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Absolute Cross Sections for He^+ Impact Single Ionization of Noble Gases

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ABSTRACT He^+ impact single ionization cross sections of noble gases have been calculated in the Modified Binary Encounter Approximation. Accurate expression of $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) and Hartree-Fock velocity distributions for the target electrons have been used throughout the calculations. The present results of single ionization cross sections are in excellent agreement with the experimental observations throughout the energy range. We have also compared our calculated results of H^+ impact ionization cross sections of noble gases with experimental measurement of Cavalcanti et al. Our present model is more suitable and gives reliable results. The calculated cross sections differs from the experimental results of H^+ impact, this shows that more theoretical calculations is required to understand the dynamics of the system.

KEYWORDS Proton, Ionization, Noble Gas, Cross-Section, Ions

INTRODUCTION

The understanding of ionization phenomena by charged particle is of considerable interest in many branches of Physics. Different physical mechanism exhibits the different physical phenomena to understand the dynamics of the system. Electrons can be ejected during the collision as the result of direct interaction of the projectile with the target electrons or as a result of a post collisional relaxation of the residual target. In the first case, processes of direct ionization with or without electron capture can contribute to multiple ionization. In the second case, inner shell vacancies produced in the first step of the reaction can be followed by Auger electron emission [1]. In the recent past, some interesting theoretical works on single and multiple ionization of noble gases by fast proton impact have been reported in the energy region where contributions of electron capture to multiple ionizations are negligible. Spranger and Kirchner [2] investigated the ionization processes for Neon and Argon using the independent particle model. Adopting a different approach, Archubi et al. [3] have developed a many electron model for multiple ionization of heavy atom by bare ions. It is based on the solution of transport equation for an ion travelling through regions and inhomogeneous electron density. The sophisticated calculations of the ionization cross-sections of many electron atoms by He^+ impact are not available in the literature. However, in the past the Modified Binary Encounter Approximation methods have been used successfully in the calculations of charged particle impact single ionization cross-sections for several atoms and ions. Using the accurate expressions of $\sigma_{\Delta E}$ as given by Vriens [4], Kumar and Roy [5] calculated proton impact double ionization of some atoms which were found to be fairly good agreement with the experimental observations.

Experimental observation of H^+ impact ionization of Magnesium shows that pure double ionization cross-sections are approaching pure single ionization cross-sections rapidly at high impact energy and the ratio of cross-sections of double ionization to the single ionization becomes 0.75. The single ionization of light atoms and molecules by structure less charged particles at high impact velocities is well described within the framework of the Bethe theory [6]. Deviation of the charged state scaling from the first Born Approximation are expected to be observed either if the collisions regime is non-perturbility or if multiple ionization occurs. These studies however concentrated on the single ionization of few electrons, ions and studies on the effect of partial screening of multiple ionizations are practically of non-existence. To the best of our knowledge there are no reliable calculations available for partial multiple ionizations of the whole set of noble gases (except Redon) by dressed, low charge state projectiles such as He^+ , although this charge state is the one that energetic alpha particles have to go through as they penetrate in matter. A scenario which appears in several applications, but not one theoretical quantal calculation is able to calculate the cross-sections for heavy atoms.

Keeping in view, the facts mentioned above seems the Binary encounter calculations give reasonable results of cross-section for heavy atoms and ions. Hence in this work, we have carried out absolute theoretical calculations of single ionization cross-sections of He^+ projectiles on Helium, Neon, Argon, Krypton and Xenon in the energy range 1.0 MeV to 3.5 MeV.

THEORETICAL METHODS

On the prediction of the first Born Approximation, the single ionization cross-sections depends on charge Z of the incoming particle and its velocity V as $Z^2 V^{-2} \ln V$, if the velocity is much larger than that corresponding to the binding of the atomic electron [7]. In the present work, we have used the accurate expressions of cross-sections as given by Vriens [4] for heavy charged particles incident on atoms. Following the theory of Catlow and Mc. Dowell [8] we have defined two dimensionless variables s and t defined by

$$s^2 = \frac{v_1^2}{v_0^2} \text{ and } t^2 = \frac{v_2^2}{v_0^2}$$

where v_1 and v_2 are the velocities in the atomic units of the incident particle and the target electron respectively and $u = v_0^2$ is the ionization potential of the target in Rydberg. Entire energies involved have also been expressed in Rydbergs. In terms of these dimensionless variables, the expressions of ionization cross-sections due to projectile of unit charge for particular incident energy and a particular velocity of a bound electron given by (see Kumar and Roy [9]).

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

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

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

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

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

where n_e is the number of electrons in shell, Z is the charge on the projectile and f (t) is the momentum distribution function of the target electron.

RESULTS AND DISCUSSION

Before we consider the discussion on the comparison of present results with the measured data, it is essential to consider the comparison of the He^+ with single ionization cross sections by protons is carried out to show the differences emerging when dressed or bare projectiles are used in the ionization processes. For protons, the projectile charge is the same for all impact parameter, while in the He^+ case the projectile charge increases if the impact parameter decreases. Thus for each energy, dressed projectiles should have effective charges that range between the ion charge and the nuclear charge, giving in principle, a total ionization cross section that is larger when compared with the proton case. However, if the collision is close enough, there is also a possibility of the projectile electron being stripped along the ionizing collision. Because the measurements are constrained to the cases where He^+ also appears in the exit channel, this restriction imposes a decrease of the ionization probability as compared with bare projectiles for close collisions. For He, Ne, Ar, Kr and Xe, the proton data are clearly below compare to our He^+ data. Indeed, as the perturbing effect of the above target over the projectile electron is not too high, the increase of the He^+ effective charge in close collision results effectively in an increase of the ionization cross section as compared with the proton case. These close values obtained for the cross sections by these two projectiles are also given by the theoretical calculation of Kirchner et al. [10,11] based on the independent particle model and considering positions involving all active electrons, both from the projectile and the target. This string saturates the electron loss probability, which becomes nearly equal to unity for impact parameters smaller than the atomic radius [12, 13]. Thus, only distant collisions are allowed if there is no electron loss, causing the effective charge of the projectile for such allowed collisions to the near one. This effect becomes more evident as the target atomic number increases. The calculation by Kirchner [10] for double and triple ionization of Ne shows the same high energy trend presented by the experiments, although the absolute values of the cross sections are higher than the values measured by Santos et al. [14].

He^+ impact ionization cross section for He, Ne, Ar, Kr and Xe have been plotted as a function of the incident energy in the Table 1 – 5 and Figure 1 – 5 respectively. We have calculated the single ionization cross sections of above mentioned targets from 1.0 MeV to 3.5 MeV impact energies. As per knowledge of the author's such theoretical calculations have never been reported earlier. We have compared our calculated single ionization cross sections with the experimental measurements made by Santos et al. [12]. The results also provide valuable checks on the results of previous calculations and measurements which exhibit unexplained discrepancies. We have also compared our theoretical results with experimental measurements of Cavalcanti et al. [15] for proton impact single ionization of Noble gases.

In Table 1 and Figure 1, we have compared our calculated results of He by He^+ and proton impact in the above mentioned energy range. Although as reported by Santos et al they have seen that some discrepancies have been found among the different measured cross section. Our calculated results throughout underestimates the experimental data at all considered impact energies. The calculated results are in good agreement with the experimental measurements. Both the results are in decreasing trend from energy 1.0 MeV to 3.5 MeV. At the energy 1.0 MeV, the ratio of calculated cross sections to the experiment cross section is about 0.74 times and having the magnitudes 65.48 x 10^{-18} cm^2 and 88 x 10^{-18} cm^2 respectively while at the energy 3.5 MeV the ratio is about 0.65 times smaller in comparison to experimental observation and having the magnitudes 21.46 x10^{-18} cm^2 and 33 x 10^{-18} cm^2 respectively.

Table 1: Single ionization of Helium atom by He^{+} impact in units of 10^{-18} cm^2

Energy (MeV)	1s	Total	Expt. [14]	T/Expt. [14]	Expt. [15]	T/Expt. [15]
1.00	65.48	65.48	88	0.74	18.9	3.46
1.25	54.59	54.59	70	0.77	-	-
1.50	46.72	46.72	66	0.70	13.1	3,56
2.00	36.19	36.19	56	0.64	11.3	3.20
2.50	29.48	29.48	45	0.65	9.4	3.13
3.00	24.85	24.85	38	0.65	8.5	2.92
3.50	21.46	21.46	33	0.65	6.6	3.25

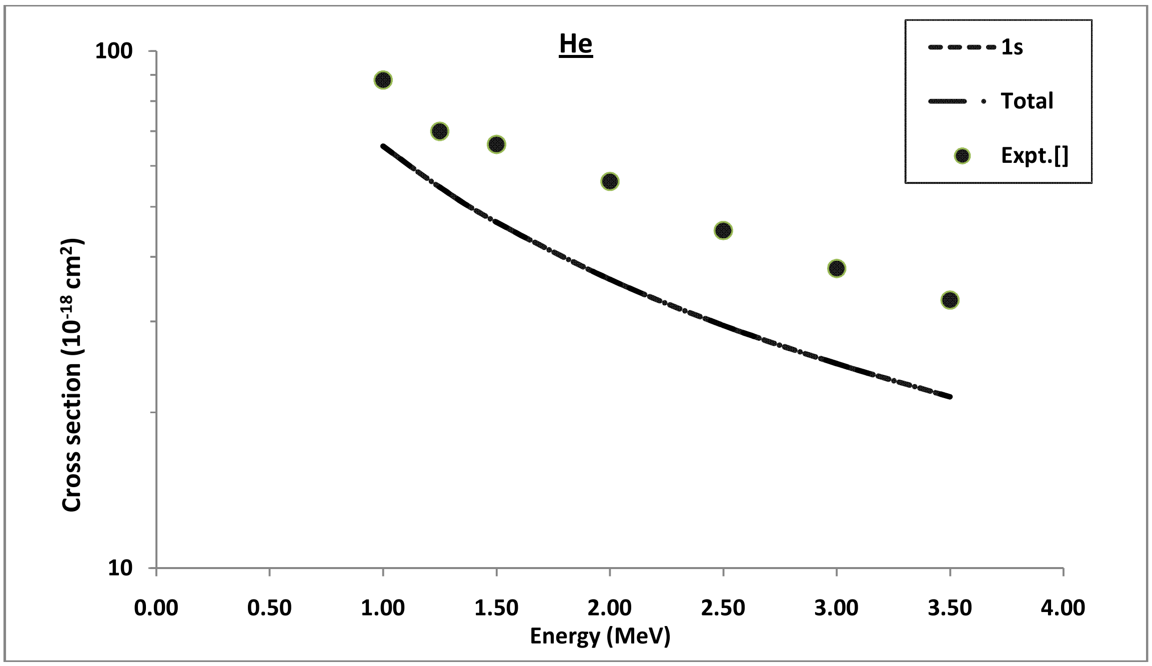

Figure 1: Single ionization of Helium atom by He^{+} impact in units of 10^{-18} cm^2

Now we would like to discuss the single ionization cross section of Ne by the impact of He^{+}. The ionization cross sections for 2p and 2s shells of Ne along with the experimental data have been presented in Table 2 and Figure 2. The calculated cross sections show reasonably good agreement with the measured data in the energy range 1.0 MeV to 3.5 MeV. The ratio of theoretical to experimental cross sections is 1.90 at 1 .0 MeV and this ratio decreases gradually with the increase in energy till it becomes 1.16 at 3.5MeV except at energy 1.50 MeV the ratio of both the cross sections is more than 2 and is 2.14 times larger than the measured cross sections. At this energy the magnitudes of theoretical cross sections and experimental values are 162.65 x 10^{-18} cm^2 and 76 x 10^{-18} cm^2 respectively. Close agreement of the present results with the experiment is achieved due to insignificant contribution from electron capture except at very low energies.

Table 2: Single ionization of Neon atom by He^+ impact in units of 10^{-18} cm^2

Energy (MeV)	2p	2s	Total	Expt. [14]	T/Expt. [14]
1.00	208.12	12.43	220.55	116	1.90
1.25	176.88	10.44	187.32	-	-
1.50	153.54	9.11	162.65	76	2.14
2.00	120.67	7.41	128.08	82	1.56
2.50	98.75	6.34	105.09	64	1.64
3.00	83.39	5.57	88.96	69	1.28
3.50	71.93	4.98	76.91	66	1.16

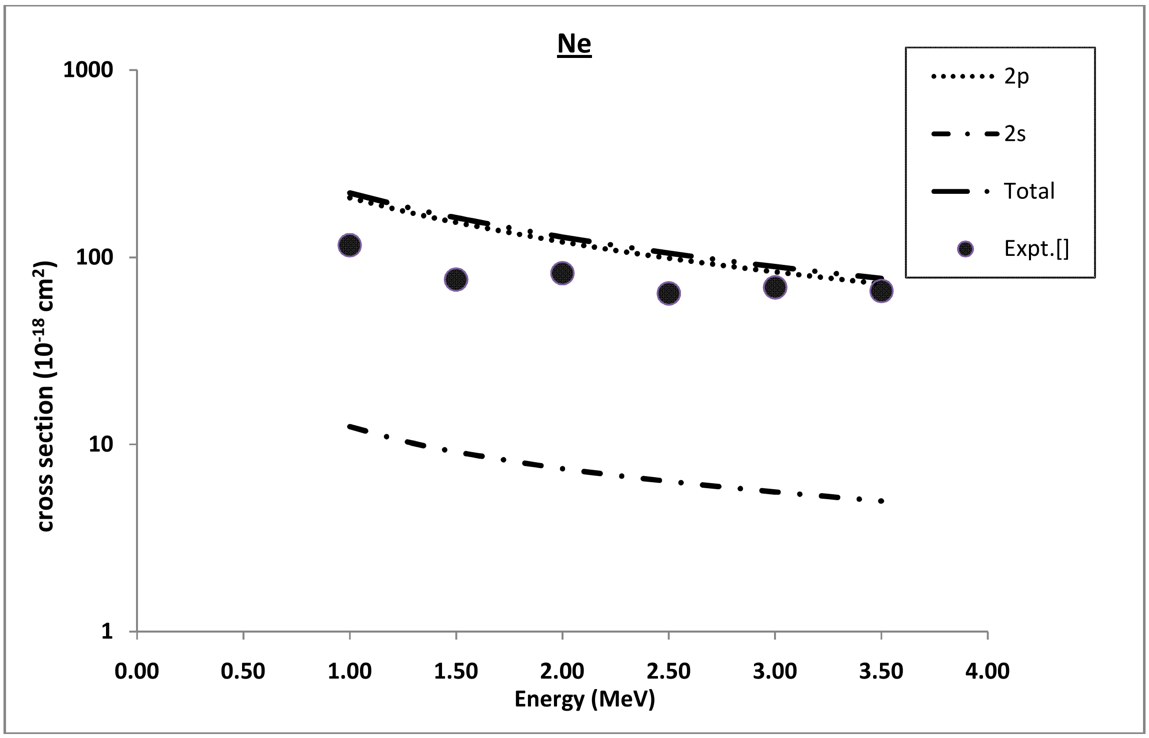

Figure 2: Single ionization of Neon atom by He^+ impact in units of 10^{-18} cm^2

In Table 3 and Figure 3 we have presented the comparison of single ionization cross sections of Ar with experimental data by the impact of He^+. Our direct calculation of ionization cross section incorporates the contributions from the inner shells 3p, 3s and 2p only. The results also provide valuable checks on the results of previous calculations as well as measured data which exhibit unexplained discrepancies. It is well known that besides direct ionization, He^+ impact ionization cross section contributed by a number of alternative processes e.g. transfer ionization and electron capture. However, in the present case no such evidence has been found in the experiment of Santos et al. The experimental result overestimates the calculated cross sections throughout the energy range considered. But from impact energy 1.0 MeV to 3.5 MeV the ratio of experimental to the theoretical calculations are always within a factor of 1.50. At impact energy 1.0 MeV the magnitudes of experimental cross sections and calculated values are 229 x 10^{-18} cm^2 and 225.60 x 10^{-18} cm^2 respectively and at this impact energy the ratio is about unity. Beyond impact energy 1MeV to 2.50 Mev the ratio lying between 1.01 to 1.23 and the ratio slightly increases at impact energies 3.0 MeV and 3.5 Mev. At these energies the ratios are 1.49 and 1.40 respectively. Overall after close inspection of the results we found that the results obtained by present method shows excellent agreement with the experiment.

Table 3: Single ionization of argon atom by He^+ impact in units of 10^{-18} cm^2

Energy (MeV)	3p	3s	2p	Total	Expt. [14]	T/Expt. [14]	Expt. [15]	T/Expt. [15]
1.00	202.81	22.79	3.08	225.60	229	0.98	128.5	1.78
1.25	170.10	19.19	3.29	189.29		-	-	-
1.50	147.57	16.46	3.39	164.03	206	0.79	95.2	1.72
2.00	117.15	12.67	3.38	129.82	162	0.80	71.0	1.82
2.50	96.51	10.23	3.23	106.74	132	0.80	65.4	1.63
3.00	81.05	8.56	3.05	89.61	134	0.66	57.1	1.57
3.50	69.50	7.36	2.85	76.86	108	0.71	44.1	1.74

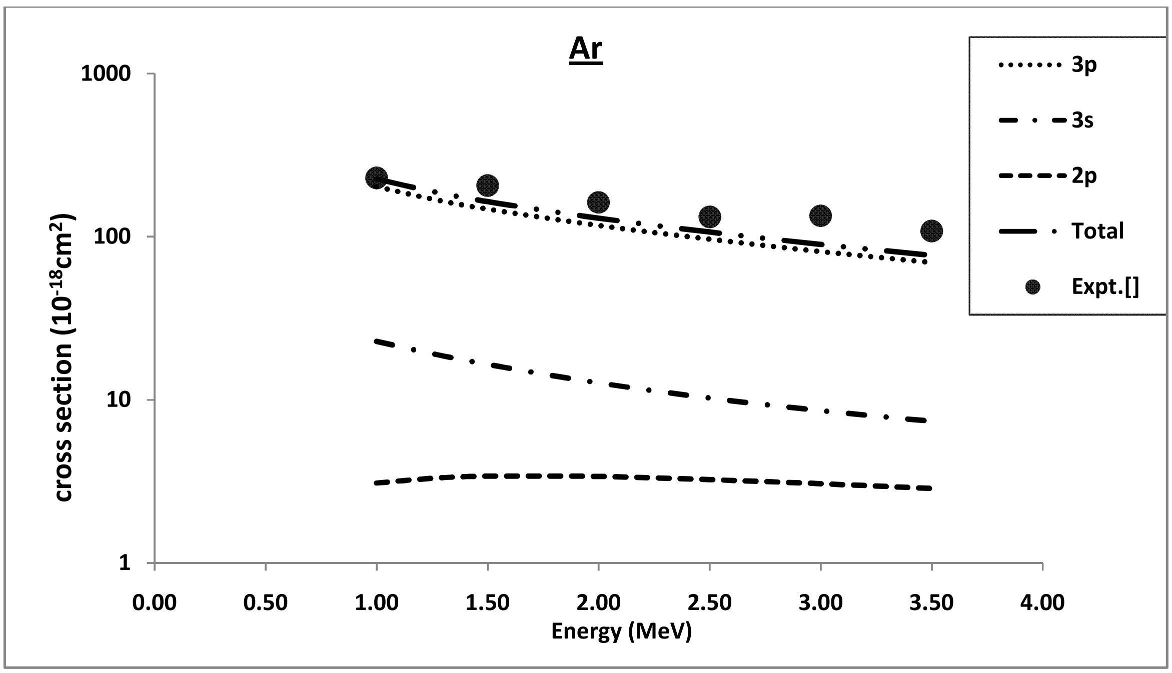

Figure 3: Single ionization of Argon atom by He^+ impact in units of 10^{-18} cm^2

We have also calculated He^+ impact ionization cross sections of Kr and Xe. The calculated cross sections of Kr and Xe along with the experimental observations of Santos et al have been presented in the Tables 4 & Table 5 and Figure 4 & Figure 5 respectively. In both the case we have calculated the ionization cross sections from 1.0 MeV to 3.5 MeV impact energies. In case of Kr we have calculated single ionization cross sections of 4p, 4s, 3d and 3p while in case of Xe we have calculated cross sections of 5p, 5s, 4d and 4p. Near the impact energy 1.0 MeV the magnitudes of the calculated cross sections are larger in comparison to the experimental data which is a usual feature of the model because the present model is valid for intermediate and high energy range. Our theoretical results come closer to the experimental data with the increase of energy value. In case of Kr the ratio of theoretical cross section to the experimental data lies between 1.28 to 0.93 while in the case of Xe the value lies between1.59 to 1.08 respectively. The magnitudes of calculated cross sections and the measured data is 302.84 x 10^{-18} cm^2 and 262 x 10^{-18} cm^2 respectively in case of Kr at impact energy 1.0 MeV while at the same energy the magnitudes of Xe are 143.77 x 10^{-18} cm^2 and 132 x 10^{-18} cm^2 respectively. From the discussion given above we found that our calculated results are in excellent agreement with the experiment in the energy region 1.0 MeV to 3.5 MeV.

Table 4: Single ionization of Krypton atom by He^+ impact in units of 10^{-18} cm^2

Energy (MeV)	4p	3d	4s	3p	Total	Expt. [14]	T/Expt. [14]	Expt. [15]	T/Expt. [15]
1.00	242.68	30.33	25.04	4.79	302.84	262	1.15	128.5	2.36
1.25	205.45	31.04	20.60	4.80	261.89		-	-	-
1.50	177.61	30.92	17.49	4.63	230.65	179	1.28	95.2	2.42
2.00	138.15	29.66	13.56	4.12	185.49	159	1.16	71.0	2.61
2.50	111.66	27.80	11.21	3.60	154.27	137	1.12	65.4	2.35
3.00	93.11	25.68	9.63	3.16	131.58	133	0.98	57.1	2.30
3.50	79.83	23.88	8.47	2.81	114.99	123	0.93	44.1	2.60

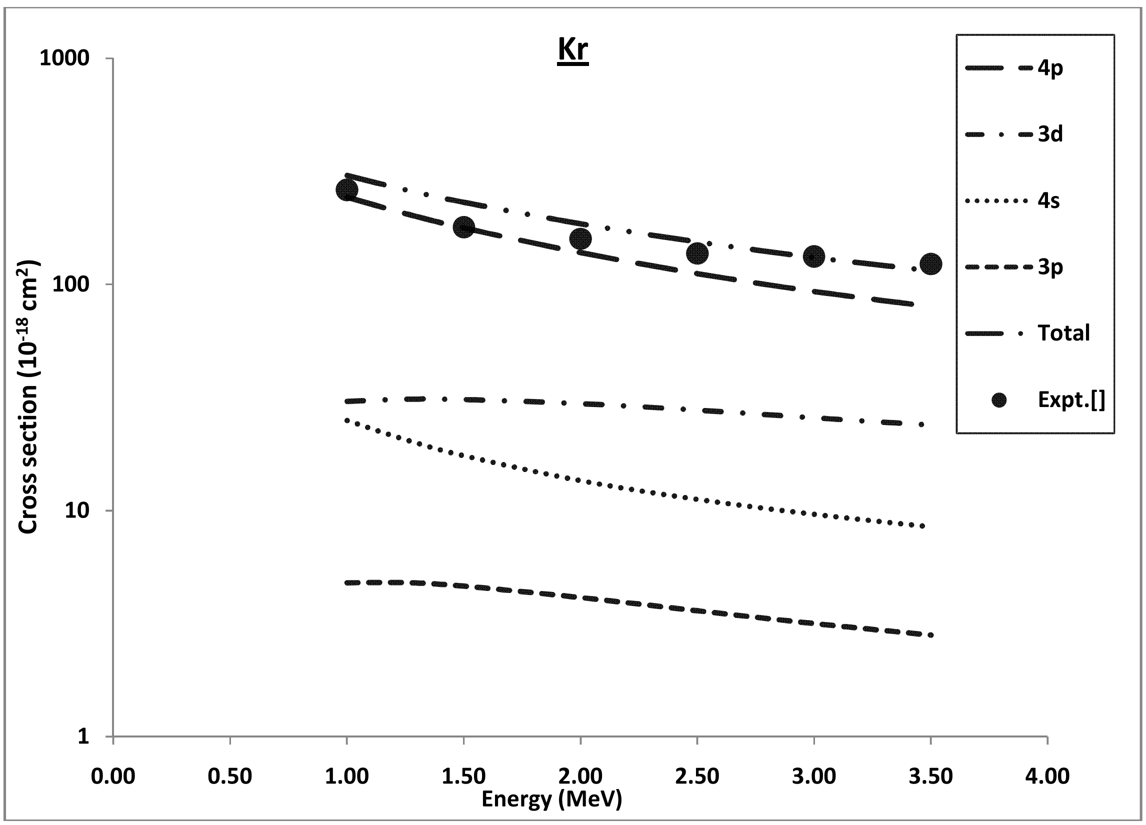

Figure 4: Single ionization of Krypton atom by He^+ impact in units of 10^{-18} cm^2

Table 5: Single ionization of Xenon atom by He^+ impact in units of 10^{-18} cm^2

Energy (MeV)	5p	4d	5s	4p	Total	Expt. [14]	T/Expt. [14]	Expt. [15]	T/Expt. [15]
1.00	369.97	59.17	30.95	2.83	462.92	290	1.59	140.9	3.29
1.25	297.11	53.70	25.93	2.55	379.29		-	-	-
1.50	248.06	47.96	22.56	2.29	320.87	219	1.46	104.7	3.06
2.00	186.57	38.81	18.10	1.90	245.38	175	1.40	73.4	3.34
2.50	149.42	32.34	15.08	1.66	198.50	168	1.18	74.2	2.68
3.00	124.56	27.77	12.83	1.49	166.65	146	1.14	55.2	3.01
3.50	106.79	24.50	11.11	1.37	143.77	132	1.08	48.9	2.94

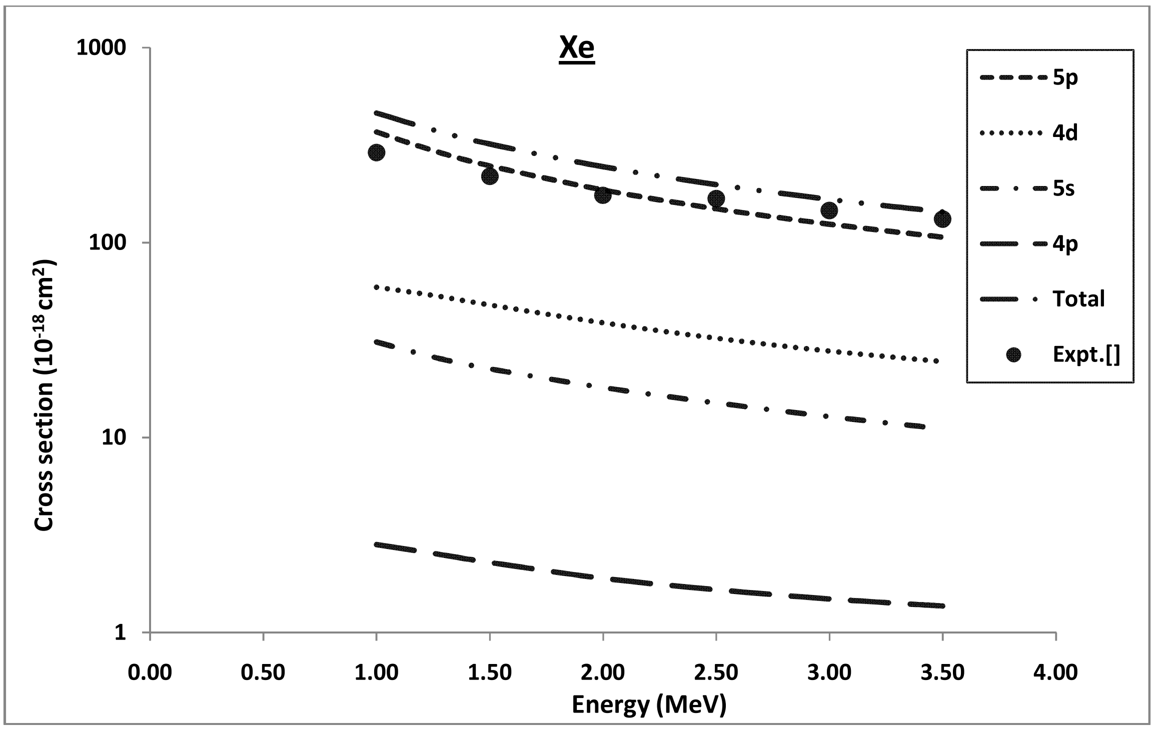

Figure 5: Single ionization of Xenon atom by He^+ impact in units of 10^{-18} cm^2

Besides this we have also compared our calculated results with the measured data of Cavalcanti et al. [15]. They have measured the absolute cross sections for multiple ionization of noble gases by swift proton impact. When we compare our calculated results of He, Ne, Ar, Kr and Xe with these measured data we find that in case of He our calculated results lies between 3.46 to 3.25 times greater in the energy range 1.0 MeV to 3.5 MeV. While in case of Ar the theoretical results are 1.76 to 1.74 times larger in the said energy region. In case of Kr the present calculated results are 2.36 to 2.60 times higher compare to measured data while in case of Xe it is lying between 3.29 to 2.94 times compare to experimental results in the energy range 1.0 MeV to 3.5 MeV.

CONCLUSION

When we are taking He^+ as a projectile then the measured data as well as calculate cross sections are larger while in case of H^+ impact, the theoretical as well as experimental cross sections are smaller.

When we concentrate our attention to find the proper reason behind such discrepancies we found that since He^+ have 2 protons and H^+ have only one proton. Hence He^+ is heavier projectile in comparison to H^+, so as soon as the projectile comes closer to the target due to Coulomb repulsion in case of He^+ the impact parameter increases while impact parameter decreases in case of H^+ impact. Therefore we conclude that in case of He^+ the projectile is slow compared to the H^+ impact. Hence in former case the cross sections are larger while in latter case the cross sections are smaller. Such trend is also available in case of experimental data.

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