular behavior of the cross section we have deal with it.

From these results, we conclude that our method of calculating (DPI) cross section is quite good for intermediate and high energies, but not good for low energies of the incident photons, mentioning we get the same behavior of the cross section in the case of Be-atom. The other reason that we didn't have a matching in the case of Mg-atom because the other researchers used a different method in calculating the double photoionization cross sections, whereas the method had been used by us was depending on fitting parameters gives a good results in some cases and reasonable in other cases.

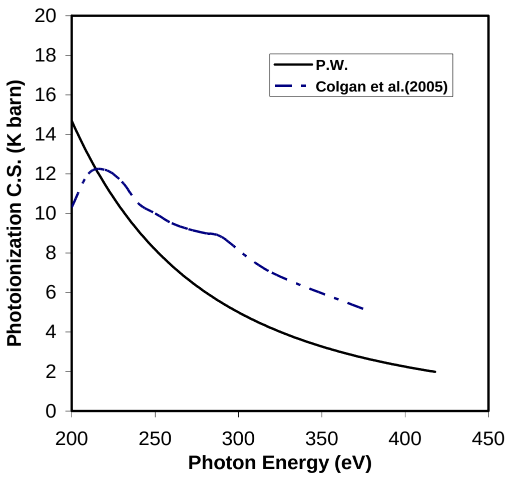

Fig. (1): The double photoionization cross section of Be-atom

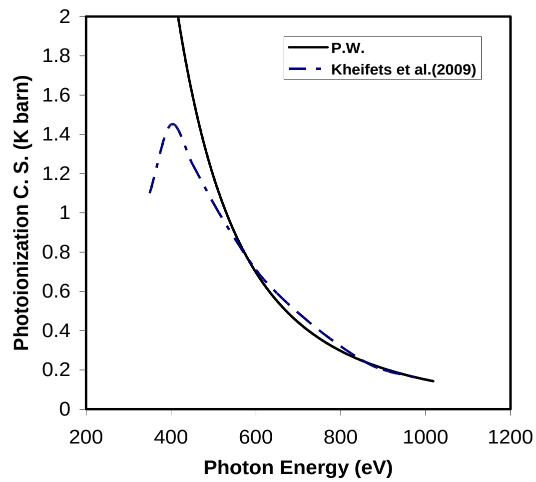

Fig. (2): The double photoionization cross section of Be-atom

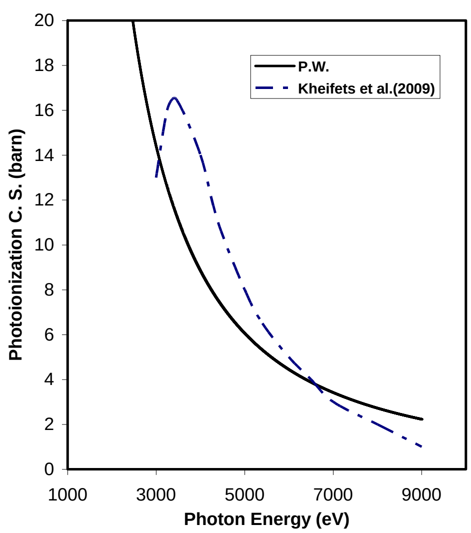

Fig. (3): The double photoionization cross section of Mg-atom

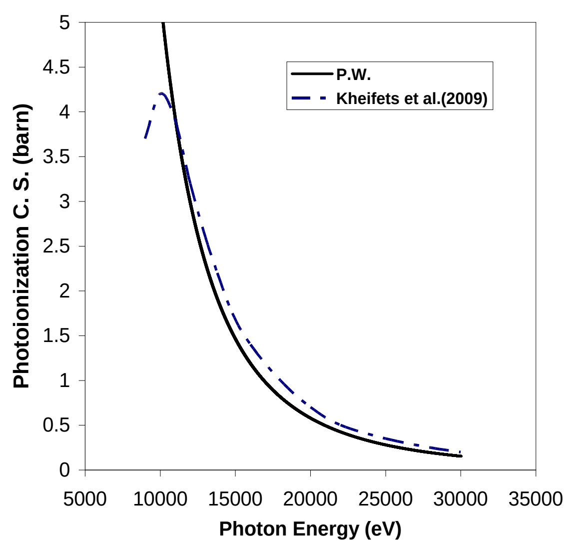

Fig. (4): The double photoionization cross section of Ca-atom

References:

[1] A. A. Khalf, "Photon-Ionization of Light Atoms at Intermediate Energies" J.Thi-Qar Sci. **2**, 207 (2010).

[2] A. I. Mikhailov, A. V. Nefiodov, G. Plunien, "About universal scaling in double K-shell photoionization", J. Phys. B **43**, 231003 (2009).

[3] A. I. Mikhailov, I. A. Mikhailov, A. N. Moskalev, A. V. Nefiodov, G. Plunien, and G. Soff, "Nonrelativistic double photoe effect on K-shell electrons" Phys.Rev.A **69**, 032703 (2004).

[4] J. Colgan and M. S. Pindzola, "Double photoionization of helium at high photon energies" J. Phys. B **37**, 1153 (2004).

[5] S. Kar and Y. K. Ho, "Ratio of double-to-single photoionization cross sections of plasma-embedded helium atoms at x-ray energies" Phys. Rev. A **77**, 022713 (2008).

[6] E. P. Kanter, R. W. Dunford, B. Krassig, S. H. Southworth, L. Young, "Double K-Photoionization of heavy atoms" Rad. Phys. Chem. **75**, 1529 (2006).

[7] K. Fennane, J. -Cl. Dousse, J. Hoszowska, M. Berset, W. Cao, Y.-P. Maillard, J. Szlachetko, and M. Szlachetko, "Double K-shell ionization of Al induced by photon and electron impact" Phys. Rev. A **79**, 032708 (2009).

[8] J. Hoszowska, A. S. Keifets, M. Berset, I. Bray, W. Cao, J.-Cl. Dousse, K. Fennane, M. Kavcic, Y. Kayser, Y.-P. Maillard, J. Szlachetko, and M. Szlachetko, "Double K-shell photoionization of low-Z atoms and He-like ions" Eurp. Phys. J. **169**, 23 (2009).

[9] R. Wehlitz, M.-T. Huang, B. D. DePaola, J. C. Levin, I. A. Sellin, T. Nagata, J. W. Cooper, and Y. Azuma, "Triple Photoionization of Lithium" Phys. Rev. Lett. **81**, 1813 (1998).

[10] R. Wehlitz, S. B. Whitfield, "Valence double photoionization of beryllium". J. Phys .B **34**, L719(2001).

[11] D. A. Verner, G. J. Ferland, K. T. Korista, D. G. Yakovlev, "Atomic Data for Astrophysics. II. New Analytic fits for photoionization cross sections of Atoms and Ions". Astrophys.J **465**, 487(1996).

[12] J. Colgan, M. S. Pindzola, F. Robicheaux, "Double and triple photoionization of Li and Be". Phys. Rev. A **72**, 022727(2005).

[13] A. S. Kheifets, I. Bray, J. Hoszowska, "K-shell double photoionization of Be, Mg, and Ca" Phys. Rev. A **79**, 042504 (2009).

التأين الضوئي المضاعف لمقاطع قشرة - K العرضية للذرات (Be, Mg and Ca)

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الملخص:

تم حساب المقاطع العرضية التأين الضوئي المضاعف للذرات (Be, Mg and Ca) باستخدام طريقة هارتري– ديراك– سليتر،وقد قورنت النتائج المستحصلة مع الحسابات النظرية لكل من الباحثين كولجان وجماعته وخيفايت وجماعته . لم يتوافر لدينا قياسات عملية للمقاطع العرضية للتاين الضوئي لغرض اجراء مقارنة مع حساباتنا النظرية. بصورة عامة نتائجنا المستحصلة للمقاطع العرضية للتاين اعطت توافق جيد مع الحسابات النظرية التي تمت المقارنة معها لذرتي البريليوم والكالسيوم وخصوصا عند الطاقات العالية، ولقد كانت النتائج لحالة ذرة المغنيسيوم متشابهه من حيث التصرف ولكن من دون الحصول على تطابق.