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Study of scattering cross sections for single and double ionization of Cu by H^+ particles impact

Suresh Prasad Gupta[1], L.K.Jha[2],Raju Khanal[3]

[1]*Patan Multiple Campus, Lalitpur, Tribhuwan University, Nepal.*

[2]*Department of Physics, B.R.A. Bihar University, Muzaffarpur-842001, Bihar, India.*

[3]*Central Department of Physic, Kirtipur, Tribhuwan University, Kathmandu,Nepal*

ABSTRACT

Theoretical calculations of H^+ impact single and double ionization cross sections for ground state Cu atoms have been performed in the binary encounter approximation(BEA) in the energies region ranging from 80 to 1440 keV/amu for single ionization and 125 to 1440 keV/amu for double ionization. The accurate expression for $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) and Hartree –Fock velocity distributions for the target electrons have been used throughout the calculations. It has been concluded that the calculated results of H^+ impact single and double ionization cross sections are in good agreement with the experimental data throughout the given energy range.

Key words: Binary Encounter Approximation, Proton impact, Single ionization, Double ionization, Hartree-Fock velocity distributions

I. INTRODUCTION

Ionization of atoms and molecules is one of the basic processes in atomic physics. Thus it has been extensively studied both experimentally and theoretically. Due to the broad range of applications and also due to its role in the study of atomic collision dynamics, there have been great effort, both experimental and theoretical, to improve our understanding of the ionization processes resulting from ion impact with atoms. From the academic point of view , the studies of the dynamics of the electron atom inelastic scattering leads to a better understanding of the physical structure of atoms and molecules and how energy and momentum are transferred between atomic particles during the collision. The description of multiple ionization is far from a simple task mainly due to the complexity of the many possible path ways leading to it. For example double ionization of atoms by fast ions is usually understood in terms of three mechanisms [1].First one is the shake off process, in which a fast electron is ejected in the direct ionization with the projectile, while the second electron is ionized by the final state rearrangement second one is the two step process, in which both electrons are simultaneously ejected by the direct interaction with the projectile and third one is the ionization of the inner shell electron with a post collision Auger decay. Both the shake off and inner shell ionization plus Auger decay yields a double ionization cross sections. The two step mechanism, which turnout to be dominant in the intermediate energy region does not follow this pattern because it is based on the action of the projectile over the two active electrons. As a general rule, the dependence of the multiple ionizations on the projectile energy and charge state are significantly different from those of single ionization cross section. The statistical distribution of the various available inelastic alternatives, as well as, the way the electrons dynamically correlates, significantly change the dependence of the multiple ionization cross section on the projectile energy and the charge state with respect to the single ionization.

A general used approach for interaction of the multiple ionization processes is the independent particle model (IPM), where it is assumed that the ionization of one electron is independent of the other and the relative probability are given by binomial distribution [2,3,4]. This method depends strongly on the quality of the calculation of the single electron ionization probability. Although some general qualitative estimates can be obtained through simple semi-classical calculations using hydrogenic wave function [4]. An alternatively theoretical approach to the IPM is the statistical energy distribution model, which has also been used by several authors [5-7]. It was formulated by Russek and Thomas [6] and further developed by Cocke [7] and Kabachnik et al.[8]. It is based on the hypothesis that the probability of multiple ionization is directly related to the energy deposited by the projectile on the target, which is, in a second step, statistically distributed among all atomic electrons and one or more of which eventually auto ionize to the final state.

In parameter to which these calculations are highly sensitive, mainly in the intermediate velocity regime is the projectile charge state. The simplest case, i.e. single ionization of light atoms and molecules by structure less charged particles at high impact velocities, is well described within the frame work of Bethe theory [9]. Derivations of the charge state scaling from the first Born approximation are expected to be observed either if the collision regime is non perturbative or if multiple ionization occurs. These studies, however, concern on the single ionization of few electrons, ions and studies on the effect of partial screening on multiple ionizations are practically on existence. To the best of our knowledge, there are no reliable calculations available for partial or total multiple ionizations.

In case of different multiple ionization processes the double ionization is the most important as the main contributions to the total ionization of the target is given by single and double ionization processes. Theoretical calculations of double ionization cross sections are considered to be of much significance because contribution from different physical processes e.g. simultaneous ejection of two electrons, inner shell ionization followed by Auger emission, resonance excitation double auto ionization process etc. can be separately estimated at various impact energies. Keeping in view the importance of the degree of ionization and convenience in calculations, we have considered it worthwhile to estimate theoretically separate contributions from the relevant physical processes leading to double ionization.

Rigorous theoretical calculation of direct double ionization cross section becomes extremely difficult as it is related to a four body Coulomb potential in the final channel[10]. Recently, some interesting theoretical calculations on single and multiple ionization of noble gases atom by fast proton impact have been reported where contribution of electron capture to multiple ionization are negligible. Spranger and Kirchner [11] investigated the ionization processes for Ne and Ar using independent particle model. They have also considered time delayed Auger like electron emission processes on the basis of a straight forward statistical model and have concluded that high projectile velocities multiple ionization is dominated by Auger like processes. Archubi et at. [12] have developed a many electrons model for multiple ionizations of heavy atoms by bare atom. It is based on the solution of transport equation for an ion travelling through an inhomogeneous electron density. Among different experimental investigations on metals, Mc Cartney et al.[13] of the Belfast group have used a cross beam technique incorporating time–of- flight analysis and coincidence counting of the collision products to carry out an interesting work on processes involving electron capture and multiple ionization in collisions of fast H^+ and He^{2+} ions with ground state Pb atoms. Measurements of this type are complex and difficult and probably for this reason the experimental data have been obtained in the limited energy ranges. They have also carried out calculations in an independent electron model for the processes experimentally investigated but unfortunately the agreements of the theoretical result with the experimental data is not satisfactory.

In the past, binary encounter approximation (BEA) has been used successfully to calculate charged particle impact single and double ionization cross section for atoms and ions. Gryzinski [14] reasonably considered two processes in a double binary encounter model to describe double ionization. In the first process the two electrons may be ejected from the system by two successive encounters of the incident particle with the target electrons. Alternatively, the incident particle may knock out only one target electron and the second electron is removed by the first ejected electron. The corresponding double ionization cross sections are denoted by Q_{sc}^{ii} (scattered part) and Q_{ej}^{ii} (ejected part) respectively. Kara et al. [15] also supported the idea of above mentioned two step interaction to describe the process of direct double ionization. In spite of certain unrealistic features and unjustified simplification in Gryzinski`s mathematical formulation for the process of double ionization, the idea of two double binary encounter process has physical justification (see Roy and Rai [16] , Vriens [17]).

Later on Roy and Rai modified Gryzinski`s theory of electron impact direct double ionization suitably. The result of double ionization cross sections, based on the modified model including contribution of indirect processe, was found to close agreement with the experimental data [118-19]. In these calculations, Hartree-Fock (HF) and hydrogenic velocity distribution were used while considering ejection of the first and second target electron respectively. Latter, Jha and Roy[20-21] and Minakshi et al.[22] used Hartree-Fock velocity distribution while considering the ejection of both electrons of the target in the calculation of direct double ionization cross section. H^+ and He^{2+} impact single and double ionization of Mg and Pb calculated in the BEA shows good agreement with experimental data. Contributions to double ionization from the Auger effect following vacancies in inner shells are theoretically substantiated by by these studies.

In the case of heavy charged particle impact (like H^+ and He^{2+}), BEA of double ionization cross section of atoms are few. Kumar and Roy [23, 24] pointed out errors and obsequies in Gryzinski`s theory for calculation of the process mentioned above and modified the mathematical frame work suitably . In comparison of the two distribution functions, Hartree Fock and Hydrogenic velocity distributions functions, they concluded that the case of HF velocity distributions for the ejection of both electrons in calculation of direct double ionization cross section will lead to improved agreement with the measured data. Keeping the facts mentioned above in mind, we consider it worthwhile to carry out calculations of H^+ impact single and double ionization cross sections for Cu atom in BEA using HF velocity distribution for the ejected electrons. This will enable us to analyze single and direct double ionization cross sections and to examine the contribution to direct double ionization from indirect physical process.

II. THEORETICAL METHOD

In terms of dimensionless variables s and t, the expressions of ionization cross section due to a projectile of unit charge of particular incident energy and a particular velocity of bound electron are given by (see Kumar and Roy [23])

$$Q_i(s,t) = \frac{4}{s^2u^2}\left[1+\frac{2t^2}{3}-\frac{1}{4(s^2-t^2)}\right]; \qquad 1 \quad \le \quad 4s(s-t)$$

$$= \frac{2}{s^2u^2t}\left[\frac{1}{4(s+t)}+t+\frac{2}{3}\left\{2s^3+t^3-(1+t^2)^{3/2}\right\}\right]; \qquad 4s(s-t)\le 1 \le 4s(s+t)$$

$$= 0; \qquad 1 > 4s(s+t)$$

(1)

In our present work we have used the accurate expression of $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) as given by Vriens [25] for heavy charged particles incident on atoms. Following Catlow and McDowell [26] the two dimensionless variables s and t are defined as $s^2 = v_1^2 / v_0^2$ and $t^2 = v_2^2 / v_0^2$, where v_1 and v_2 are the velocities in atomic units of the incident particle and the target electron respectively and $u = v_0^2$ is the ionization potential of the target in rydbergs. All other energies involved are also expressed in rydbergs.

Numerical integration of $Q_i(s,t)$ has been carried out over Hartree Fock velocity distribution of the bound electrons to obtain the total ionization cross section. Thus the expression of total single ionization cross section for heavy charged particle impact for a particular shell of the target is given by

$$Q_i(s) = n_e \int_0^{\infty} Q_i(s,t)\, f(t) u^{1/2} dt (\pi a_0^2)$$

(2)

where n_e is number of electron in a shell and $f(t)$ is the momentum distribution function of the target electron.

Total double ionization cross section of an atom for charged particle impact can be given as

$$Q^{ii}(T) = Q_D^{ii} + Q_A^{ii}$$

When ionization from Auger effect is not considered then heavy charged particle impact total direct double ionization cross section Q_D^{ii} is given by

$$Q_D^{ii} = Q_{sc}^{ii} + Q_{ej}^{ii}$$

(3)

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In In accordance of the idea given by Gryzinski [14] in double binary encounter model, these cross sections involving integrals over energy transfer are given by

$$Q_{sc}^{ii} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2} \times \int_{u_i}^{\Delta E_{\max}} \sigma_{\Delta E}(E_q) \left(\int_{u_{ii}}^{\Delta E_{\max}} \sigma_{\Delta E}(E_q - \Delta E) d(\Delta E') \right) d(\Delta E)$$

(4)

and

$$Q_{ej}^{ii} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2} \times \int_{u_i+u_{ii}}^{\Delta E_{\max}} \sigma_{\Delta E}(E_q) \left(\int_{u_{ii}}^{\Delta E - u_i} \sigma_{\Delta E'}(\Delta E) d(\Delta E') \right) d(\Delta E)$$

(5)

The symbols used in the above expressions have been defined by Gryzinski [14]. Here ΔE and $\Delta E'$ stand for energy transfer during the first and the second collisions respectively and $\bar{r}$ denotes the mean distance between the electrons in the shell given by $\bar{r} = \frac{R}{n_e^{1/3}}$ (R being the radius of the shell of the target atom), u_i and u_{ii} are the ionization potentials corresponding to ejection of the electrons of the target. The symbol E_q represents the energy of the projectile. . The factor $\frac{n_e(n_e-1)}{4\pi\bar{r}^2}$ has been suitably modified considering the mode of ionization in which the electrons are ejected from different shells. In this case $n_e(n_e-1)$ has been replaced by $n_{e1} \times n_{e2}$; where n_{e1} and n_{e2} stand for number of electrons in the shells under consideration. The binding energies of the shells of Cu, the expectation values of the shell radii and HF radial wave functions have been taken from the data reported by Clementi and Roetti [27]

In terms of dimensionless variables s and t discussed earlier, the expression for $\sigma_{\Delta E}$ in the case of a projectile of unit charge is given by (see Kumar and Roy [24])

$$\sigma_{\Delta E} d(\Delta E) = \left\{ \begin{array}{cc} Ad(\Delta E); & \Delta E \leq 4su(s-t) \\ Bd(\Delta E); & 4su(s-t) \leq \Delta E \leq 4su(s+t) \\ 0; & \Delta E > 4su(s+t) \end{array} \right\}$$

(6)

where

$$A = \frac{4}{s^2 u}\left(\frac{1}{(\Delta E)^2} + \frac{4t^2 u}{3(\Delta E)^3} \right) \quad \text{and} \quad B = \frac{2}{3t(\Delta E)^3}\left(8s - \frac{\left| (\Delta E + t^2 u)^{1/2} - tu^{1/2} \right|^3}{s^2 u^{3/2}} \right)$$

The above expressions of the scattered part and ejected part of the direct double ionization cross sections showing the relevant integrals involving energy transfer and Hartree-Fock velocity distributions for the ejection of the two electrons are given below.

$$Q_{sc}^{ii} = \frac{n_e(n_e-1)Z^2}{4\pi\bar{r}^2} \times \left(\int_{t=0}^{s-\frac{1}{4s}} \left\{ \int_{u_i}^{4su_i(s-t)} A\alpha d(\Delta E) + \int_{4su_i(s-t)}^{4su_i(s+t)} B\alpha d(\Delta E) \right\} f(t) u_i^{1/2} dt + \int_{t=s-\frac{1}{4s}}^{\infty} \int_{u_i}^{4su_i(s+t)} B\alpha f(t) u_i^{1/2} d(\Delta E) dt \right) (\pi a_0^2)$$

(7)

when $(s-1/4s)$ is positive and

$$Q_{sc}^{ii} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2} \times \left(\int_{t=\frac{1}{4s}-s}^{\infty} \int_{u_i}^{4su_i(s+t)} B\alpha f(t) u_i^{1/2} d(\Delta E) dt \right) (\pi a_0^2) \quad \text{when} \quad (s-1/4s) \quad \text{is} \quad \text{negative}$$

(8)

In the above expressions $\alpha = \int_0^{\infty} Q_i(s', t) f'(t) u_{ii}^{1/2} dt (\pi a_0^2)$

(9)

and s' is given by

$$s'^2 = \frac{E_q - \Delta E}{1836 u_{ii}} \quad for \quad H^+ \quad impact$$

(10)

Similarly equations for ejected part are

$$Q_{ej}^{ii} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2} \times \left(\int_{t=0}^{s-(1+\frac{u_{ii}}{u_i})/4s} \left\{ \int_{u_i+u_{ii}}^{4su_i(s-t)} A\alpha' d(\Delta E) + \int_{4su_i(s-t)}^{4su_i(s+t)} B\alpha' d(\Delta E) \right\} f(t) u_i^{1/2} dt + \int_{t=s-(1+\frac{u_{ii}}{u_i})/4s}^{\infty} \int_{u_i+u_{ii}}^{4su_i(s+t)} B\alpha' f(t) u_i^{1/2} d(\Delta E) dt \right) (\pi a_0^2)$$

(11)

when $s-(1+\frac{u_{ii}}{u_i})/4s$ is positive and

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$$Q_{ej}^{ii} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2} \times \left(\int_{t=(1+\frac{u_{ii}}{u_i})/4s-s}^{\infty} \int_{u_i+u_{ii}}^{4su_i(s+t)} B\alpha' f(t) u_i^{1/2} d(\Delta E) dt \right) (\pi a_0^2)$$

(12)

when $s-(1+\frac{u_{ii}}{u_i})/4s$ is negative with

$$\alpha' = \int_0^{\infty} q_i(s',t) f'(t) u_{ii}^{1/2} dt (\pi a_0^2)$$

(13)

Here $q_i(s',t)$ is the expression for electron impact ionization cross section of atoms (see Jha and Roy [21]) and s' is given by $s'^2 = \frac{\Delta E - u_i}{u_{ii}}$ for H^+.

The integral appearing in Q_{sc}^{ii} and Q_{ej}^{ii} have been evaluated numerically. In the above equations the functions $f(t)$ and $f'(t)$ are momentum distribution functions corresponding to the first and the second ejected electron respectively. These have been constructed from HF radial wave functions (see Catlow and McDowell [26], Jha and Roy [20]). We have considered total cross section for heavy charged particle impact direct double ionization of Cu as given by

$$Q_D^{ii} = Q_D^{ii}(4s,3d) + Q_D^{ii}(4s,3p)$$

(14)

where $Q_D^{ii}(4s,3d)$ and $Q_D^{ii}(4s,3p)$ stand for the direct double ionization cross sections corresponding to ejection of one electron from $4s$ shell and the other either from the $3d$ shell or from $3p$ shell respectively.

III. RESULT AND DISCUSSION

3.1 H$^+$ impact single ionization cross section

Our calculated cross section for single ionization along with experimental data of Patton et al.[28] due to H$^+$ impact of Cu has been shown in Table 1 and Fig.1. In order to obtain single ionization cross section for Cu, we have considered ionization from 4*s*, 3*d* and 3*p* shells only. Ionization from deeper inner shells (3*s*, 2*p*, 2*s*) have not been included in the present calculations as a single vacancy in the shells lead to Auger emission. In the figure we have plotted the single ionization cross sections considering ionization from 4*s* shell including contribution due to only one electron from 3*d* shell and 3*p* shell respectively. The ionization from 4*s* and 3*d* shells has been shown separately in the Table1. First of all we would like to discuss our results by considering ionization from 4s shell only. At low incident energies from 80 keV/amu to 175 keV/amu , the experimental data of the calculated values are within the factor of 2. Beyond this energy range the discrepancy goes on

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increasing and at 1440 keV/amu the experimental result is about 3.3 times larger than the calculated value. The magnitudes of calculated and experimental cross sections at this energy are 0.23×10^{-16} cm^2 and 0.78×10^{-16} cm^2 respectively.

If the contribution of 10 electrons of 3*d* shells is included in the calculation, the cross sections becomes 6 to 8 times larger than the experimental data at all incident energies below 500KeV/amu. In this connection it may be mentioned that_calculation of single ionization cross section in BE approach shows good agreement with experimental data at high energy region, being always within a factor of 2. At this point it is worth mentioning that the observation made by Lotz [28] who calculated electron impact ionization cross section of the atoms with the help of empirical formula found reasonable agreement with experimental data in most of the cases. In absence of the theoretical calculation, experimental data are generally compared with the results obtained by Lotz formula. But in the case of electron impact single ionization of Cu, Lotz has pointed out that, he had to reduce the cross section of $3d^{10}$ electrons drastically in order to get satisfactory agreement with the experiment. Almost similar difficulties have been observed by Lotz in the case of silver [$4d^{10}$, $5s^1$] which has electronic configuration of similar nature as that of Cu.

Keeping in view, the observation of Lotz, we have made an approximate assumption to include contribution of one *3d* electron in order to examine the results. It can be observed from the figure and table that the results so obtained are in excellent agreement with the experimental data throughout the energy range investigated.

From the fact given above it is apparent that one faces difficulties in calculation of *3d* shell single ionization cross section of Cu. If contribution from all the 10 electrons is taken into account, similar difficulties have been experienced by earlier worker in the case of other atoms and ions involving ionization from full occupied *d* shells. Jha and Roy [30] have observed similar difficulties in the calculations of electron impact ionization of In^+ and Cu respectively. Bell el al. has obtained satisfactory agreement with experiment. The contribution to the ionization cross section from electrons in the 4*d* shell was added in at any one half of its calculated value in the configuration averaged distorted wave (CADW) approximation. Use of only half of the *d* sub shell contribution was proposed by Roger et al. [31] earlier and was found to fit the experimental data better in the case of other experiments.

Besides this, we would like to discuss the different physical processes consequent upon ionization of 3*d* electron in the case of Cu. After removal of one electron from 3*d* shell, the target is left in $3d^9$ 4s state. This is not an auto ionization state and hence auto ionization is not possible.

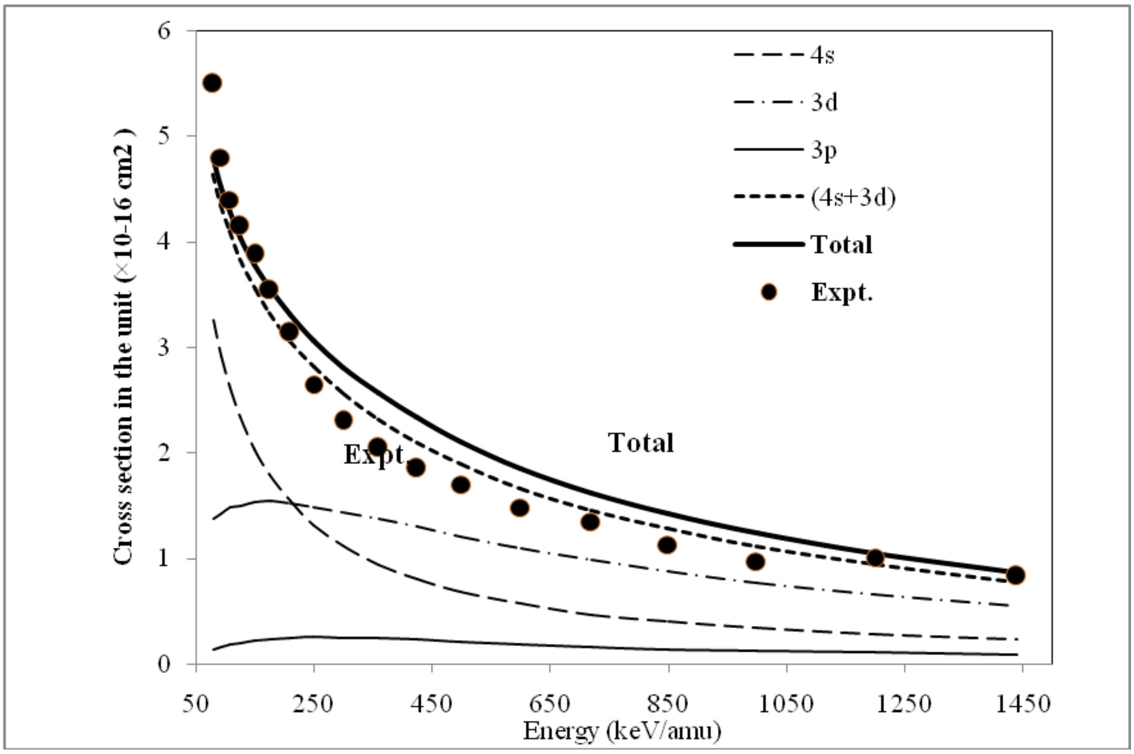

Figure1: Proton impact single ionization cross sections of Cu in the unit of ×10-^{16} cm^{2}.

[Here 4*s*, 3*d* and 3*p* stand for the ionization cross sections of the respective shells, **Total** stands for the total calculated single ionization cross sections and **Expt** stands for variations in experimental values.]

Table 1. Proton impact single ionization cross sections of Cu in the unit of ×10^{-16} cm^{2}

E(keV/amu)	Contribution of 4s	Contribution of 3d	Contribution of 3p	Contribution of (4s+3d)	Total	Expt. [28]
80	3.26	1.38	0.14	4.64	4.78	5.50
93	2.92	1.43	0.16	4.35	4.51	4.80
108	2.62	1.48	0.18	4.10	4.28	4.40
125	2.34	1.50	0.2	3.84	4.04	4.15
150	2.03	1.53	0.22	3.56	3.78	3.88
175	1.79	1.54	0.23	3.33	3.56	3.54
210	1.54	1.52	0.25	3.06	3.31	3.14
250	1.32	1.49	0.26	2.81	3.07	2.65
300	1.12	1.44	0.25	2.56	2.81	2.30
360	0.94	1.38	0.24	2.32	2.56	2.05
425	0.80	1.30	0.23	2.10	2.33	1.85
500	0.68	1.21	0.21	1.89	2.10	1.70

600	0.57	1.09	0.19	1.66	1.85	1.48
720	0.47	0.99	0.16	1.46	1.62	1.35
850	0.40	0.88	0.14	1.28	1.42	1.13
1000	0.34	0.77	0.13	1.11	1.24	0.97
1200	0.28	0.66	0.11	0.94	1.05	1.01
1440	0.23	0.55	0.09	0.78	0.87	0.83

Now we would like to discuss the general feature of the calculated results along with the experimental data. From the energy range of 80KeV/amu to 175 KeV/amu the ratio varies from 0.84 to 0.94. Beyond this energy range from 175 keV /amu to 1000 keV/amu the ratios are varying from 0.97 to 1.14 respectively. At the highest energy of 1440 keV/amu the magnitude of calculated and experimental value of cross sections are 0.78×10^{-16} cm^2 and 0.82×10^{-16} cm^2 respectively and their ratio is 0.93.From the close observation of the calculated results it shows that at the lowest energy 80 keV/amu the magnitude is 4.64×10^{-16} cm^2 and at the highest energy 1440 keV/amu the magnitude is $0.78 \times 10^{-16} cm^2$. It means the variation of data is about six time in the case of calculated cross section while in the case of experimental data almost similar features has been exhibited, which is also 6.6 times. The theoretical results are in excellent agreement throughout the given energy range.

The discussion given above clearly explains why the inclusion of one 3*d* electron brings our calculated results in excellent agreement with the experiment. More elaborate theoretical investigation is required for quantitatively understanding of the process of single ionization from the 3*d* shell of Cu. It is expected that this work will stimulates other theoretical workers. To take up further study of the problem more theoretical calculations are required to understand the dynamics of the system properly.

3.2 H^+ impact double ionization cross section

In the present work, an attempt has been made to obtain double ionization cross section by proton impact of Cu. In this case direct double ionization cross sections have been calculated to take contributions from the ejection of (4*s*,3*d*) and (4*s*,3*p*) shells only. These calculations have been performed from 125- 1440 keV/amu impact energies using BEA. The calculated results along with experimental data have been presented in the Table 2 and Fig. 2. In the energy range 125 – 300 keV/amu the calculated results differ by a factor of more than 2 from the experimental data. Further it is observed that in the region 360 – 1440 keV/amu the theoretical and experimental results differ by a factor 2. In this connection it may be mentioned that calculation of double ionizations in the BEA using Hatree - Fock velocity distribution for target electrons show good agreement with experimental data in high energy region being always within the factor of 2. It can be seen from the Table 2 that at impact energies 720 keV/amu and 850 keV/amu the calculated results agree well with the experimental data. At these impact energies, the magnitude of the calculated cross sections are $1.49 \times 10^{-17} cm^2$ and 1.15×10^{-17} cm^2 while the experimental data for these impact energies have cross sections of magnitudes 1.43×10^{-17} cm^2 and $1.21 \times 10^{-17} cm^2$ respectively. At the corresponding energies the ratio of these two cross sections are 1.04 and 0.95. From the energy range 125 – 720 keV/amu the calculated results overestimates the experimental data. Beyond this energy to highest energy we have considered the calculated results underestimate the experimental values. The magnitude of the lowest and the highest value of calculated cross sections are 10.3×10^{-17} cm^2 and $0.52\times10^{-17}cm^2$ respectively. It is further seen that the ratio of the lowest and highest values is about more than 19 times. This shows that the theoretical value decreases very rapidly with the increase of the impact energies. But in the case of experimental data the magnitudes of the lowest and highest cross sections are $2.3\times10^{-17}cm^2$ and $0.86\times10^{-17}cm^2$ and it differs more than 2 times. The experimental data decreases very slowly with the increase of impact energy. At the impact energy 125 keV/amu, 150 keV/amu, 175 keV/amu and 250 keV/amu the calculated cross sections are more than 5 times, 4 times, 3 times and 2 times greater than the experimental cross sections. The increase of the impact energy both the results are coming closer to each other and at impact energy 720 keV it is almost similar. In close inspection of the calculated results it seems that at higher energies range the possibility of some other physical process may require. In view of the discussion given above, it is clearly seen that the ionization of (4*s*,3*d*) shells dominates the cross section throughout the energy region we considered.

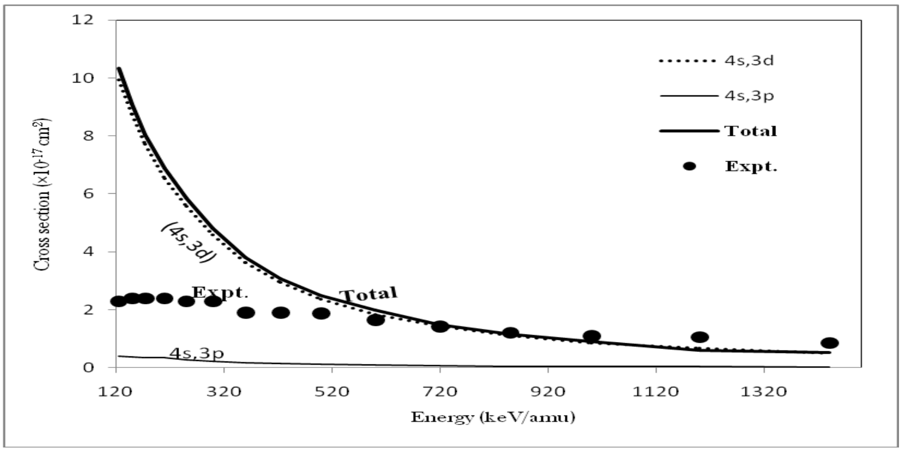

Figure2: Proton impact double ionization cross sections of Cu in the unit of $\times10^{-17}$ cm^2.

[Here (4*s*, 3*d*) and (4*s*,3*p*) stand for double ionization coss sections corresponding to ionization of 4*s* shell followed by ionization of 3*d* and 3*p* respectively, **Total** stands for total theoretical double ionization cross sections and **Expt.** represents variations in total experimental values.]

Table 2. Proton impact double ionization cross sections of Cu in unit of $\times10^{-17}cm^2$

E (keV/amu)	Contributions of (4s,3d)	Contributions of (4s,3p)	Total	Expt. [28]
125	9.94	0.39	10.33	2.30
150	8.74	0.37	9.11	2.40
175	7.71	0.34	8.05	2.40
210	6.54	0.34	6.88	2.40
250	5.58	0.26	5.84	2.30
300	4.58	0.22	4.80	2.30
360	3.62	0.18	3.80	1.90

425	2.94	0.14	3.08	1.90
500	2.37	0.11	2.48	1.88
600	1.84	0.09	1.93	1.65
720	1.42	0.07	1.49	1.43
850	1.10	0.05	1.15	1.21
1000	0.85	0.04	0.89	1.09
1200	0.67	0.03	0.60	1.06
1440	0.50	0.02	0.52	0.86

IV. CONCLUSION

In the case of H^+ impact single ionization of Cu the theoretical values throughout the given energy range is in excellent agreement with the experimental values. Inclusion of 3d shell brings our results close to the experimental results in the case of single ionization. In the case of H^+ impact double ionization in BEA using HF velocity distribution shows good agreement with experimental data in intermediate and high energy range from 360 to 1440 keV/amu.

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