STUDY OF CROSS SECTION FOR IONIZATION AND ELECTRON CAPTURE PROCESS

A THESIS SUBMITTED TO THE

CENTRAL DEPARTMENT OF PHYSICS

INSTITUTE OF SCIENCE AND TECHNOLOGY

TRIBHUVAN UNIVERSITY

NEPAL

FOR THE AWARD OF

DOCTOR OF PHILOSOPHY

IN PHYSICS

BY

SURESH PRASAD GUPTA

MARCH 2018

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DECLARATION

Thesis entitled **"STUDY OF CROSS SECTION FOR IONIZATION AND ELECTRON CAPTURE PROCESS"** which is being submitted to the Central Department of Physics, Institute of Science and Technology (IoST), Tribhuvan University, Nepal for the award of the degree of Doctor of Philosophy (Ph.D.), is a research work carried out by me under the supervision of Prof. Dr. Raju Khanal, Central Department of Physics, Tribhuvan University, Nepal and co-supervised by Prof. Dr. Lalan Kumar Jha, University Department of Physics, Babasaheb Bhimrao Ambedkar (B. R. A.) Bihar University, India.

This research is original and has not been submitted earlier in part or full in this or any other form to any university or institute, here or elsewhere, for the award of any degree.

…..........................

Suresh Prasad Gupta

RECOMMENDATION

This is to recommend that **Mr. Suresh Prasad Gupta** has carried out research entitled “**Study of cross section for ionization and electron capture process**” for the award of Doctor of Philosophy (Ph.D.) in **Physics** under our supervision. To our knowledge, this work has not been submitted for any other degree.

He has fulfilled all the requirements laid down by the Institute of Science and Technology (IoST), Tribhuvan University, Kirtipur for the submission of the thesis for the award of Ph. D. degree.

…………………

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March 2018

LETTER OF APPROVAL

Date: Feb.23/2020

On the recommendation of supervisor **Prof. Dr. Raju Khanal** and co-supervisor **Prof. Dr. Lalan Kumar Jha** this Ph.D. thesis submitted by **Mr. Suresh Prasad Gupta**, entitled "**Study of cross section for ionization and electron capture process**" is forwarded by Central Department Research Committee (CDRC) to the Dean, Institute of Science and Technology (IoST), Tribhuvan University (TU).

………………………

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ACKNOWLEDGEMENTS

I am extremely grateful to my able and competent guide Prof. Dr. Raju Khanal, Central Department of Physics (CDP), Tribhuvan University (TU) and co-supervisor Prof. Dr. Lalan Kumar Jha, University Department of Physics, B. R. A. Bihar University for supervising the progress of work with keen interest.

I am extremely grateful to Prof. Dr. Binil Aryal, Head of CDP, Prof. Dr. Narayan Adhikari, Prof. Dr. Om Prakash Niraula, Prof. Dr. Ishwor Koirala, Dr. Gopi Chandra Kafle, Dr. Balram Ghimire, Dr. Sanju Shrestha, Dr. Ajay Kumar Jha of CDP and Prof. Dr. Khem Narayan Poudyal of Pulchowk Engineering College for their moral support and encouragements during my thesis work. I would like to express my thanks to all the faculty members and administrative staffs of CDP.

I am thankful to Patan Multiple Campus and Institute of Science and Technology (TU) for providing me study leave to carry out my research work. My special thank goes to my senior friends Prof. Dr. Hom Nath Poudyal, Prof. Dr. Narayan Chapagain, Dr. Lekh Nath Mishra, Dr. Kishori Yadav, Mr. Prakash Man Shrestha, Mr. Rajesh Kumar Bachchan and Mr. Suresh Basnet for their moral and technical supports during the progress of my work. I would like to express my indebtedness to late. Prof. Dr. B. N. Roy of the University Department of Physics and Ex-Pro Vice Chancellor, B. R. A. Bihar University, Muzaffarpur for helpful discussions during the progress of my work. Finally, my special thank goes to my late mother Parvati Devi, father Raghubir Prasad Gupta and all the family members who were always source of inspiration to complete my research work. Lastly, I would like to express my gratitude to my wife Ranjana Gupta, my beloved sons Shovit and Ujjwal for their support, love and understanding throughout my research work.

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Suresh Prasad Gupta

March 2018

ABSTRACT

Collision of electron and ions with atoms and molecules is common technique for extracting information from such small entities. Electron impact ionization and excitation have been actively studied by many research groups. In spite of successes of using different quantal approximations in the case of light atoms, there exist difficulty in the calculation of electron impact single and multiple ionization cross sections for heavy atoms due to mathematical complexities. The binary encounter approximation (BEA) for the investigation of single and multiple ionizations of atoms by electron and heavy charged particles impact is found to be suitable. The approximation gives reliable results consistent with the experiments. Vriens (1966) derived a more reliable classical formalism of electron impact ionization including effect of exchange and interference. Various theoretical approaches have contributed in the development of binary encounter approximation for electron-atom, ion-atom collision processes. Double ionization of atoms and ions is a four particle interaction and hence it is still impossible to carry out exact calculations for these processes. Gryzinski and Kune (1999) have derived general analytical expression for electron impact double ionization cross sections in binary encounter model to describe the direct double ionization. In the first case the two electrons may be ejected from target atom by two successive encounters of the incident particle and secondly the incident particle may knock out one target active electron and the second electron of the target is removed by first elected electron.

In this work heavy charged particles impact single and double ionization cross section for Cu and Fe atoms have been calculated in binary encounter approximation using Hartree-Fock momentum distribution for the target electrons. Electron impact single ionization cross sections for Kr, Xe and single and double ionization cross sections for Fe has been carried out. Our theoretical results for electron impact single ionization of Kr, Xe and Fe using binary encounter approximation are in good agreement with the experimental data. About 94.7 % in the case of Kr, 71 % in the case of Xe, and 93.9% in the case of Fe are within ratio factor of two and hence results are in close agreement with experimental data in the given energy range. In the case of proton impact single ionization cross section of Cu about 72 % results have ratio factor less

than 1.12 and 50% have less than 1.1. Same nature is observed in the case of Fe and about 94.7 % fall under validity region of ratio factor 2. In the case of He^{2+} impact single ionization cross section of Cu and Fe the results agree well in intermediate and high energy region. For the He^{2+} impact double ionization cross section of Cu and Fe about 75 % and 76.9 % of calculated results are in agreement with experimental results respectively. The direct double ionization of Fe is considered to be due to the ejection of loosely bound 3d and 4s electrons and also considered ionization of 3s electron to lead an excited state which results double ionization through auto ionization. Alpha particle impact double ionization of Fe and Cu have random fluctuations in the experimental observations in low energy range which are not observed in theoretical results. Further investigations are required both in experimental and theoretical methods. In different cases of single and double ionization by electron and heavy charged particles the calculated results are found to be in satisfactory agreement with the available experimental data.

Theoretical knowledge of ionization cross section and collision dynamics find wide application in different fields of science. Phenomena involving electron collisions have important roles such as astrophysics, upper atmosphere of Titan, electron driven chemistry, low temperature plasma diagnostics, modeling of plasma in Tokomak, plasma processes in cometary, radiation effects, biomedical applications, display technology, astrophysics, Stellar model, radiative process in the earth's upper atmosphere and medical application. Using a technique of Monte Carlo simulations track structure is usually used in micro and nano dosimeter to find radiation transport index in medical science. Better the results of cross sections used as simulation codes better the results of treatment in medical science. Projectile particles of ions like protons and helium deposit a large amount of their energy in a volume of a few micrometers or even nanometers and cause extensive damage to the microscopic structure of matter and results cell death in the DNA. With different suitable theoretical models one can predict reliable values of cross sections of different atoms/ions.

LIST OF ACRONYMS AND ABBREVIATIONS

BEA	Binary encounter approximation
BET	Binary encounter theory
BOA	Born-Oppenheimer approximation
CA	Correlation approximation
CADW	Configuration averaged distorted wave
CBA	Coulomb-Born approximation
CBE	Coulomb-Born exchange
CCA	Close coupling approximation
CFA	Central field approximation
CS	Cross section
CTMC	Classical trajectory Monte Carlo simulation method
DDI	Direct double ionization
DI	Double ionization
DMF	Detusch-Mark formalism
DWA	Distorted wave approximation
DWBEA	Distorted wave Born exchange approximation
FBA	First Born approximation
FDCS	Fully differential cross section
HF	Hartree-Fock
IA	Indirect auto ionization
TCS	Total cross section
TICS	Total ionization cross section

LIST OF TABLES

LIST OF FIGURES

Page No.

TABLE OF CONTENTS

CHAPTER 1

1. INTRODUCTION

1.1 Introduction

Atomic collision phenomena are of fundamental importance in atomic and molecular physics. It plays an important role in other fields of interest such as astrophysics, chemistry, plasma physics and laser physics. Basically, these phenomena involve collisions between an elementary particle and an atomic system. The collision of a charged particle with a gas atom or molecule may result in a number of effects. These effects may first be distinguished as elastic, inelastic or super elastic. In an elastic collision no energy exchange takes place between the internal motion of the atom and the incident particle. In case of inelastic collision some kinetic energy is lost by the incident particle and the systems undergo a change of their internal structure. Further, the inelastic collisions is distinguished as ionizing and non-ionizing collisions, depending on whether or not sufficient energy is transferred to lead to ejection of one or more electrons from the atom. Ionizing collisions may be analysed further in terms of number and energy of the electrons ejected from the atom and in terms of excitation of the ions. Non-ionizing inelastic collision will involve excitation of distinct atomic states. Another inelastic collision is the charge transfer process in which the incident positively charged particle captures one or more electrons from target atom. In case of electron impact, super elastic collision can occur when the electron gains energy from the internal motion of the excited atom. Collision of this type occurs between incident electrons and meta-stable atoms.

Theoretical studies of collisions of charged particles with atoms and ions for different atomic collision processes are necessarily required in explaining the structure and nature of the interaction forces existing therein. Depending upon the energy exchange taking place in interaction, various collision processes can be defined. When a positively charged projectile A^{n+} (n being an integer) moving with velocity v, is allowed to strike a target B^{q+} (atomic and ionic system, q being integer including zero), one of the following reactions may take place (Kumari, 2011).

$$A(v) + B^{q^+}(0) \rightarrow \begin{cases} A^{n^+} + B^{q^+} & (1.1a) \\ A^{n^+} + (B^{q^+})^* & (1.1b) \\ A^{n^+} + B^{(q+p)^+} + pe & (1.1c) \\ A^{(n-p)^+} + B^{(q+p)^+} & (1.1d) \\ A^{(n-k)^+} + B^{(q+r)^+} + (r-k)e & (1.1e) \end{cases}$$

where $p = 1, 2, 3, ...$ Here the target $B^{q+}(0)$ is taken initially to be at rest in the frame of reference with respect to which v is measured. The different processes as given by equations (1.1a) is designated as elastic scattering, equation (1.1b) designated as excitation, equation (1.1c) is designated as pure single or multiple ionization, equation (1.1d) is designated as charge transfer and equation (1.1e) is designated as transfer ionization respectively. Equations (1.1d) and (1.1e) are simply single or multiple charge transfer and charge transfer ionization respectively. Besides these there may be combination of the above processes like transfer ionization etc. If electron is taken as projectile and the target is an atom or ion, the corresponding processes can be assigned to be as

$$\mathrm{e}^-(v) + \mathrm{B}^{q+}(o) \rightarrow \begin{cases} \mathrm{e}^- + \mathrm{B}^{q+} \text{ (Elasticscattering)} & (1.2a) \\ \mathrm{e}^- + (\mathrm{B}^{q+})^* \text{ (Excitation)} & (1.2b) \\ \mathrm{e}^- + \mathrm{B}^{(q+p)+} + \mathrm{Pe}\text{(Ionization)} & (1.2c) \end{cases}$$

In an elastic scattering, the total kinetic energy of the interacting systems is conserved and hence there is no change in the internal energy of the systems involved. However, these collision processes are relatively less important but useful in explaining the interaction forces existing between the colliding systems. The inelastic collision is that in which some kinetic energy is lost by the incident particle. This loss in kinetic energy changes the internal state of the target which may give rise to the process of excitation, ionization, charge transfer etc. The asterisk mark in the above reactions represents excitation due to the change in the internal energy. Study of these processes is important in giving valuable information about the structure of the target and other associated features.

It is quite necessary to introduce a physical quantity Cross section in terms of which the interaction can be measured or different collision phenomena can be quantitatively expressed. Before defining cross section we would like to give a brief idea of a typical collision experiment. In the experiment a well collimated beam of mono-energetic particles is made incident on a target. After collision with target, the energy and the angular distribution of outgoing particles are studied by a suitable detector. The schematic diagram of a scattering experiment is given in Figure 1.

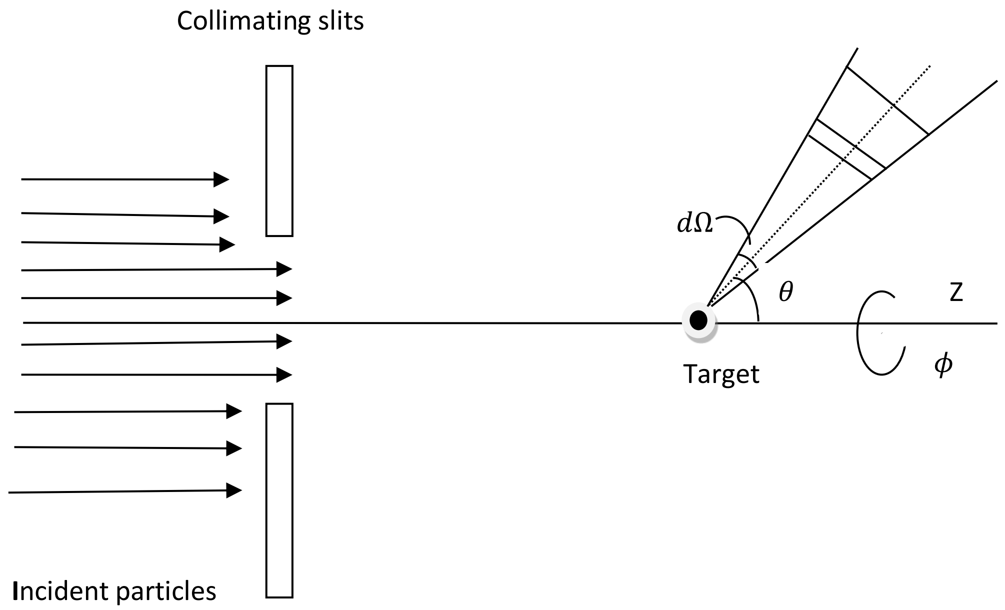

Figure 1: A systematic diagram of scattering experiment (Kumari, 2011).

As stated earlier, the result of collision experiment is usually expressed in terms of cross section. If we restrict our attention to a small solid angle about a particular direction, cross section is designated as differential cross section. After collision with target, the angular distribution of incident and scattered particles is expressed in term of differential scattering cross section. Let N be the number of incident particles crossing per unit time per unit area perpendicular to the beam so that N represents the flux of incident particles. Let $\mathrm{d}N^{'}$ be the number of incident particles scattered per unit time in a small solid angle $\mathrm{d}\Omega$ along direction (θ, ϕ) with respect to Z-axis. Under the experimental conditions described above the number $\mathrm{d}N'$ of incident particles is proportional to N, n (the number of target electrons) and $\mathrm{d}\Omega$, so that one can write

$$\mathrm{d}N' = Nn\sigma(\theta, \phi)\mathrm{d}\Omega \tag{1.3}$$

The proportionality factor $\sigma(\theta, \phi)$ is known as scattering cross section.Scattering cross section may be defined as the ratio of the number of particles scattered per unit solid angle per unit time and the incident flux for one target centre. It gives the quantitative measure of probability of particular interaction between two colliding particles and often written as

$$\sigma(\theta,\phi) = \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\theta,\phi) \tag{1.4}$$

Right side term is known as differential scattering cross section. The cross section that is function of one of the collision results (i.e. angle scattered, energy transferred) is known as differential cross section. The total scattering cross section is obtained by integrating the differential cross section over all scattering angles or energies i.e.

$$\sigma_{\mathrm{tot}} = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\theta,\phi)\, d\Omega = \int_0^{\pi}\int_0^{2\pi} \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\theta,\phi)\, \sin\theta \mathrm{d}\theta \mathrm{d}\phi \tag{1.5}$$

The relative probabilities of various collision processes are different. Both the differential and total scattering cross section have the dimension of area. This definition holds well in classical as well as in quantum mechanics.

The ionization process occurs when an incident electron collides with a target followed by a removal of one or more electrons from the target. There are many types of ionization processes. The first type is single ionization where the incident electron releases one electron from the target. The second type is multiple ionization of the target where more than one electron is released after interaction with projectile and target atom. Consider the case of electron impact single ionization which is normally called an (e, 2e) process. Symbolically, the direct electron impact single ionization can be expressed as (Hagan, 2010).

$$\mathrm{e}^-_{\mathrm{in}}(E_{\mathrm{in}}, p_{\mathrm{in}}) + X \rightarrow X^+ + \mathrm{e}^-_{\mathrm{a}}(E_{\mathrm{a}},\, p_{\mathrm{a}}) + \mathrm{e}^-_{\mathrm{b}}(E_{\mathrm{b}}, p_{\mathrm{b}}) \tag{1.6}$$

where X is the target assumed to be in the ground state, $\mathrm{e}^-_{\mathrm{a}}$ and $\mathrm{e}^-_{\mathrm{b}}$ are scattered and ejected electrons, X^+ is ion generated after collision. The ion motion can be neglected since the ion mass is very large compared to the mass of the electron. Let E_{in}, E_{a}, E_{b} and $\vec{p}_{\mathrm{in}}, \overrightarrow{p}_{\mathrm{a}}$, $\vec{p}_{\mathrm{a}}$ are the kinetic energies and momenta of the incident, scattered and ejected electrons respectively. Total energy of the collision must be conserved and their incident energy is given by

$$E_{\mathrm{in}} = \varepsilon_{\mathrm{i}} + E_{\mathrm{a}} + E_{\mathrm{b}} \tag{1.7}$$

where ε_{i} is ionization potential.

The total momentum is also conserved i.e $\vec{p}_{\mathrm{in}} = \vec{p}_{\mathrm{a}} + \vec{p}_{\mathrm{b}} + \vec{P}$, where $\vec{P}$ is momentum of the residual atom. Momentum transferred by the scattered electron will be $\Delta\vec{p} = \vec{p}_{\mathrm{i}} - \vec{p}_{\mathrm{a}}$ .The results of these kinds of collisions are typically expressed as a cross section. In electron impact ionization, the probability for the (e, 2e) process is expressed in terms of differential cross section. There are different types of cross sections. They are normally termed as: the total cross section, the singly, doubly and triply differential cross section. The singly differential cross section ($\mathrm{d}\sigma/\mathrm{d}\Omega$) describes the angular distribution of the scattered electron. The double differential cross section ($\mathrm{d}^2\sigma/\mathrm{d}\Omega_\mathrm{a}\,\mathrm{d}E_a$) describes the energy and the angular distribution of the scattered electron after the ionization. The triply or fully differential cross section (FDCS) is given by ($\mathrm{d}^3\sigma/\mathrm{d}\Omega_\mathrm{a}\,\mathrm{d}\Omega_b\mathrm{d}E_a$) . It describes the probability that the two out-going electrons with energies of E_a and E_b will be found in solid angles $\mathrm{d}\Omega_\mathrm{a}$ and $\mathrm{d}\Omega_\mathrm{b}$ after the ionization. In order to gain information about (e, 2e) ionization process, one measure the fully differential cross section which is proportional to the probability that the two outgoing electrons will be moving in a particular direction with particular energies after the ionization event.

1.2 General theoretical approach

The prime aim of any theoretical description of the scattering process is to yield the experimentally observed cross sections. With suitable theoretical description one can predict reliable values of cross sections.

After the discovery of atomic model by Rutherford (1911), the classical methods were used to describe collision processes. With the advent of quantum mechanics, classical methods were abandoned in atomic physics. It is well known that in certain cases the classical approach provides the same results as the semi-classical and pure quantum mechanical approaches. In quantum mechanics few-body problem arises from the fact that the Schrodinger equation is not analytically solvable for more than two mutually interacting particles. As a result, for three or more particles theory must be resort to significant modeling efforts using approximations and their validity are determined by comparison with experimental results. Various theoretical approaches used for calculating collision cross sections can be broadly classified under the following categories:

(i) Quantal methods

(ii) Semi-classical and semi-empirical methods and

(iii) Pure classical and binary encounter approximations.

Several quantal approximations have been proposed for the atomic collision processes in different energy regions. Quantum mechanical methods frequently used for investigation of collision processes in the low energy region are the Close coupling approximation (CCA), Correlation approximation (CA), Polarised pseudo state approximation (PPSA), R-matrix theory, Many-body methods and Quantum defect theory (QDT). In the intermediate energy range, few times the ionization threshold i.e. less than 10 V_{IP} (Pflüger et al., 2012),the method frequently used are Optical potential method, Eikonal Born series (EBS), Distorted wave methods and Coulomb projected Born-approximation. At sufficient high energies the first Born approximation (FBA) is found to give accurate results. Bates and McDonough (1972) have derived the key formula of the classical binary encounter approximation from the Born approximation for the differential cross section for a general inelastic collision.

Theoretical models for low to intermediate energies, where ionization probability is highest, must consider many factors including distortion in wave functions describing the projectile and target, target polarization due to the Coulomb interaction between the projectile, nucleus and bound electrons, exchange effects, multiple scattering and post collision interaction between particles emerging from the reaction. In case of high incident energy greater than 20 V_{IP} (Pflüger et al., 2012) and weak interaction, perturbation theory can be used for calculating differential cross sections. There are several ways of obtaining the first order perturbation approximation to the differential cross section. The particular method used here to discuss Born approximation is based on the time dependent perturbation theory and the system is described by Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r},t) \tag{1.8}$$

This equation can also be written as

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla^2\right]\psi(\boldsymbol{r},t) = V(\boldsymbol{r})\psi(\boldsymbol{r},t) \tag{1.9}$$

Since the interaction $V(\boldsymbol{r})$ is time independent, there exist stationary solutions of this equation corresponding to incident energy $E(k) = \hbar^2k^2/(2m)$:

$$\psi(\boldsymbol{r},t) = (2\pi)^{-3/2}\psi_k(\boldsymbol{r})\exp[-iE(k)t/\hbar] \tag{1.10}$$

where the time-independent wave function $\psi_k(\boldsymbol{r})$ is a solution of Schrödinger equation

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}) \tag{1.11}$$

satisfying the asymptotic boundary condition

$$\psi_k(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} e^{i\boldsymbol{k}.\boldsymbol{r}} + f(k,\theta,\phi)\frac{e^{ikr}}{r} \tag{1.12}$$

The factor $(2\pi)^{-3/2}$ has been inserted in equation (1.10) so that the unperturbed wave function

$$\phi(\boldsymbol{k},\boldsymbol{r},t) = (2\pi)^{-\frac{3}{2}}\exp\left\{i\left[\boldsymbol{k}.\boldsymbol{r} - \frac{E(k)t}{\hbar}\right]\right\} \tag{1.13}$$

has the standard normalization

$$\int \phi^*(\boldsymbol{k}',\boldsymbol{r},t)\phi(\boldsymbol{k},\boldsymbol{r},t)d\boldsymbol{r} = \delta(\boldsymbol{k}-\boldsymbol{k}') \tag{1.14}$$

The function $\phi(\boldsymbol{k},\boldsymbol{r},t)$ form a complete set, so that the exact solution $\psi(\boldsymbol{r},t)$ can be expanded as

$$\psi(\boldsymbol{r},t) = \int C(\boldsymbol{k},t)\,\phi(\boldsymbol{k},\boldsymbol{r},t)d\boldsymbol{k} \tag{1.15}$$

Let us insert this expansion in the left side of equation (1.9). Multiplying both sides of the equation on the left by $\phi^*(\boldsymbol{k}',\boldsymbol{r},t)$, integrating over all space and using expression (1.14) together with the fact that the unperturbed wave functions (1.13) satisfy the equation (1.9) with $V = 0$, we find that

$$i\hbar\dot{C}(\boldsymbol{k}',t) = \int \phi^*(\boldsymbol{k}',\boldsymbol{r},t)V(\boldsymbol{r})\psi(\boldsymbol{r},t)d\boldsymbol{r} \tag{1.16}$$

or using equations (1.10) and (1.13),

$$i\hbar\dot{C}(\boldsymbol{k}',\mathrm{t}) = (2\pi)^{-3}\exp\left\{\frac{i[E(k')-E(k)]t}{\hbar}\right\}\int \exp(-i\boldsymbol{k}'.\boldsymbol{r})\,V(\boldsymbol{r})\psi_k \tag{1.17}$$

The integral

$$T(\boldsymbol{k}',\boldsymbol{k}) = \int \exp(-i\boldsymbol{k}'.\boldsymbol{r})\,V(\boldsymbol{r})\psi_k(\boldsymbol{r})d\boldsymbol{r} \tag{1.18}$$

which appears on the right of equation (1.17) is called a transition matrix element. Equations (1.16) and (1.17) hold during the period $0 \le t \le \tau$.For $t < 0$, the amplitudes $C(\boldsymbol{k}',t)$ are all zero and integrating with respect to t from 0 to τ. We find that

$$C(\boldsymbol{k}',\tau) = (2\pi)^{-3}(\hbar\omega)^{-1}[1-\exp(i\omega\tau)]T(\boldsymbol{k}',\boldsymbol{k}) \tag{1.19}$$

where

$$\omega = \frac{E(\boldsymbol{k}')-E(\boldsymbol{k})}{\hbar} \tag{1.20}$$

The transition rate $W(\boldsymbol{k}')\mathrm{d}\boldsymbol{k}'$ for scattering into a final unperturbed state in which the wave vector $\boldsymbol{k}'$lies in the interval $\boldsymbol{k}'$ to $\boldsymbol{k}' + \mathrm{d}\boldsymbol{k}'$is then

$$W(\boldsymbol{k}')d\boldsymbol{k}' = \frac{1}{\tau}|C(\boldsymbol{k}',\tau)|^2\mathrm{d}\boldsymbol{k} = (2\pi)^{-6}\hbar^{-2}|T(\boldsymbol{k}',\boldsymbol{k})|^2 2[F(\tau,\omega)/\tau]\mathrm{d}\boldsymbol{k}' \quad (1.21)$$

where

$$F(\tau,\omega) = \frac{(1-\cos\omega\tau)}{\omega^2} \quad (1.22)$$

For large $\tau, [F(\tau,\omega)/\tau]$ becomes equal to $\pi\delta(\omega)$. Let the polar angles of $\boldsymbol{k}'$ with respect to the direction of incidence be (θ,ϕ). We then have

$$\mathrm{d}\boldsymbol{k}' = \kappa'^2\mathrm{d}\kappa' d\Omega = \frac{m\kappa'}{\hbar}\mathrm{d}\omega\mathrm{d}\Omega \quad (1.23)$$

where we have used equation (1.20) and the relation $E(k') = \hbar^2 k'^2/(2m)$ to deduce that $\mathrm{d}\omega/\mathrm{d}k' = (\hbar k'/m)\mathrm{d}k'$. The transition rate for scattering can be obtained by integrating over ω. That is

$$W\mathrm{d}\Omega = (2\pi)^{-6}\hbar^{-2}\left(\frac{m}{\hbar}\right)d\Omega\int \left|T(\boldsymbol{k}',\boldsymbol{k})\right|^2 2\pi\delta(\omega)k\mathrm{d}\omega$$

$$= (2\pi)^{-5}m\hbar^{-3}\left|T(\boldsymbol{k}',\boldsymbol{k})\right|^2 k'\mathrm{d}\Omega \quad (1.24)$$

where $E(k') = E(k)$, i.e. $k' = k$. To calculate differential cross section, we divide W by the incident flux. With the normalization (1.14), this flux equals $(2\pi)^{-3}\nu = (2\pi)^{-3}\hbar k/m$. Hence,

$$\frac{\mathrm{d}\sigma}{d\Omega} = \frac{(2\pi)^3 m}{\hbar k}\mathrm{W} = (2\pi)^{-2}m^2\hbar^{-4}\left|T(\boldsymbol{k}',\boldsymbol{k})\right|^2 \quad (1.25)$$

Comparing equation (1.25) with differential cross section, we get

$$\frac{\mathrm{d}\sigma}{d\Omega} = |f(k,\theta,\phi)|^2 \;\; = |f(k,\theta,\phi)|^2 = (2\pi)^{-2}m^2\hbar^{-4}\left|T(\boldsymbol{k}',\boldsymbol{k})\right|^2 \quad (1.26)$$

so that with a conventional choice of phase we can write

$$f(k,\theta,\phi) = \frac{-m}{2\pi\hbar^2}\int \exp(-i\boldsymbol{k}'.\boldsymbol{r})\,V(\boldsymbol{r})\psi_k(\boldsymbol{r})d\boldsymbol{r}$$

$$= -\frac{1}{4\pi}\int \exp(-i\boldsymbol{k}'.\boldsymbol{r})\,V(\boldsymbol{r})\psi_k(\boldsymbol{r})d\boldsymbol{r} \quad (1.27)$$

where vector $\boldsymbol{k}'$ has polar co-ordinates (k,θ,ϕ), the polar axis being along the direction $\boldsymbol{k}$ of incidence.

To obtain first-order perturbation approximation to the transition matrix called the first Born approximation $T^{\mathrm{B}}(\boldsymbol{k}',\boldsymbol{k})$ we assume that the wave function $\psi_k(\boldsymbol{r})$ can be approximated by the unperturbed incident wave $\exp(i\boldsymbol{k}.\boldsymbol{r})$. Upon substitution in equation (1.18), we find that

$$T^{\mathrm{B}}(\boldsymbol{k}',\boldsymbol{k}) = \int \exp(-i\boldsymbol{k}'.\boldsymbol{r})\, V(\boldsymbol{r}) \exp(i\boldsymbol{k}.\boldsymbol{r})\, d\boldsymbol{r}$$

$$= \int \exp(i\Delta.\boldsymbol{r})\, V(\boldsymbol{r}) d\boldsymbol{r} \qquad (1.28)$$

Where $\Delta = \boldsymbol{k} - \boldsymbol{k}'$ is the wave vector transfered and $\hbar\Delta$ being the momentum transfer. Since for the elastic scattering case considered here, $k = k'$ and $\boldsymbol{k}.\boldsymbol{k}' = k^2\cos\theta$, the magnitude of Δ is

$$\Delta = 2k\sin\frac{\theta}{2} \qquad (1.29)$$

where θ is the angle of scattering. From equation (1.27), the scattering amplitude corresponding to first Born approximation to the scattering amplitude is

$$f^{\mathrm{B}} = -\frac{1}{4\pi}\int \exp(i\Delta.\boldsymbol{r})\, V(\boldsymbol{r}) d\boldsymbol{r} \qquad (1.30)$$

It is apparent from (1.28) and (1.30) that the first born quantities T^{B} and f^{B} are proportional to the Fourier transform of the potential $V(\boldsymbol{r})$. We also note that the first Born differential cross section is

$$\frac{\mathrm{d}\sigma^{\mathrm{B}}}{d\Omega} = |f^{\mathrm{B}}|^2 \qquad (1.31)$$

remains unchanged when the sign of the potential is reversed.

The Born approximation gives satisfactory results at high energy. For the intermediate region, the high energy method can't be used without modification. Thus, impulse approximation, DWA, etc. may work satisfactorily for intermediate energy regions. All experimental results on any microscopic event should have some classical form as experiments are performed with classical equipment. A lot of attempts have been made to find the classical limit of quantum mechanical formalism. No general conclusion has yet been achieved like the transparent reduction of relativistic laws to classical laws in a definite way. For this reason, attempts from Büttiker and Landauer, (1982). Home and Sengupta,(1984). and Bohm and Hiley, (1985) have been made to find the classical limit of quantum mechanical formalism with a view to getting some general conclusion. Regarding accuracy it is very difficult to expect to have very accurate results in comparison to the results obtained in quantum mechanical formalism. However, the theoretical results are found fairly accurate to the experimental data over a certain energy range. In general, the two types of familiar methods are:

- Binary encounter approximation (BEA)
- Classical trajectory Monte Carlo (CTMC) simulation method

1.2.1 Binary encounter approximation

In binary encounter approximation target electrons are considered as free particles, before collision; having a velocity distribution which is characteristic of the binding forces. Mutual interaction between the atomic electrons and nucleus is disregarded during the collision. The target nucleus and the other bound electrons behave like spectators. This assumption is known as impulse hypothesis. Bates and Kingston (1970) discussed the validity of BEA in the case of proton impact for wide range of impact energy. Percival(1966) and Vriens (1966) have pointed out that a necessary condition for ionization is that the energy transferred to the bound electron is greater than the binding energy. From a number of theoretical works done by different workers are in favor of using binary encounter theory (BET) for calculating ionization cross section are:

(a) The great simplicity and wide applicability of related formulae.

(b) Such formulae give reasonable estimates (within a factor of 2) of ionization cross sections over a significant range of energies of the incident particles.

(c) The binary encounter theory gives a correct description of the close collisions. The argument against application of the binary encounter or classical theory is that the distant collisions are not described correctly.

1.2.2 Monte Carlo simulation method

The classical trajectory Monte Carlo (CTMC) procedure is basically a treatment of three body problems viz: the projectile ion, active electron and the target core in the three-dimensional framework. Monte Carlo simulation method takes account of the dynamics on the whole system where time evolution of the system is determined by some laws of classical mechanics. In some cases, the classical limit of quantum mechanical formalism reduces to ensemble interpretation. So, we may expect that, if we solve any problem in classical formalism in an ensemble environment we may get some meaningful results. We believe that this is the main theme of CTMC method.

Out of the two above mentioned method the Monte Carlo method is quite complex and take much computational time. On the other hand, the BEA has been extensively used for the study of different atomic collision process. This is mainly due to the simplicity of the method.

1.3 Semi-classical and semi-empirical approach

Theoretical calculations of the double ionization cross sections becomes quite complicated as it involves the consideration of the four charged particles in the final channel interacting through the long range Coulomb potential. Sophisticated calculations of the double and higher multiple ionization cross sections of atoms and ions by electron impact are not available in literature. As a consequence of this, semi-empirical and semi-classical approaches have been developed for calculation of multiple ionization cross sections.

The semi-classical methods are used in an attempt to circumvent the formidable theoretical problems by making classical approximations to the quantum scattering problem. In some-classical methods an attempt is made to improve their accuracy by the use of adjustable parameters determined by comparison of the basic theory to known ionization cross section data. The use of classical mechanics with the incorporation of certain features of the quantal treatment to describe electron impact ionization is useful.

According to Rudge (1968) following three basic approximations are used in treating electron impact ionization by classical methods:

(a) A classical description must be considered for the initial state of the bound electron. Several descriptions have been used assuming the electron to be at rest or to have a fixed velocity or to have some prescribed velocity distribution.

(b) The collision has to be described in the frame of classical laws of motion.

(c) Even for the simplest case, (e.g. $\mathrm{H} + e^{-} \rightarrow \mathrm{H}^{+} + 2\,e^{-}$) the collision is three body problem. In most treatments the collision process has been described as though it were a two body like binary encounter approximation.

Total and partial cross sections for single electron capture by H^{+} impact on Mg atoms have been calculated by Amaya-Tapia et al.(2001) using semi-classical impact parameters.

The general goal of empirical and semi-empirical formulae is to represent observed cross section data by a relatively simple expression containing a few parameters determined largely from experimental data. Because of the great need for reasonable estimates of ionization cross section functions and scarcity of accurate data, a number of empirical formulas for the ionization cross section function have appeared in the literature as reported by Percival (1966), Lotz (1967, 1970), Rudge (1968), Burgess, A and Percival, I.(1976).

Deutsch et al. (1993) extended the semi-classical Detusch and Mark (1987) formalism (DM) to study the double and triple ionization. The DM formula for the total ionization cross section (σ) of an atom is given by

$$\sigma = \sum_{\mathrm{nl}} g_{\mathrm{nl}} \pi (r_{nl})^2 \xi_{\mathrm{nl}} f(U) \tag{1.32}$$

where $(r_{\mathrm{nl}})^2$ is the mean square radius of the nl-shell, ξ_{nl} is the number of electrons in the nl-shell, g_{nl} is a weighting factor and $f(U)$ is a energy dependent function. Later on, Deutsch and Mark (1987) modified the equation (1.32) as follows

$$\sigma^{m+} = g^m \sum_k \pi (r_k)^2 \xi_k f_k(U) \tag{1.33}$$

The summation extends over the various sub shells with $k = 1$ referring to the outermost sub shell, $\mathrm{k} = 2$ to the second outermost sub shell etc. The weighting factor g^{m} are different from g_{nl}. The energy dependent function $f_{\mathrm{k}}(U)$ are different for contributing sub-shells. Belenger et al.(1997) reported semi-empirical formula for calculation of double ionization cross sections for neutral atoms, positive and negative ions.

1.4 Different theoretical models used in calculating cross section

1.4.1 Rutherford cross section

The scattering of charged particles has been under the scope of scientists since the beginning of last century. Scattering in Coulomb field is of particular interest for physists that study charged particles interactions. Experiments on scattering of alpha particle on numerous targets have played an important role in the development of atomic models. Rutherford formula is correct both in classical theory and quantum except for scattering of identical particles. Consider a case of collision of a particle with charge $Z_1 e$ with a free electron.The interaction of collision is described by

Rutherford cross section in terms of energy distribution of the ejected electron given as

$$\frac{\mathrm{d}\sigma(W,T)}{\mathrm{dW}} = \frac{4\pi a_0^2 Z_1^2 R^2}{T\mathrm{W}^2} \tag{1.34}$$

where W is kinetic energy of the ejected electron, a_0 is Bohr radius 5.29×10^{-11} m, R is the Rydberg energy (13.6 eV) and $T$is the non-relativistic kinetic energy of incident electron defined by $T = mv^2/2$, with the relative speed $v$and the electron mass$m$regardless of the actual mass of the projectile. It is seen that the equation diverges for $W \to 0$, although we know that for a real atom, the cross section for ejecting an electron with $W = 0$ is finite. To overcome this difficulty we replace W by the energy transfer $E = W + B$ where B the binding energy of the ejected-electron. With the substitution, the Rutherford cross section becomes

$$\frac{\mathrm{d}\sigma(W,T)}{\mathrm{dW}} = \frac{d\sigma}{dE} = \frac{4\pi a_0^2 Z_1^2 R^2}{T\mathrm{E}^2} \tag{1.35}$$

1.4.2 J. J. Thomson model

The earliest treatment of ionizing collisions using the classical Binary encounter approximation was done first by Thomson assuming that the target electron is at rest. Thomson (1912) used classical mechanics to derive an expression for the atomic electron impact ionization cross section.

Collision of electron with atom, the transfer of energy ε from the incident electron 1 (say) to a bound electron 2 (say) is equated to the energy transfer between two free electrons. It is assumed that during the period of interaction between these electrons, the other electrons and the nucleolus plays no role. A necessary condition for this is that the period should be short compared with the orbiting time of atomic electron 2. This condition is easier to satisfy for collision with large energy transfers, occurring in ionizing collisions. For large energy transfer the binary encounter takes place in a region which is small relative to the size of atom.

J. J. Thomson used classical mechanics to derive an expression for the atomic electron impact ionization cross section. Consider a Coulomb-collision between a particle of mass m_1 and charge $Z_1 e$ with initial kinetic energy E_1 and a particle of mass m_2 and charge $Z_2 e$ with initial kinetic energy $E_2 = 0$. The cross section for energy transfer in range $\varepsilon_1 \leq \varepsilon \leq \varepsilon_2$ can be given as

$$Q(\varepsilon_1, \varepsilon_2) = \pi Z_1^2 Z_2^2 \frac{m_1 e^4}{m_2 E_1} \left[\frac{1}{\varepsilon_1} - \frac{1}{\varepsilon_2}\right] \tag{1.36}$$

In the case of collision between two electrons, $Z_1 = Z_2 = -1$ and $m_1 = m_2 = m$ and we consider $U \leq \varepsilon \leq E_1$ and obtain Thomson`s ionization cross section

$$\frac{\pi e^4 N}{E_1}\left[\frac{1}{U} - \frac{1}{E_1}\right] \tag{1.37}$$

where N is the effective number of electrons in the atom and U is the ionization energy of the atom.

1.4.3 Thomas and William model

Thomas (1927) and William (1927) generalized the case of Thomson`s model supposing $E_2 \neq 0$. They considered symmetrically distribution of velocity of the atomic electrons. Thomas (1927) obtained result of cross section dQ (p, ε) for energy transfer between ε and $(\varepsilon + \mathrm{d}\varepsilon)$ and simultaneous momentum transfer between p and $(p + \mathrm{dp})$. For the case of $m_1 = m_2 = m$ and $Z_1 = Z_2 = -1$;$\varepsilon > 0$ the energy transfer cross section finally can be given as (Burgess and Percival, 1968)

$$\frac{\mathrm{d}Q(\varepsilon)}{\mathrm{d}\varepsilon} = \frac{\pi e^4}{E_1}\left[\frac{1}{\varepsilon^2} + \frac{4E_2}{3\varepsilon^3}\right] \tag{1.38}$$

Since the binary encounter take place effectively in a small region, Thomson also introduced an idea that the incoming particle should gain kinetic energy by interacting with the nucleus and electrons in the atom. Younger and Märk (1985) gave an expression of cross section for general case $Z_1 \neq Z_2$ and $m_1 \neq m_2$ as

$$\frac{\mathrm{d}Q(\varepsilon)}{\mathrm{d}\varepsilon} = \frac{\pi e^4 Z_1^2 Z_2^2 m_1}{m_2 E_1}\left[\frac{1}{\varepsilon^2} + \frac{4E_2}{3\varepsilon^3}\right] \tag{1.39}$$

1.4.4 Mott cross section

Mott (1930) generalized the Rutherford cross sections for collision between two electrons by taking exchange into account. New progress was made when Mott derived the quantum mechanical cross section formulae for Coulomb scattering of identical particles in both the center of mass system and the coordinate frame in which one of the particles is initially at rest. The Mott cross section is given in the form of singly differential cross section (SDCS) or energy distribution of the ejected electron. The generalized formula for non-relativistic case is

$$\frac{\mathrm{d}\sigma(W,T)}{\mathrm{d}W} = \frac{4\pi a_0^2 Z_1^2 R^2}{T}\left[\frac{1}{W^2} - \frac{1}{W(T-W)} + \frac{1}{(T-W)^2}\right] \tag{1.40}$$

This is an exact solution for the collision of two free electrons. Here, $T$is the kinetic energy of incident electron, $(T - W)$ is kinetic energy of the scattered electrons and$W$is the kinetic energy of ejected electron. Since the scattered and ejected electrons are indistinguishable the faster one is called primary electron and slower one is called secondary electron after collision. The first term in the square brackets in above equation is the direct collision term, the second term represents the interference term (between the direct and exchange collision) and third term is the exchange collision term. The binding energy must be overcome for a bound electron to be ejected. Keeping this fact in mind, Mott ionization cross sections are modified by replacing W by energy transfer$E = W + B$, where B binding energy of the ejected electron. Modified Mott cross section for a sub shell is obtained by replacing W by E and T by $(T + B)$

$$\frac{\mathrm{d}\sigma(W,T)}{\mathrm{d}W} = \frac{\mathrm{d}\sigma}{\mathrm{d}E} = \frac{4\pi a_0^2 \mathrm{NR}^2}{T}\left[\frac{1}{E^2} - \frac{1}{E(T-W)} + \frac{1}{(T-W)^2}\right] \tag{1.41}$$

where N is the number of bound electrons in the sub-shells.

This is an approximation for a bound target electron and becomes a good approximation for ejecting a fast electron only when $W \gg B$ i.e. when the kinetic energy of ejected electron is much greater than its binding energy.

1.4.5 Gryzinski's theory

In the beginning theoretical studies on applications of the BEA were carried out by Gryzinski (1965a,b,c). Interest in the binary encounter theory was revived after the work of Gryzinski, who obtained classical relations for Coulombic collision of two moving charged particles and applied them for theoretical studies of variety of charged particle atom collision processes. In Gryzinski's theory the atomic electrons are assumed to have a distribution of velocities or a single average velocity. He developed a theory giving excitation and ionizations cross section. The excitation cross section is for a transition to a principal quantum level (n) not to the individual sublevels. Gryzinski assumed $s - s$ transitions to take place only by the exchange process.

Gryzinski improved the Thomson's equation by assuming a continuous velocity distribution for the atomic electron leading to the following expression (Younger and Märk, 1985)

$$\sigma = \sum 4\pi a_0^2\, N_n \left(\frac{E_{\mathrm{i}}^{\mathrm{H}}}{E_{\mathrm{in}}}\right)^2 f(u) \tag{1.42}$$

where

$$f(u) = \frac{1}{u}\left[\frac{(u-1)}{(u+1)}\right]^{3/2}\left[1+\frac{2}{3}\left(1-\frac{1}{2u}\right)\text{In}\{2.7+(u-1)^{1/2}\}\right] \quad (1.43)$$

and a_0 is the Bohr`s radius, N_n is the number of electrons in the n^{th} sub shell, E_{in} is the ionization potential of n^{th} sub-shell, E_{i}^{H} is the ionization potential of the hydrogen atom and $u = E/E_{\text{in}}$, where E is the incident potential energy.

Further improvement in the theory requires the incorporation of the quantum factors such as exchange and interference effects. Vriens (1969) modified the Gryzinski's theory and incorporate the quantal effects of exchange and interference.

1.4.6 Binary encounter cross section

In the binary encounter theory (BET) an incident electron is supposed to interact with only one of the atomic electrons at a time and the cross sections for the electron-atom collisions are obtained by integrating the cross sections for the binary encounter collision between incident and atomic electrons over the momentum distribution of the atomic electron. To better describe the ionization of an atom by an electron, Vriens, following the work of Gryzinski, proposed that the target electron should be assigned a velocity or momentum distribution to represent its orbital motion. Such momentum distribution is derived from bound electron wave function.

As derived by Vriens (1969), the expression consists of direct, exchange and interference terms. The expression of symmetric form of the (for the primary and secondary electrons) binary encounter cross section can be given as:

$$\frac{\text{d}\sigma(W,T)}{\text{dW}} = \frac{4\pi a_0^2 \text{NR}^2}{(T+U+B)}\left\{\frac{1}{E^2} - \frac{1}{E(E-W)} + \frac{1}{(T-W)^2} + \frac{4U}{3}\left(\frac{1}{E^2} + \frac{1}{(T-W)^3}\right)\right\} \quad (1.44)$$

Deriving the binary encounter cross section for the collision between two electrons we can, from first principle, arrive at an exact solution for a collision between an incident electron with kinetic energy$T$and atarget electron with an average kinetic energy U which equivalent to ionization potential energy [= $\text{p}^2/(2m)$], where P is momentum operator in a given sub-shell and rest symbols have usual meaning as in Section 1.4.4.

1.5 Justification of classical approximation for charged particles-atoms/ions collision

The use of classical approximation in the studies of atomic scattering problems is based on the following grounds.

1.5.1 Rutherford scattering identity

Rutherford (1911) postulated that all the positive charge and almost all the mass of an atom is concentrated in a positively charged nucleus of very small dimension ($\approx 10^{-14}$ m) compared with the dimension of the whole atom ($\approx 10^{-10}$ m). The prediction of Rutherford's theory of α particle scattering, based on this nuclear atom model, was fully confirmed further by Geiger and Marsden(1913). It is a special feature of the coulomb interaction that classical mechanics yields differential cross sections identical to quantum mechanics for the Coulomb scattering of two non-identical particles. When identical particles are involved, the two results differ because of contribution from the interference between the direct and exchange terms in quantum mechanical description of the process. Rutherford's identity does not directly apply to the processes involving interaction between three or more particles.

1.5.2 Correspondence principle

The correspondence principle was introduced by Bohr in 1923. It is an effort to make use of classical theory as a limiting case of quantum theory to infer some properties of atomic systems. In other words, classical physics results are macroscopically correct and may be considered as limiting cases of quantum mechanical results when the quantum discontinuities may be neglected.

The connection between quantum mechanics and classical mechanics is provided by correspondence principle. It states that whenever the action variables associated with the systems and their changes are large in comparison to Planck's constant, the classical mechanics can be used to a good approximation. Consequently, classical methods can be used for the study of collisions between atoms and simple molecules in the absence of any resulting transition between the electronic states. Further classical methods can also be used for the study of collisions involving highly excited atoms and ions for large change in quantum numbers. In this connection it is worthwhile to mention that specific quantum phenomena such as interference, resonance etc. cannot be explained in terms of classical theory alone and small modifications are necessary to incorporate such effects approximately in the classical calculations. The binary encounter approximation has been used with great simplicity for the study of various collision processes. In the next chapter, more detail discussion on the binary encounter approximation has been presented.

1.6 Motivation

Theoretical knowledge of ionization cross section and collision dynamics find wide application in different fields of science such as Display technology, Aerospace industry, Astrophysics, Nuclear Astrophysics, Stellar model, Radiative process in the earth's upper atmosphere, Medical application and many more.

With suitable theoretical description one can predict reliable values of cross sections of different atoms/ions. Closeness of theoretical results provides physics behind the experimental data of particular target atom. When experimental and theoretical results are not available an approximate formulas is used to generate data of cross sections. In order to calculate cross sections of atoms and ions by the impact of light and heavy charged particles different types of theoretical as well as experimental works are available in literature.

Theoretical calculations based upon quantal treatment are very sophisticated and it fails to calculate the cross sections in case of heavy particles. Several quantal approximations have been successfully developed for accurate calculation of electron impact single ionization cross sections of atoms/ions. In the case of double ionization cross section the situation is less satisfactory and is confined to helium and helium-like ions. In the beginning, electron impact integrated double ionization cross sections in the Born approximation were reported for a few light targets e.g. H^+, He and Li^+ (McGuire et al., 1981; Tweed, 1973). In recent past quantal calculations of double ionization cross section of multi-electron systems have become available in the literature. Pindzola et al. (2009) carried out calculations of electron impact double ionization cross sections of Ba atoms. Later on Pindzola et al. (2010) calculated electron impact direct double ionization cross sections of Mg for simultaneous ejection of 3s electron using a non-perterbative time-dependent close coupling method. Indirect contributions to double ionization, involving the ionization of 2p and 2s electrons followed by auto ionization, have been calculated using a perturbative time independent distorted wave method. The direct and indirect ionization cross sections are found to be in good agreement with experiments at low and high impact

energies respectively. Recently, Pindzola et. al.(2011) has reported calculations of electron impact double ionization cross sections of B^+ ions. The process of DDI in which the incident electron simulates the simultaneous emission of two electrons results in a four-body Coulomb problem in the final channel. Due to mathematical complexities and extremely heavy computational task, ab-initio theoretical investigation of electron impact direct double ionization cross sections of atoms/ions remains a challenging problem. Therefore, as the degree of ionization increases, the problem becomes complicated in solving the wave functions quantum mechanically.
Difficulties in carrying out sophisticated calculations quantum mechanically, the BEA can be considered to provide a suitable theoretical description of the double ionization process. In the past, BEA has been used successfully in the calculations of charged particle impact single and double ionization cross sections for several atoms and ions. Further, the success of the work by (Roy and Rai, 1973, 1979), Kumar and Roy (1977, 1978, 1979, 1981), Tan and Lee (1981), Shrivastava and Roy(1984) and Minakshi et al. (2009) supported this conclusion.Keeping in view the facts mentioned above we are motivated to calculate the ionization cross section of different atoms via different processes using BEA.

1.7 Objectives

Despite of detail theoretical knowledge of collision dynamics our main objectives in the present thesis are as follows:

1. To Study single and double ionization cross sections of Kr and Xe by electron impact.
2. To Study single and double ionization cross sections of Fe by electron impact.
3. To Study single and double ionization cross section of Cu and Fe by H^+ and He^{2+} impact.

1.8 Brief account of the problem undertaken

Different theoretical models are used to calculate ionization cross sections of various atoms depending upon range of impact energy and nature of colliding particles. Keeping in view, we have carried out theoretical calculations of ionization cross section under binary encounter approximation (BEA). Accurate expressions of $\sigma_{\Delta E}$(cross section for energy transfer ΔE) given by Vriens (1969) and Hartree-Fock velocity distributions for the target electrons have been used throughout the calculations.

Our theoretical work of electron impact single ionisation cross sections of Kr and Xe is compared with the experimental work carried out by Rejoub et.al. (2002) and electron impact single and double ionization cross sections of Fe is compared with experimental work of Shah et al.(1993).Further proton and alpha particles impact single and double ionization of Cu and Fe are calculated theoretically and compared with the experimental data available in the literature of Patton et al. (1995). Since no theoretical works are available till date the experimental results mentioned in the above papers are compared with our theoretical calculated results using Vriens symmetrical model and the model modified by Roy and Rai (1979). In Chapter1, the theoretical background of scattering cross sections and different theoretical methods used in the calculation of cross sections of various atoms and ions and charged particles have been described. Further, motivation and objective about the present work is given at the end of this chapter. In Chapter 2, the description for the justification of the use, its development and validity along with the description of different types of calculation have been presented. At the end of this chapter, the literature survey and further development of this field have been discussed. In Chapter 3, the thesis contains the theoretical methodology of electron impact single and double ionization of Kr, Xe and Fe . Beyond this the methods of calculation of proton and alpha particle impact single and double ionization of Fe and Cu have been discussed. In Chapter 4, result and discussion of the above-mentioned calculation have been presented and discussed in detail. The above mentioned are the brief descriptions of the problem undertaken.

CHAPTER 2

2. LITERATURE REVIEW

2.1 Many electrons Schrödinger equation

Quantum mechanics employed the conceptual framework which drastically differs from that of classical physics and makes a genuine revolution in our understanding of the physical world. Just like Newton's second law in classical physics, the Schrödinger equation is the corner stone in quantum physics (Afnan, 2011). The mathematical equation that describes the time evolution of a physical system in which quantum effects, wave particle duality are significant is called the Schrödinger equation.

Properties of a material strongly depend on the electrons in the system and need to be addressed by quantum mechanical methods. The way to govern the problems related to the electronic structure of the matter is the Schrödinger equation including the time, developed by a German physicist Erwin Schrödinger (1887-1961). But, in our case we only concern on atoms and molecules but not on time interaction. Thus we only focus on the time independent Schrödinger wave equation. The main vision of most quantum mechanical phenomenon is obtaining the approximate solution of the time independent, non-relativistic Schrödinger wave equation. Therefore, the Schrödinger equation is the basic relationship for determining wave functions and energy levels. We apply it to several systems including H atom and other atoms and molecules having many electrons and nuclei. The essential feature of this theory is to describe the behavior of atomic systems and their interaction with other particles and electromagnetic radiation.

The Schrödinger equation is the conventional point to begin the description of many electron systems. For stationary state problems, the Schrödinger equation for the system of many electron and nuclei in mutual interaction can be expressed as:

$$\overrightarrow{H}|\psi\rangle = i\hbar\frac{\partial|\psi\rangle}{\partial t} = E|\psi\rangle \tag{2.1}$$

where $\overrightarrow{H}$ represents the Hamiltonian of an N electrons system and can be written as (in Hatree units)

$$\vec{H} = -\sum_{I=1}^{N_e}\frac{\nabla_I^2}{2M_\mathrm{I}} - \sum_{i=1}^{N}\frac{\nabla_i^2}{2m} + \frac{1}{2}\sum_{ij}\frac{1}{r_{ij}} + V_\mathrm{el}(\{r_i\},\{R_I\}) + V_\mathrm{II}(\{R_I\}) \tag{2.2}$$

The notation used can be expressed as

$$\vec{H} = \vec{T}_\mathrm{N} + \vec{T}_\mathrm{e} + \vec{V}_\mathrm{int} + \vec{V}_\mathrm{ext} + \vec{V}_{II} \tag{2.3}$$

such that,

$$\vec{T}_\mathrm{N} = -\sum_{I=1}^{N_e}\frac{\nabla_I^2}{2M_I} \qquad \text{K E of nuclei } \left(\mathrm{i^{th}} \text{ ion core having a mass } M1\right)$$

$$\vec{T}_\mathrm{e} = -\sum_{i=1}^{N}\frac{\nabla_i^2}{2m} \qquad \text{KE of electrons } \left(\mathrm{i^{th}} \text{ valence electron with mass } m\right)$$

$$\vec{V}_\mathrm{int} = \frac{1}{2}\sum_{ij}\frac{1}{\left[r_i - r_j\right]} \qquad \text{electron} - \text{electron interaction energy}$$

$$\vec{V}_\mathrm{ext} = -\frac{1}{2}\sum_{ij}\frac{Z_I e^2}{\left[r_i - R_I\right]} \qquad \text{ion} - \text{electron interaction energy}$$

$$\vec{V}_\mathrm{II} = \frac{1}{2}\frac{1}{\left[R_I - R_J\right]} \qquad \text{ion – ion interaction energy}$$

Hence the terms V_II and V_el are the Coulomb interactions between the ion-ion and between the electron and ion respectively, r_{ij} is the distance between the i^th and the j^th electron. The term V_ext makes the term inseparable. The energy term related to the spin and magnetic moments of the particles in the interaction are omitted. The analytical solution of this equation is tedious and almost impossible for larger systems. Mathematical solution of single atom and very small molecules are available. In order to solve this equation analytically, some reasonable and well controlled approximation has to be made so that we can able to handle most of the systems. Some of the important approximations are explained below.

2.2 Born-Oppenheimer approximation

The Born–Oppenheimer approximation (BOA) is based upon the fact that the mass of an atomic nucleus in an atom is much larger than the mass of an electron. Because of such difference in masses, the electron moves much faster than that of the nucleus. Since electron and nucleus have opposite charges, there exist mutual attractive forces (e^2/r^2) between them which cause both the particles to be accelerated. So acceleration produced in the electron is much larger compared to the nuclei. To describe the electronic states of the atoms or molecules, one can make a good approximation by assuming that nuclei are not moving or supposed to be being stationary. So, instead of solving the Schrödinger equation for a collection of mobile electrons and nuclei, one can solve it for electrons only moving in the stationary potential generated by the frozen nuclei.

The equation above is complex and crucial to solve because it deals with a large number of interacting ions and electrons having different masses. The first step towards the simplification of the above equation is the Born-Oppenheimer approximation. As we know ions are much heavier than electrons and they move much slower compared to electrons and hence the electrons respond instantaneously to any external effect. The electronic and the ionic degrees of freedom can be decoupled and the electronic properties can be calculated by assuming that the ions are fixed to a particular configuration. Following this approximation, the kinetic energy of ions can be neglected and the ion-ion interaction is assumed to be constant i.e., frozen core approximation (FCA). So under BOA, the many body Hamiltonian for a system of N interacting electrons moving in the field of fixed ion cores can be expressed as,

$$\vec{H} = -\sum_{i=1}^{N}\frac{\nabla_i^2}{2m} - \frac{1}{2}\sum_{i,j}\frac{1}{[R_I - r_{ij}]} + \sum_{i>j}\frac{1}{[r_i - r_j]} \tag{2.4}$$

Schrödinger equation for the electrons (for the given position of the ion- core R_I) can be written as

$$\left[-\sum_{i=1}^{N}\frac{\nabla_i^2}{2m} + V_{\mathrm{el}}(\{r_i\}|\{R_{\mathrm{I}}\}) + \frac{1}{2}\sum_{ij}\frac{1}{[r_i - r_j]}\right]\psi(\{r_i\}|\{R_{\mathrm{I}}\})$$

$$= E_{\mathrm{e}}(\{R_{\mathrm{I}}\})\psi(\{r_i\}|\{R_{\mathrm{I}}\})\psi \tag{2.5}$$

It is not possible to get exact solution from the equation and hence different approximations are needed to simplify the Schrodinger equation.

2.3 Central field approximation

An atom, in general, consists of a large number of electrons and dynamics of these particles in general cannot be considered separately. We assume that nucleus is fixed in a given configuration so that one can focus on electronic dynamics. We can obtain a good approximate description of a many-electron atom by supposing that each electron moves independently in an average potential due to the nucleus and the other electrons. This independent particle model reduces many-electron problem to independent single electron problem. The concept or assumption in which potential around nucleus is assumed spherically symmetric is known as central field approximation (CFA). The central field approximation for many electron atoms takes the combined electric field of the nucleus and all the electrons acting on any of the electrons and to be the same for all the electrons in the atom. That is, every electron sees an identical potential and is only the function of its distance from the nucleus. Among the approaches to the many electron system, we consider the historic Hartree-Fock theory which is based on the concept of self-consistency.

2.4 Binary encounter approximation

The basic idea and assumption of binary encounter theory has been briefly discussed in sub-section 1.2.1. Among classical methods the binary encounter approximation has been found quite suitable for the study of charged particle impact ionization of atoms. On the other side, distorted wave methods are being widely used for quantal calculations of the differential cross section for the study of electron–ion or electron-atom collisions. These methods have been found successful in the investigation of atomic collision processes at intermediate energies.

Formulations of the problem for different collision channels in the framework of BEA have been done separately by Gryzinski (1965a,b,c), Gerjuoy (1966), Stabler (1964). These works have been reviewed by Burgess and Percival (1968) and proceeded further by Vriens (1966, 1967, 1969).The binary encounter model is based on the following two assumptions:

(i) During the collision the incident particle interacts with one target particle usually a bound electron at a time. This is equivalent to the fact that electrons of the target atom are regarded completely independent of each other and they do not interact with each other in course of collision.

(ii) Prior to the collision; target electrons are considered as free particles having a velocity distribution which is characteristic of the target binding forces. Mutual interaction between the atomic electrons and nucleus is disregarded during the collision. This assumption is known as impulse hypothesis. The condition for the validity of the second assumption is that time of interaction between the incident particle and target electron should be small compared to the orbital period of the target electron.

According to the first assumption, the atomic electron and the nucleus are assumed to be independent scattering centre. The effective region of interaction between the incident particle and the target electron is small compared to the atomic dimension. Under this condition, the momentum transferred by the incident particle to one of the target electrons would be larger than the momentum associated with the atomic electrons and the energy transferred would be much larger than the binding energy of the bound electron (Vriens, 1969).

The two steps involved in obtaining cross section in BEA are discussed as below. First of all collision between the incident particle and the target electrons is considered. Next differential cross section for this process is related to the cross section per unit energy and momentum transfer from which the relevant cross sections for different collision processes can be estimated. Using classical mechanics the first step can be treated exactly if the projectile is other than electron. However, approximations are involved when the Coulomb differential cross sections are related with the cross section for the particular collision process between the charged particle and the atom. In this approximation no assumption is made about the position or the orbit of the atom in an atom but knowledge about the velocity distribution of the target electron is required. In this connection it is to be noted that the complete classical theory requires a simultaneous knowledge of position and the velocity of atomic electron. The binary encounter approximation has been found useful in the study of ionization and charge transfer processes.

2.5 Development of the binary encounter approximation

Interest in the binary encounter theory was revived after the work of Gryzinski, who obtained classical relations for Columbic collision of two moving charged particles and applied them for theoretical studies of a variety of charged particle atom collision processes. Besides this, Gryzinski and Kune (1999) introduced some new physical ideas e.g., the concept of double binary encounter between the projectile and the target electrons as a mechanism of double ionization of the target and the idea that a single binary encounter between the incident particle and the bound electron, with energy transfer lying between two specified limits, may also lead to electron capture. Gryzinski's ideas have been applied and extended successfully by various workers to investigate different types of collision processes. After publications of Gryzinski's works some errors and unrealistic assumptions were detected in his theoretical expressions. In case of electron impact, Vriens (1966) obtained accurate expressions of $\sigma_{\Delta E}$ and ionization cross sections in symmetrical model including exchange and interference for atomic and ionic target. Later on he derived correct expressions of $\sigma_{\Delta E}$ and ionization cross sections for bare ion impact (Vriens, 1967). Thomas and Garcia(1969) have modified the binary encounter model of ionization by charged particles to evaluate electron impact ionization cross sections of positive ions. The development and applications of the BEA have been presented in the review articles by Burgess and Percival (1968), Vriens (1969), Bates and Kingston (1970), Garcia et al. (1973).Use of accurate quantum mechanical velocity distribution in the BEA improves the results of collision cross sections but fails to exhibit high energy dependence of cross sections. This high energy dependence is due to contribution from the distance encounters (Burgess and Percival, 1968) which is not taken in classical impulse approximation.

Despite use of quantum mechanics in calculation of electron impact single ionization cross sections of atoms and ions, some interesting BEA studies of this process have been reported with reasonable success. In a large number of cases experimentally observed single ionization cross section curves shows structure which has been attributed, in most cases, to the excitation of an inner shell electron to an auto ionizing state of the system and its subsequent ionization. Contributions of this indirect mechanism to electron impact single ionization cross section have been incorporated in the BE calculations by Roy and Rai (1973) in the case of alkaline earth ions. In all these calculations Vriens (1966) expression for ionization cross section has been used along with Hartree-Fock momentum distribution for the bound electron. In addition to the theory of single ionization, Gryzinski has also described a method for calculation of charged particle impact double ionization cross sections of atoms. Roy and Rai

(1977) proposed a modified binary encounter model for calculation of proton impact double ionization cross sections of atoms and Chatterjee and Roy (1987) have studied electron impact double ionization of Ar^{2+}, Ar^{3+} and Xe^{+} in BEA. In the case of bare ion impact, Kumar and Roy (1977) used successfully the binary encounter expression developed by Vriens (1967) along with accurate quantum mechanical velocity distribution for the bound electron in both encounters to obtain proton impact double ionization cross section of helium. Later on electron impact double ionization cross sections based on the modified model of Roy and Rai (1973) including contributions of indirect physical processes were found to be in close agreement with experimental data. Hartree-Fock and hydrogenic velocity distributions were used while considering the ejection of the first and second target electron respectively.

It is worthwhile to discuss the development in calculations of bare ion impact ionization of atoms in the BEA. In the recent past Minakshi et al. (2009) calculated single and double ionization of Pb by H^{+} and He^{2+}impact and results calculated for H^{+} impact single and double ionization are found in good agreement with experimental data but in the case of He^{2+}impact limited success is observed probably due to the fact that the experimental results are confined to low energy region only.

Charge transfer and transfer ionization is also one event in the atomic collision process where electron get captured either by projectile or positively charged target. In the beginning Thomas (1927) applied the classical impulse approximation to the calculation of cross section for electron capture from a heavy atom by fast light nucleus. After this work the classical theories remained dormant for more than three decades. The pioneering work of Gryziniski revived interest towards BEA and pure classical collision theories. Several workers carried out the theoretical investigations on ionization and charge transfer processes using the above mentioned theories. In the recent past Pandey et al. (2007) carried out differential, total and partial cross sections of H^{+} and D^{+} ions incident on Mg and Ca atoms using CTMC method in energy range of 1 keV to 100keV. Total capture cross sections are found to be in good agreement with the experimental observations. A remarkable development in the BEA was made by Bates and Mapleton (1967) who modified the theory of Thomas (1927) for electron capture and developed a theory which is capable of explaining the experimental observations to a good extent. Later on Roy and Rai (1979) derived new limits for energy transfer and used in Gryzinski's model which requires only one binary encounter for charge transfer to take place. Further, Kumar and Roy (1979) calculated single electron capture cross sections for nobel gas atoms by H^+ and He^{2+} impact. Tam and Lee (1981) pointed out shortcoming in theoretical approach of Roy and Rai (1979) and introduce some modifications. Later on Chatterjee and Roy (1985) extended binary encounter approach of Tan and Lee (1981) to double electron capture cross sections by light bare ion from heavy atomic targets. He assumed that the projectile is scattered ones by the target and captures one electron via a binary encounter. After this the projectile with its reduced charge is still in the interaction region. It is scattered second time capturing another electron via a second binary encounter resulting in double electron capture process. Their theoretical results of H^{2+} impact double electron capture cross sections of He, Li, Ar and Kr have found in reasonable good agreement with available experimental data and other theoretical calculations.

2.6 Validity of the binary encounter approximation

The validity of any theoretical approach lies in its ability to unveil the mystery of any physical phenomena experimentally observed and consequently depends upon the degree of closeness of theoretical results with the experimental results. The ultimate and utmost goal and success of theoretical formalism for the investigation of scattering phenomena lies in its ability to explain the experimental observations. Exact solutions of atomic collision processes are not possible. Various approximation methods based on physical justification have often been used with rapid development in quantum mechanics. Several quantal approximations have been developed for different energy ranges.

Now we discuss the case of the binary encounter approximations. As we discussed earlier, the main assumption in this approximation is that during the collision of the projectile with the bound electron, the target nucleus and the other bound electrons behave like spectators. The interaction time is considered to be short compared to the orbital time of the bound electron. This condition is easily satisfied if collision involves transfer of large energy and momentum (Burgess and Percival,1968).The use of accurate velocity distribution in the BEA gives reasonable estimates of cross sections for ionization and charge transfer processes. The BE theory is not valid for the excitation cross section. It is because in the classical theory neither energy nor angular momentum quantization can be taken into account. Hence this approximation does not take into account properly the quantization of energy and angular momentum required in the case of excitation. In case of ionization the final state lies in the continuum.

Bates and Kingston (1970) have discussed the validity of the BEA in case of proton impact in energy regions (i) 10 keV to 100 keV (ii) 100 keV to 1 MeV and (iii) 1 MeVto 10 MeV. The charge transfer process is expected to be important in the energy range from 10 keV to 100 keV. Percival and Valentine (1966) have pointed out that a necessary condition for ionization is that the energy transferred to the bound electron is greater than the binding energy. This condition is not sufficient as the ejected electron may become bound to the incident charged particle. Thus the calculated cross sections are found to be higher than the true ionization cross sections and lower than the electron removal cross sections. Total cross section is given by the sum of ionization cross section and electron capture cross sections. Due to this situation one cannot draw a definite conclusion about the suitability of the BEA in this energy region. The binary encounter theory gives reasonably good agreement with experimental data in case of ionization in energy range (ii). The success of the calculations in the energy range (iii) depends on the nature of the target. For lighter target the theory underestimates the cross sections because of the fact that under this condition distant encounters have an important contribution in producing ionization of the target. In the case of heavier atoms the energy range in which the distant collision becomes important shifts beyond 10 MeV and the agreement in the energy range (iii) becomes satisfactory. The arguments in favour of using binary encounter theory for calculating ionization cross section have been discussed in subsection 1.2.1.

Vriens (1969) designed the expression for $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) in the binary encounter approximation using the expression for generalized oscillator strength given by the first Born approximation and assuming that the target electron to be free. He has further shown that the expression for $\sigma_{\Delta E}$ follows from the solution of Schrödinger equation both in the symmetrical and the unsymmetrical model. Starting from the Born approximation, Bates and McDonough (1972) have also given the derivation of the binary encounter approximation. A comparative study of the BEA and Born approximation has been given by Harberger et al.(1973). They have compared the generalized oscillator strength in the Bethe and Binary encounter approximation and studied the effect of velocity distribution for the target electron on the binary encounter cross sections. They conclude that the two approximations give identical results provided the energy and momentum transfer during the collision are large and accurate velocity distribution for the atomic electron is used. Further, they have pointed out that except the binary character of the collision; the binary encounter theory has the same justification as the first Born approximation.

2.7 Gryzinski and Kune model of double ionization

The process of electron-impact double ionization of atoms (e^- + X =3e^- + X^{2+}) is very difficult to describe theoretically since the interaction of the incident electron with the atomic electrons has a collective character. Gryzinski and Kune (1999) presented a general model of electron-impact double ionization of atoms that have atomic numbers $Z \geq 20$.

Gryzinski and Kune (1999) have derived general expression for electron impact double ionization cross sections of atoms using the formalism of the binary encounter approach of the classical impulse approximation with atomic number Z≥ 20 and s or d outer shells with two electrons. The model treats the process of double ionization in the statistical way. There is no consideration of wave function representation of bound electron. However, this model is not applicable in case of Mg where there used wave functions representing the bound electrons as characteristic of the target atom. The process of ionization of an atom by an electron is pictured in the BEA as a result of a superposition of binary encounter of the incident electron with the electrons of the target atom. This is in conflict with the reality of atomic double ionization, where there is encounters of the incident electron with the two 'active' electrons (to be removed from the atom) and the encounter is not binary as encounters are influenced by other atomic electrons..

In addition, there can be several processes (direct ionization, ionization due to excitation–auto ionization, Auger transitions, etc.) of ionization involving the 'active' atomic electrons in the ionization process. Gryzinski and Kune (1999) modified the original approach of the BEA (where the participation of the 'active' electrons in the ionization process is only through their direct ionization) and treat the process of the removal of the two 'active' electrons from the atom in a 'statistical' way.

2.7.1 The model mechanism of the double ionization

According to the idea suggested by Gryzinski and Kune (1999), the double ionization of an atomic target by projectile may proceed via two alternative processes.

(i) The two electrons may be ejected from the atom by two successive encounters of the incident charged particle with the target electrons.

(ii) Alternatively the incident particle may knock out only one electron and the second electron is removed by the second electron. The total double ionization cross section for the target is given by the sum of contributions of double ionization from the two alternative processes (Figure 2).

The electron-impact double ionization of atoms is a result of two consecutive electronic encounters. The transfers of energy to the two particles are also treated in this model in a 'statistical' way. The electron-impact double ionization of an atom proceeds by two 'direct' and 'indirect', mechanisms. The 'direct' ionization consists of two consecutive scatterings (Figure 2a). First the incident electron e of velocity $\boldsymbol{v}$ (kinetic energy$E_k = m_e v^2/2,\ m_e$ is the electron mass) is scattered from one of the atomic 'active' electrons e_1 which has a shell-averaged velocity $\boldsymbol{v}_1$ and a kinetic energy $E_{1,k}$ .The scattering of the electron e from the electron e_1 takes place in the 'collision region I' and it results in ejection of electron e_1 from the atom. The ejected

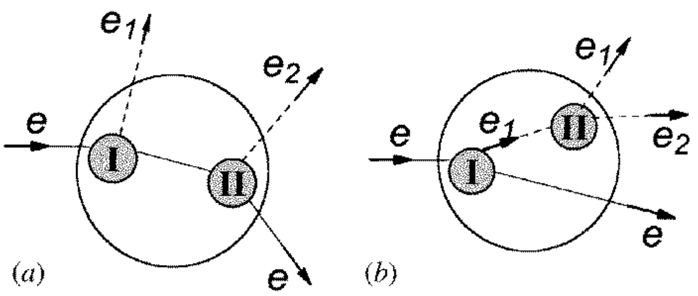

Figure2: Gryzinski-Kun model of double ionization.(a)The'direct'mechanism and (b) the'indirect' mechanism of electron impact double ionization of atoms. (Gryzinski and Kun, 1999)]

electron leaves the atom with velocity $\boldsymbol{v}_1'$and kineticenergy $E_{1,k}$, while the incident electron e leaves the collision region I with some average velocity$\boldsymbol{v}'$and average kinetic energy E_k. In the second scattering, the electron enters the 'collision region II'with the velocity $\boldsymbol{v}'$and collides there with the electron e_2 which has a shell-averaged velocity $\boldsymbol{v}_2$ having shell-averaged kinetic energy $E_{2,k}$. This second scattering results in ejection of the electron e_2 from the atom. The ejected electron leaves the atom with velocity $\boldsymbol{v}_2$ and kinetic energy $E_{2,k}$ while the electron e leaves the atom with velocity v'' and kinetic energy E_k''.

The ‘indirect’ double ionization also consists of two consecutive scatterings (Figure 2b). In the first scattering, the incident electron e is scattered from the electron e_1 in the collision region I, and, as a result, the electron e_1 leaves the region and moves towards the collision region II while the electron e leaves the atom. In the second scattering (taking place in the collision region II), the electron e_1 collides with the electron e_2. This second scattering results in removal of the electron e_2 from the atom. In this model of double ionization of atoms by electron impact, the ‘active’ electrons in the undisturbed atom have Dirac energy distributions. The approach developed in this work applies to atoms with outer shells where the motion of the ‘active’ electrons is confined to s and d shells.

Hartree-Fock and hydrogenic velocity distributions were used while considering the first and second target electrons respectively. Electron impact total double ionization cross section of an atom including the contribution from the Auger emission can be written as

$$Q^{\mathrm{ii}}(T) = Q^{\mathrm{ii}}_{\mathrm{D}} + Q^{\mathrm{ii}}_{\mathrm{A}} \tag{2.6}$$

where $Q^{\mathrm{ii}}_{\mathrm{D}}$ denotes the contribution from direct ejection of the two electrons including contribution from inner shells and $Q^{\mathrm{ii}}_{\mathrm{A}}$ contribution from the Auger emission.

The expressions for cross sections corresponding to the above two processes of the double binary encounter model leading to direct double ionization (when Auger emission is not considered) is given by

$$Q^{\mathrm{ii}}_{\mathrm{D}} = Q^{\mathrm{ii}}_{\mathrm{SC}} + Q^{\mathrm{ii}}_{\mathrm{ej}} \tag{2.7}$$

where $Q^{\mathrm{ii}}_{\mathrm{SC}}$ and $Q^{\mathrm{ii}}_{\mathrm{ej}}$ are double ionizations cross sections under two alternative processes. In the first process, the two target electrons are ejected from two successive encounters by the incident electron denoted by $Q^{\mathrm{ii}}_{\mathrm{SC}}$. Alternatively, the incident electron may knock out only one target electron and the second electron is removed by the first ejected electron denoted by $Q^{\mathrm{ii}}_{\mathrm{ej}}$.The expressions for $Q^{\mathrm{ii}}_{\mathrm{SC}}$ and $Q^{\mathrm{ii}}_{\mathrm{ej}}$ have been integrated numerically over energy transfer and Hartree-Fock momentum distribution for ejection of the two electrons. For example, in the case of gallium, the total cross section for electron impact direct double ionization is given by

$$Q^{\mathrm{ii}}_{\mathrm{D}} = Q^{\mathrm{ii}}_{\mathrm{D}}(4\mathrm{s}, 4\mathrm{p}) + Q^{\mathrm{ii}}_{\mathrm{D}}(4\mathrm{s}, 4\mathrm{s}) \tag{2.8}$$

where $Q^{\mathrm{ii}}_{\mathrm{D}}(4\mathrm{s}, 4\mathrm{p})$ stands for the double ionization cross section corresponding to the one electron ejected from the 4p shell and the other from the 4s shell and $Q^{\mathrm{ii}}_{\mathrm{D}}(4s, 4s)$ stands for ejection of the two electrons from same shell.

2.8 Electron impact single ionization cross section of Kr, Xe and Fe and double ionization cross section of Fe atom

Electron impact ionization of atoms and ions is one of the most fundamental collision processes in atomic and molecular physics. Knowledge of ionization and excitation cross sections is of fundamental importance for understanding collision dynamics and electron -atom interactions, as well as in several applied fields such as radiation science, astrophysics, Auger electron spectroscopy (AES), electron energy loss spectroscopy (EELS). These areas of study need enormous and continuous quantities of data, within a certain accuracy level, for different targets over a wide range of energy values. Electron impact ionization and excitation have been actively studied by many research groups since the 1920's. Most of the work produced was based on classical collision theory and several first principle theories were developed. The most important work in the field of electron-atom collision was made by Bethe (1930) who derived the correct form of the ionization cross section for high-energy collision using the plane-wave Born approximation (PWBA). Since then, several empirical, semi-empirical and semi-classical approximations have been proposed to describe electron impact ionization of atoms and molecules and several reviews on them were published.

Electron-atom collision can be divided into two broad types: soft or distant collisions with large impact parameters and hard or close collision with small impact parameters. The Mott theory (1930) which describes the collision of two free electrons, accounts for hard collisions well but not the soft collision. Bethe (1930) has shown that soft collision takes place essentially through the dipole interaction between the incident particle and the target electron.

In the last one hundred years, the atomic physics community devoted a lot of effort into the study of particle collision. Many methods and approximations derived throughout the times are still used in the interpretation of particle interactions. Till date a large number of investigations dealing with electron impact single ionization of atoms have been carried out. A number of reviews covering the developments in this field in recent years are available. Different quantum mechanical methods have been employed for electron impact ionization by Younger (1981, 1982). To obtain total ionization cross sections for complex targets over a wide range, a number of semi-classical and semi-empirical formulae have also been developed by Younger (1985). An elegant discussion on electron impact ionization of alkali metals have been given by Roy and Rai (1973) and others. There applied plane wave Born approximation (PWBA) to calculate electron impact ionization cross sections for atoms including exchange effect in quintal calculation. In spite of all these successes, the difficulty still lays in the calculation of electron impact single ionization cross sections for heavy atoms in quantal approximations due to mathematical complexities.

The structures observed in the experiments have been clearly explained by different theoretical approaches. Peach (1966) performed a quantal calculation of electron and proton impact ionization of sodium and magnesium and Vainshtein et al.(1971) used the Born approximation and the classical binary encounter theory (BET) to explain the experimentally observed structures for magnesium, calcium, strontium and barium. Though, these calculations have shown good agreement between theory and experiment, the calculations suffer from two deficiencies. First, the Born approximation is not well suited for low incident energy in which the structures are present. Secondly, in case of binary encounter calculations, Vainshtein et al.(1971) has modified Stabler's (1964) expression by considering the acceleration of the incident electron by the field of neutral atom but have used a δ-function velocity distribution for the bound electron and has not taken exchange into consideration. On the other hand, a binary encounter theory for the investigation of electron impact ionization cross sections of atoms has been found to be suitable as it gives reliable results consistent with the experiments. The earlier classical model did not take into account the in distinguishability of the incident and the bound electron (unsymmetrical collision model) and is not reliable at low impact energies. At low incident energies, exchange plays an important role. To remove these difficulties, a more reliable classical formalism of electron impact ionization including the effect of exchange and interference, has been given by Vriens (1966) (symmetrical collision model).Some more calculations on electron impact ionization have been reported by McFarland (1967), Tripathi et al.(1969) and Mann (1967)for the alkaline earths. Roy and Rai (1973) have used symmetrical collision model including exchange and interference to investigate the structures observed in the ionization curves of heavier alkali atoms and alkaline earths. They have used the correct Hartree-Fock velocity distribution for the bound electron to obtain single ionization cross-sections. The contribution of inner cell as well as excitation auto ionization has been explicitly included. The results obtained are in fairly good agreement with the experimental observations.

Keeping the above-mentioned fact in view we have used this symmetrical collision model of Vriens including exchange and interference the semi-classical BEA has been found useful in explaining contribution of inner shell ionization for electron impact single ionization cross sections of atoms. In the present calculations, momentum distribution function for bound electrons has been formulated using Hartree-Fock radial wave functions reported by Clementi and Roetti (1974).

There are some theoretical workers e.g. Chatterjee and Roy (1984, 1987), Roy and Rai (1973), Shrivastava and Roy (1984), Jha and Roy (2000, 2002, 2004, 2006) and Kumar and Roy (1977, 1978, 1979), whose contribution to the development of the BEA and theoretical investigations for ion-atom collision processes are particular important. Various processes can contribute to electron impact double ionization of atoms and ions depending on the incident electron energy and on the structure of parent and intermediate atomic states. For direct ejection of two outer shell electrons, two different types of mechanism are identified: shake off and two state mechanism. In addition, many indirect double ionization processes are associated with the formation of auto ionizing states following inner shells ionization or excitation. In the case of direct double ionization (DDI) via shake off process, the incident electron interacts with a bound electron and ejects it with outer bound electrons being left in the state which is not an eigen state of the residual ion. In the subsequent relaxation process there is finite probability of a second ionization. Electron impact double ionization of atoms and ions is a four particle (one ion and three electrons) problem. In the final channel, these four charged particles interacts with each other via long range Coulomb potential and makes this many body problem extremely difficult. For this reason, it is still impossible to carry out exact calculations for these processes. The full theoretical calculation and detail experimental investigations remain scare in such cases. The most detailed description of the process is given by means of full differential cross sections allowing the analysis of angular and energy distributions for each one of the ejected or scattered electrons.

Experimental investigation of ionization cross section for metals lead to several difficulties and have been carried out by only very few experimental groups for limited number of elements. Accurate experimental measurement of multiple ionization of iron by electron impact have been carried out by Shah et al.(1993) using pulse cross beam technique incorporating time-of-flight spectroscopy of the collision products to study the electron impact ionization of ground state Fe atom within the energy range from respective thresholds to 1250 eV. Experimental data obtained by Shah et al.(1993) would not be compared with previous theoretical calculation of double ionization cross section due to non-availability of the data in the literature.

Freund et al.(1990) performed crossed beam experiment in the presence of meta-stable atom of Fe and measured cross sections that exhibit evidence of contribution from inner shell electrons. Rigorous theoretical calculation of double ionization cross section becomes very complicated as it is related with the consideration of the four charged particles in the final channel interacting through the long range Coulomb potential (Berakdar, 1996). Quantal calculation of the double ionization cross sections of atoms/ions by electron impact have not been reported so far. Belenger et al. (1997) have reported a semi empirical formula for evaluation of double ionization cross section of neutral atoms, positive and negative ions by electron impact and presented results for Cu target. The shape of the cross section is described by analytical expression and approximation parameters are estimated by fitting the model cross sections to reliable experimental data. Besides this, similar methods have been reported by Deutsch et al.(1996). Few attempts have been made to calculate electron impact double ionization cross section for light target e.g., H^+, He and Li^+ using Born approximation (Tweed, 1973; McGuire,1982). In a promising approach the time dependent close coupling method was used by Pindzola et al. (2007) in the calculation of electron impact double ionization of cross section of He. Afterward Pindzola and his coworkers carried out calculations of electron impact double ionization cross section of Mg (Pindzola et al., 2009), Be (Pindzola et al., 2010) and B^+ ion (Pindzola et al., 2011) using a non-perterbative time dependent close coupling method. However, such calculations are restricted so far to essentially two electrons system. Using classical binary encounter approximation (BEA). Gryzinski and Kune (1999) have derived general analytical expression for electron impact double ionization cross section of atoms with atomic number Z $\geq$20 and s or d outer shell with two electrons. They have compared their calculations only with experimental data for Ca, Sr, Ba and Hg atoms and found satisfactory agreement. However, this model is not applicable in case of Fe.

Keeping in view the above-mentioned fact, we have used the semi-classical BE symmetrical collision model of Vriens (1966) including exchange and interference in the present work along with Hartree-Fock velocity distribution for the target electrons. We have also taken into consideration of the inner shells. In the past, the BE approximation has been found successful in the calculation of electron impact single and double ionization of atoms (Jha et al., 2000, 2002, 2004).

2.9 Heavy particle impact single and double ionization cross sections of Cu and Fe atoms

Collision between heavy charged particles, say H^+ or He^{2+}, with target atoms may results pure ionization, excitation, excitation-auto-ionization, electron capture, charge transfer and transfer ionization. Continuous data of ionization cross sections of respective processes have great importance in different fields of science. Proton (H^+) impact ionization from various atoms and molecules has attracted many researchers over many years since it serves important and challenging problem in atomic physics. It is one of the most fundamental process in various applications such as Fusion reactor (Plasma edge process cooling rate estimates), radiation damage in biological matter (including cancer treatment, energy loss of heavy ions in solid targets and ion beam technology (etching and thin film manufacture). Charge exchange reactions in various types of ion-atom collisions are of considerable interest due to their applications in different branches of physics. It plays an important role in controlled thermonuclear fusion development, astrophysics, ion penetration in solids and radiation physics. Charge changing phenomena find applications in the production of vacuum ultraviolet radiation and X-rays and in the study of Solar Corona (Bayfield and Khayrallah, 1975). Since a large number of elements both in neutral and ionic forms exist in the upper atmosphere, the capture processes are particularly relevant to upper atmosphere research (Roy and Rai,1979). Furthermore it is helpful in understanding some auroral phenomena (Basu et al.,1978). Charge exchange processes contribute to the production of negatively charged ions, which play an important role in accelerator technology, particularly in the design of Tandem accelerators (Roy and Rai,1979). Practical applications of single and double electron capture by alpha particles incident on atoms have been discussed by Post et al. (1979). From theoretical point of view physical insight in mechanisms of interaction during charge changing processes is considered to be important. Considerable interest has developed, owing to a number of possible applications, in the studies of single and multiple electron transfer collisions of highly ionized ions with atoms and molecules.

Simplest of all such collisions is He^{2+} incident on some neutral atoms and molecules. Besides contributing to the understanding of certain high temperature systems such as the sun, the solar wind and fusion reactions these processes have some direct applications. It has been proposed by Post et al. (1979) to use single and double electron capture processes in generation of magnetically confined fusion plasmas. From astrophysical point of view the charge exchange in alpha particle-atom collisions is important because the emission spectrum of solar chromospheres contains the spectral line $\lambda = 4686\text{A}^{\circ}$ whose origin has been attributed to the presence of ionized helium formed due to the process of electron capture by fast alpha particles produced in nuclear reactions (Basu et al., 1978).

Correct description of ionization process with high precision, probabilities of other concurrent process, in a particular elastic scattering, target excitation and electron capture to the projectile should be considered simultaneously in low-to-intermediate collision energies. It is not possible to describe one process accurately without treating all on equal footing. It is because ionization is strongly entertained with other inelastic and elastic process. Bare ion impact single and double electron capture cross sections of atoms have been investigated experimentally by many workers and sufficient experimental results are available. Various quantal approximations have been used by a number of workers to calculate single electron capture cross sections but mathematical complexities have prevented applications of such methods to heavy targets. Theoretical studies of double electron transfer processes using different quantum mechanical approximations are also limited to lighter targets only due to complexities involved in theoretical calculation. Various theoretical methods applied in the investigation of charge transfer processes have been critically reviewed by Mapleton (1972) and Belkic and Gayet (1977). Tan and Lee (1981) have also discussed different classical and quantal approximations which have been used in calculations of electron capture cross sections. Full quantum mechanical four body formulations for double electron capture by bare ions from helium atoms have been proposed by Belkic and Mancev (1993) using the continuum distorted wave approximation. Here it is important to mention that electron capture by He^{2+} from molecular targets such as H_2, D_2, N_2, O_2, Co and Co_2 are relevant to many phenomena observed in interstellar space and planetary magnetosphere matter. Much attention has been attracted in recent past to emission of X-ray from some comets whose origin has been interpreted as being due to charge transfer by solar-wind ions from cometary gases. Kusakabe et al. (2006) and de Silva et al. (2007) have reported their experimental observations of single and double electron capture cross sections for He^{2+} impact on a number of molecular targets. Theoretical studies of such processes using close coupling method have been carried out by Shimakura et al. (1993) and Kusakabe et al. (2006). These results have been compared with the experimental observations by Kusakabe et al. (2006) and de Silva et al. (2007).

Now we like to discuss the developments in the BEA for the study of charge transfer processes. In the beginning Thomas (1927) applied the classical impulse approximation to the calculation of cross section for electron capture from a heavy atom by fast light nucleus. Several workers carried out the theoretical investigations on ionization and charge transfer processes using modified Gryziniski's model. In a remarkable development in the BEA Bates and Mapleton (1966, 1967) modified and improved the theory of Thomas (1927) for electron capture and developed a theory which is capable of explaining the experimental observations to a good extent. This theory like the original theory of Thomas requires two binary encounters to explain electron capture and is akin to a second order process. Later on Roy and Rai (1979), based on Thomas classical theory of electron capture, derived new limits for energy transfer to be used in Gryzinski's model which requires only one binary encounter for charge transfer to take place. They adopted an empirical procedure to determine the maximum value of the angle between the directions of the incident ion and the ejected electron, which may still permit capture to take place. Single electron capture cross sections for noble gas atoms due to H^+ and He^+impact were calculated by Roy and Rai (1979) and Kumar and Roy (1979) respectively. After the publication of these results Tan and Lee (1981) pointed out shortcomings in the theoretical approach of Roy and Rai (1979). They introduced some modifications. Instead of using an empirical method as applied by Roy and Rai (1979) Tan and Lee (1981) used Thomas condition for electron capture. The Thomas condition of electron capture is satisfied even if the energy transferred by the projectile to the target electron is smaller than ΔE_l (lower limit of energy transfer). Their calculated results of H^+ and He^+ impact single electron capture cross sections for N, O and the noble gas atoms showed satisfactory agreement with the experimental data. Later on Chatterjee and Roy (1985) extended the binary encounter approach of Tan and Lee (1981) to calculation of double electron capture cross sections by light bare ion from heavy atomic targets. In this context they applied Gryzinski's (1965c) double binary encounter idea to describe direct double ionization of atoms. In their work Chatterjee and Roy (1985) assumed that the projectile is scattered once by the target and captures one electron via a binary encounter. After this the projectile with its reduced charge is still in the interaction region. It is scattered second time, capturing another electron via a second binary encounter, resulting in double electron capture process. Their theoretical results of He^{2+} impact double electron capture cross sections of He, Li, Ar and Kr have been found in reasonable good agreement with available experiments and other theoretical calculations. During last two decades remarkable experimental investigations on H^+ and He^{2+} impact pure single and multiple ionization, pure single and double electrons capture (in case of He^{2+}only), and transfer ionization cross sections of atoms have been carried out by the Belfast group (Shah et al.,1992).

In the past BEA has been used successfully by many workers to calculate charge particle impact single ionization cross sections of several atoms and ions. There used accurate expression for $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) given by Vriens (1967) and Hartree-Fock velocity distribution. Recently, Minakshi et al.(2009) has calculated H^+ and He^{2+} impact single and double ionization of lead and satisfactory results were obtained. A general used approach for interaction of the multiple ionization processes is the independent particle model (IPM). It is assumed that the ionization of one electron is independent of the other and the relative probability are given by binomial distribution (McGuire, 1982; Kirchner et al.,1999; McGuire et al., 1981). 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 (Sant Anna et al. 1998). An alternative theoretical approach to the IPM is the statistical energy distribution model. This model has also been used by several authors (Russek and Thomas, 1958 , McGuire et al., 1981) and further developed by Kabachniket et al.(1997). The model is based on the hypothesis that the probability of multiple ionizations is directly related to the energy deposited by the projectile on the target. The energy deposited is statistically distributed among all atomic electrons and one or more of which eventually auto ionize to the final state.

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. Therefore 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 (Berakdar, 1996). Recently, some interesting theoretical calculations on single and multiple ionization of noble gases atom by fast proton impact have been reported where contributions of electron capture to multiple ionizations are negligible. Spranger and Kirchner(2004) 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 statistical model and concluded that high projectile velocities multiple ionization is dominated by Auger like processes. Archubi et at. (2007) have developed a many electron model for multiple ionizations of heavy atoms by bare atom adopting a different approach. It is based on the solution of transport equation for an ion travelling through an inhomogeneous electron density. Among different experimental investigations on metals, McCartney et al. (1999) 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. Because of this reason the experimental data have been obtained in the limited energy ranges. They have also carried out theoretical calculations in an independent electron model but unfortunately the agreement 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 and Kune reasonably considered two processes in a double binary encounter model to describe the 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 electron. The corresponding double ionization cross sections are denoted by $Q_{\mathrm{SC}}^{\mathrm{ii}}$ (scattered part) and $Q_{\mathrm{ej}}^{\mathrm{ii}}$ (ejected part) respectively. Kara et al.(1997) also supported the idea of above mentioned two step interactions to describe the process of direct double ionization. Roy and Rai (1973) modified Gryzinski`s theory of electron impact double ionization suitably and, the result of double ionization cross sections based on the modified model including contribution of indirect processes were found to close agreement with the experimental data (Chatterjee and Roy, 1984,1987). Hartree-Fock and hydrogenic velocity distribution were used while considering ejection of the first and second target electron respectively. Later on, Jha and Roy (2002) and Minakshi et al. (2009) 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 these studies. In the case of heavy charged particle impact, BEA of double ionization cross section of atoms are few. Kumar and Roy (1977) pointed out error and obsequies in Gryzinski's theory for calculation of the process mentioned above and modified the mathematical framework suitably incorporating the necessary correction. From comparison of the two distribution 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^+ and He^{2+} impact single and double ionization cross sections for Cu and Fe atoms 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.

CHAPTER 3

3. MATERIALS AND METHODS

In our research work, we performed theoretical calculation of single and double ionization cross sections of four different types of atoms namely Kr, Xe, Fe and Cu. There used binary encounter approximation developed by Gryzinski (1965a,b,c) and modified by Vriens (1966, 1967, 1969). Later on, the above-mentioned model was modified by Roy and Rai (1973) and Kumar and Roy (1977). Recent past the above-mentioned calculation was further modified by Jha and Roy (2000) on the basis of proper physical justification and makes the calculation of cross sections of different atoms and ions.

3.1 Methods of calculation

3.1.1 Electron impact single ionization cross sections

A negatively charged particle (electron) experiences Columbic force of attraction when it approaches towards the ionic target. It causes the projectile to change its velocity discussed in detail by Thomas and Garcia (1969).This causes an appreciable increase in its kinetic energy and substantial decrease in impact parameter of the incident electron. The expression for the increased kinetic energy of the incident electron at a distance ξ from the nucleus of the ion can be given by

$$E_1' = E_1 + \frac{Z'e^2}{\xi} \tag{3.1}$$

where E_1 is the initial kinetic energy of the incident electron and $Z'e$ is the net nuclear charge of the target ion.

Thomas and Garcia (1969) have modified the expression of the of the ionization cross section for positive ion by taking the two effects e.g., increase in the kinetic energy and decrease in impact parameter of the incident electron. The resulting expression for the ionization cross section can be given as

$$\sigma_1(E_1) = \sigma_1(E_1') \left[\frac{1}{2} + \frac{1}{2}\left\{1 + \frac{2Z'e^2\pi}{E_1\sigma_1(E_1')} \times \left[\xi - \left(\xi^2 - \frac{\sigma_1(E_1')}{\pi}\right)^{\frac{1}{2}}\right]\right\}^{\frac{1}{2}}\right] \quad (3.2)$$

where $\sigma_1(E_1)$ is the expression for cross section at increased electron energy E_1' given by equation (3.1) and ξ is the collision radius whose value depends upon the ionic radius.

In this work, we begin from Vriens (1966) expression for electron impact ionization cross section including exchange and interference for the calculation of electron impact single ionization cross sections of Kr and Xe. There used Hartree-Fock velocity distribution for the target electrons. We have also taken into consideration the contributions of inner shells. In the past, the BEA has been found successful in the calculation of electron impact single ionization cross sections of atoms (Gupta et al., 2015). A brief outline of the method of calculation is given below. Expression for electron impact ionization, including exchange and interference due to Vriens (1966) is given by

$$Q' = \frac{\pi e^2}{E_1 + E_2 + U}\left\{\left(\frac{1}{U} - \frac{1}{E_1}\right) + \frac{2E_2}{3}\left(\frac{1}{U^2} - \frac{1}{E_1^2}\right) - \frac{\Phi' \ln\left(\frac{E_1}{U}\right)}{E_1 + U}\right\} \quad (3.3)$$

where

$$\Phi' = \cos\left[\left(\frac{R}{E_1 + U}\right)^{\frac{1}{2}} \mathrm{In}\left(\frac{E_1}{U}\right)\right] \quad (3.4)$$

In the above expressions E_1 and E_2 are kinetic energies of incident and particular bound electron of the target respectively and R is Rydberg constant.

McDowell (1966) adopted two dimensionless variables s and t relating to the ratio of kinetic energy of incoming and orbiting electrons to the ionization potential energy U. Catlow and McDowell (1967) extended it to formulate the expression of ionization cross section of atoms interms of the two dimensionless quantities s and t defined as

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

where $U = {v_0}^2$ is the ionization potential of the shell under consideration expressed in Rydbergs and v_1 and v_2 are the velocities of the incident and the bound electrons respectively, in atomic units. All other energies have also been expressed in Rydberg. In terms of these dimensionless quantities, Vriens expression for electron impact ionization cross section takes the form

$$Q_i\,(s,t) = \frac{4}{(s^2+t^2+1)}\left[\frac{(S^2-1)}{U^2s^2} + \frac{2t^2(s^2-1)}{3U^2s^4} - \frac{\phi'}{u^2(s^2+1)}\ln s^2\right]\pi a_0^2 \quad (3.5)$$

where

$$\phi' = \left[\left(\frac{1}{s^2\;U+U}\right)^{\frac{1}{2}}\ln s^2\right] \quad (3.6)$$

The expression (3.5) has been integrated over Hartree-Fock velocity distribution for the bound electron of the target and given as

$$Q_i(s) = n_{\mathrm{e}}\int_0^{\infty} Q_i\,(s,t) f(t) U^{\frac{1}{2}} dt \quad (3.7)$$

where n_{e} is the number of equivalent electrons in the shell under consideration and $f(t)$ is the momentum distribution function for the bound electron which is defined as

$$f(t) = 4\pi t^2 U \rho_{\mathrm{nl}}\left(U^{\frac{1}{2}}t\right) \quad (3.8)$$

Here

$$\rho_{\mathrm{nl}} = \frac{1}{2l+1}\sum_{m=-1}^{+1}[\psi_{\mathrm{nlm}}(\chi)]^2 \quad (3.9)$$

where

$$\psi_{\mathrm{nlm}}(\chi) = \frac{1}{(2\pi)^{\frac{1}{2}}}\int \Phi_{\mathrm{nlm}}(r)\, e^{ik.r} dr \quad (3.10)$$

is the Fourier transform of the one electron orbital. Complete wave function or Slater orbitals is given by

$$\Phi_{\mathrm{nlm}}(r) = N_{\mathrm{nl}} R_{\mathrm{nl}}(r) Y_{\mathrm{lm}}(\Omega) \quad (3.11)$$

where $R_{\mathrm{nl}}(r)$ and N_{nl} are the analytical Hartree-Fock radial function and normalization constant given as

$$N_{nl} = [(2n)!]^{-\frac{1}{2}}(2\xi)^{n+\frac{1}{2}} \quad (3.12)$$

and

$$R_{\mathrm{nl}} = r^{n-1}e^{-\xi r} \quad (3.13)$$

Spherical harmonic $Y_{\mathrm{lm}}(\Omega)$ have different form depending upon the value of quantum numbers ℓ, m. Inner shell electrons in heavy atoms have high velocity and they are relativistic in nature. Hence, relativistic effect plays an important role for such targets. In present work, ionization from valence shells and a few inner shells have only been considered and ignored relativistic effects for outer shell electrons of the atom. Keeping this fact in account we have used non-relativistic wave function in the present work.

In the present calculations, momentum distribution functions for the bound electrons have been constructed using Hartree-Forck radial functions reported by Clementi and Roetti (1974). For shell radii and binding energies of electrons, quantum mechanical value of radial distance of maximum probability given by Desclanx (1973) and quantum mechanical values of orbital energies given by Clementi and Roetti (1974) have, respectively, been used in the calculations.

3.1.2 H^+ and He^{2+} impact single ionization cross section

In the present work, we have used the accurate expression of $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) as given by Vriens (1967) for heavy charged particles incident on atoms. Following Catlow and McDowell (1967), there introduced two dimensionless variables *s* and *t* defined by

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

where v_1 and v_2 are the velocities in atomic units of the incident particle and the target electron respectively and $U = {v_0}^2$ where $v_0$is root mean square velocity of orbital electrons) and U is the ionization potential of the target in Rydberg. All other energies involved are also expressed in Rydbergs. In terms of these variables, the expressions of ionization cross section due to a projectile of unit charge for particular incident energy and a particular velocity of bound electron are given by (Singh et al., 2009)

$$Q_{\mathrm{i}}(s,t) = \frac{4}{s^2U^2}\left[1 + \frac{2t^2}{3} - \frac{1}{4(s^2-t^2)}\right], \quad 1 \le 4s(s-t) \tag{3.14}$$

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

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

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 for heavy charged particle impact single ionization cross section for a particular shell of the target is given by

$$Q_{\mathrm{i}}(s) = n_{\mathrm{e}} Z^2 \int_0^{\infty} Q_i\,(s,t) f(t) U^{\frac{1}{2}} dt \pi a_0^2 \tag{3.15}$$

$f(t)$, ρ_{nl} , $\psi_{\mathrm{nlm}}(\chi)$, $\phi_{\mathrm{nlm}}(r)$ and rest of the symbols are defined in the Section 3.1.1

Complete wave function or Slater Orbitals wave function is given by

$$\Phi_{\mathrm{nlm}}(r) = N_{\mathrm{nl}} R_{\mathrm{nl}}(r) Y_{\mathrm{lm}}(\Omega) \tag{3.16}$$

3.1.3 Electron impact double ionization cross section

The method of calculating electron impact double ionization cross section of atoms in double binary encounter model has been discussed in detail in earlier publications (Roy and Rai, 1973; Chatterjee and Roy, 1984; Jha and Roy, 2002). Electron impact double ionization cross sections including contribution from Auger emission can be written as

$$Q^{\mathrm{ii}}(T) = Q_{\mathrm{D}}^{\mathrm{ii}} + Q_{\mathrm{A}}^{\mathrm{ii}} \tag{3.17}$$

where $Q_{\mathrm{D}}^{\mathrm{ii}}$ denotes the contribution from direct double ionization (DDI) and Q_A^{ii} that from Auger emission. When Auger effect is ignored the total DDI is

$$Q_{\mathrm{D}}^{\mathrm{ii}} = Q_{\mathrm{SC}}^{\mathrm{ii}} + Q_{\mathrm{ej}}^{\mathrm{ii}} \tag{3.18}$$

The expressions for $Q_{\mathrm{SC}}^{\mathrm{ii}}$ and $Q_{\mathrm{ej}}^{\mathrm{ii}}$ given by Gryzinski (1965c) and modified by Roy and Rai (1973) are

$$Q_{\mathrm{SC}}^{\mathrm{ii}} = \frac{n_{\mathrm{e}}(n_{\mathrm{e}}-1)}{4\pi\bar{r}^2} \int_{U_i}^{E_q-U} \sigma_{\Delta E} \left[\int_{U_{\mathrm{ii}}}^{E_q-\Delta E} \sigma_{\Delta E} d(\Delta E) \right] d(\Delta E) \tag{3.19}$$

and

$$Q_{\mathrm{ej}}^{\mathrm{ii}} = \frac{n_{\mathrm{e}}(n_{\mathrm{e}}-1)}{4\pi\bar{r}^2} \int_{U_{\mathrm{i}}+U_{\mathrm{ii}}}^{E_q} \sigma_{\Delta E} \left[\int_{U_{\mathrm{ii}}}^{E_q-\Delta E} \sigma_{\Delta E} d(\Delta E) \right] d(\Delta E) \tag{3.20}$$

The above two expressions have been integrated numerically over energy transfers and the Hartree Fock velocity distributions for the ejection of the two electrons under double BEM leading to direct double ionization are given by (Gupta et al., 2017)

$$Q_{\mathrm{SC}}^{\mathrm{ii}} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2} \int_{t=0}^{\infty} \int_{U_{\mathrm{i}}}^{E_q-U_{ii}} \sigma_{\Delta E} \left[\int_{t=0}^{\infty} \int_{U_{\mathrm{i}}}^{E_q-\Delta E} \sigma_{\Delta E'}\, f(t) U_{\mathrm{ii}}^{\frac{1}{2}} d(\Delta E^{\mathrm{i}}) dt \right]$$

$$\times f(t)U_{\mathrm{i}}^{\frac{1}{2}}d(\Delta E)dt \times 8.797 \times 10^{-17}(\pi a_0^2) \tag{3.21}$$

and

$$Q_{\mathrm{ej}}^{\mathrm{ii}} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int_{t=0}^{\infty}\int_{U_{\mathrm{i}}+U_{\mathrm{ii}}}^{E_q}\sigma_{\Delta E}\left[\int_{t=0}^{\infty}\int_{U_{\mathrm{ii}}}^{\Delta E-U_{\mathrm{i}}}\sigma_{\Delta E'}\,f(t)U_{\mathrm{ii}}^{\frac{1}{2}}d(\Delta E^{\mathrm{i}})dt\right]$$

$$\times f(t)U_i^{\frac{1}{2}}d(\Delta E)dt \times 8.797 \times 10^{-17}(\pi a_0^2) \tag{3.22}$$

Here n_{e} is the numbers of electrons in the shell under consideration, ΔE and $\Delta E'$ stands for energy transfers during the first and second collision respectively, $\bar{r}$ denotes the mean distance between the electrons in the shell given by $\bar{r} = R/n_{\mathrm{e}}^{1/3}$ where R being radius of the shell of the target. Also U_{i} and U_{ii} are the ionization potentials corresponding to the ejection of the two electrons of the target.

Using dimensionless variables introduced by Catlow and McDowell (1967), the accurate expression of cross section $\sigma_{\Delta E}$ (Varien, 1966) as used by Kumar and Roy (1978), can be given as

$$\sigma_{\Delta E} = \frac{2}{(s^2+t^2+1)u}\left[\left(\frac{1}{\Delta E^2}+\frac{4t^2u}{3\Delta E^3}\right)+\left(\frac{1}{(s^2u+u-\Delta E)^2}+\frac{4t^2u}{3(s^2u+u-\Delta E)^3}\right)\right.$$
$$\left.-\frac{\phi}{\Delta E(s^2u+u-\Delta E)}\right]\pi a_0^2 \tag{3.23}$$

where

$$\phi = \cos\left\{\left(\frac{1}{s^2u+u}\right)^{\frac{1}{2}}\ln s^2\right\} \tag{3.24}$$

Due to in distinguishability of electron in the symmetrical model of Vriens the cross sections corresponding to the two processes are exactly equal at all incident energies (Kumar and Roy, 1978) and hence in order to obtain the direct double ionization cross section, either of the cross sections should be multiplied by 2. In equation (3.21) u and s^2 have been replaced by U_i and E_q/U_{i} in expression for $\sigma_{\Delta E}$ and by U_{ii} and $(E_q-\Delta E)/U_{\mathrm{ii}}$ in the case of $\sigma_{\Delta E'}$. The symbol E_q is the energy of the projectile. The only difference in the equation (3.22) is that s^2 assumes the value $(\Delta E - U_i)/U_{ii}$ in the expression for $\sigma_{\Delta E'}$. The function $f(t)$ appearing in the above equations is the momentum distribution function. In case of double ionization $f(t)$ has been constructed replacing ionization potential energy u by U_{i} and U_{ii} for ejection of first and the second electron respectively. In order to obtain $Q_{\mathrm{A}}^{\mathrm{ii}}$ (double ionization cross section from Auger effect), the single ionization cross section should be multiplied by Auger yield of the shell under consideration. The expression of $Q_{\mathrm{A}}^{\mathrm{ii}}$ incorporating the Columbic effect is given by (Kumar and Roy, 1979)

$$Q_{\mathrm{A}}^{\mathrm{ii}} = (1-f)n_{\mathrm{e}} \int_0^\infty \left\{ \frac{(s-s')^2}{s^2u^2(s'^2+t^2+1)} \times \left[\frac{s'^2-1}{s'^2} + \frac{2t^2}{3}\left(\frac{s'^4-1}{s'^4}\right) - \frac{\Phi(r)\ln s'^2}{s'^2+1} \right] \right\}$$
$$\times f(t) u^{\frac{1}{2}} dt (\pi a_0^2) \qquad (3.25)$$

where f is the fluorescence branching ratio of the intermediate ion state and

$$s'^2 = s^2 + \frac{2Z}{\xi u} \qquad (3.26)$$

Here s' is dimensionless variable for second encounter with second active electron of the target.

$$E_1' = E_1 + \frac{Ze^2}{\xi} \qquad (3.27)$$

We have considered orbitals 4s, 3d and 3p of outer shells only. Total cross section for electron impact direct double ionization of Fe

$$Q_{\mathrm{D}}^{\mathrm{ii}} = Q_{\mathrm{D}}^{\mathrm{ii}}(4s,4s) + Q_{\mathrm{D}}^{\mathrm{ii}}(4s,3d) + Q_{\mathrm{D}}^{\mathrm{ii}}(4s,3p) \qquad (3.28)$$

where $Q_{\mathrm{D}}^{\mathrm{ii}}(4s,3d)$ stands for the double ionization cross section corresponding to one electron ejected from 4s shell and the other from the 3d shell. The factor $n_{\mathrm{e}}(n_{\mathrm{e}}-1)/4\pi\bar{r}^2$ has been suitably modified for considering the modes of ionization in which the electrons are ejected from different shells The factor $n_{\mathrm{e}}(n_{\mathrm{e}}-1)$ has been replaced by $n_{e1} \times n_{e2}$ for pair of different orbitals In order to obtain the value $\bar{r}$, the atomic radius has been replaced by the mean of the expectation value of radii of the shell given by $\overline{r} = R/n_{\mathrm{e}}^{1/3}$ where R being radius of the shell of the target. (Jha and Roy, 2002). Binding energies, orbital energies of the sub shells and expectation values of radii are taken as given by Climenti and Roetti (1974) and Desclaux (1973).

3.1.4 H^+ and He^{2+} impact double ionization cross section

In accordance with the predictions of the first Born approximation, the single ionization cross section depends on the charge Z of the incoming particle and its velocity v as $Z^2v^2 \mathrm{In} v$ if the velocity is much larger than corresponding to the binding energy of the atomic electron (Melo et al.,2002). We have assumed Z^2 dependence in calculations of direct double ionization cross sections (DDICS) in the present double binary encounter model. Heavy charged particle impact total double ionization cross section $Q^{\mathrm{ii}}(T)$ including the contribution from Auger emission $Q_{\mathrm{A}}^{\mathrm{ii}}$ can be written as

$$Q^{\mathrm{ii}}(T) = Q_{\mathrm{D}}^{\mathrm{ii}} + Q_{\mathrm{A}}^{\mathrm{ii}} \tag{3.29}$$

When Auger effect is ignored, the direct double ionization (DDI) $Q_{\mathrm{D}}^{\mathrm{ii}}$ is

$$Q_{\mathrm{D}}^{\mathrm{ii}} = Q_{\mathrm{SC}}^{\mathrm{ii}} + Q_{\mathrm{ej}}^{\mathrm{ii}} \tag{3.30}$$

In accordance of the idea given by Gryzinski (1965c) in double binary encounter model, these cross sections involving integrals over energy transfer are given by (Singh et el., 2009)

$$Q_{\mathrm{SC}}^{\mathrm{ii}} = \frac{n_{\mathrm{e}}(n_{\mathrm{e}}-1)}{4\pi\bar{r}^2}\int_{U_{\mathrm{i}}+U_{\mathrm{ii}}}^{\Delta E_{\max}} \sigma_{\Delta E}\left(E_q\right)\left[\int_{U_{\mathrm{ii}}}^{\Delta E_{\max}} \sigma_{\Delta E}\left(E_q-\Delta E\right) d(\Delta E')\right] d(\Delta E) \tag{3.31}$$

and

$$Q_{\mathrm{ej}}^{\mathrm{ii}} = \frac{n_{\mathrm{e}}(n_{\mathrm{e}}-1)}{4\pi\bar{r}^2}\int_{u_{\mathrm{i}}+u_{\mathrm{ii}}}^{\Delta E_{\max}} \sigma_{\Delta E}\left[\int_{u_{\mathrm{ii}}}^{\Delta E-u_{\mathrm{i}}} \sigma_{\Delta E}(\Delta E) d(\Delta E')\right] d(\Delta E) \tag{3.32}$$

The various symbols used in the above expressions have been defined by Gryzinski (1965c). 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 $\bar{r} = R/n_{\mathrm{e}}^{1/3}$ (R being the radius of the shell of the target atom), u_i and u_{ii} are the first and second ionization potentials corresponding to ejection of the electrons from the target. The symbol E_q represents the energy of the projectile.

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 (Singh et al., 2009)

$$\sigma_{\Delta E} d(\Delta E) = \begin{cases} Ad(\Delta E); & \Delta E \leq 4su(s-t) \\ Bd(\Delta E); & 4su(s-t) \leq \Delta E \leq 4su(s+t) \\ 0; & \Delta E > 4su(s+t) \end{cases} \tag{3.33}$$

where

$$\mathrm{A} = \frac{1}{s^2 u}\left(\frac{1}{(\Delta E)^2} + \frac{4t^2 u}{3(\Delta E)^3}\right) \tag{3.34}$$

and

$$\mathrm{B} = \frac{2}{3t(\Delta E)^3}\left(8s - \frac{1}{s^2 u^{\frac{3}{2}}}\left[(\Delta E + t^2 u)^{\frac{1}{2}} - tu^{\frac{1}{2}}\right]^3\right) \tag{3.35}$$

The expressions of the scattered and ejected part of the DDICS showing the relevant integrals involving energy transfer and Hartree-Fock velocity distributions for the target electrons are given below as (Singh et al., 2009)

$$Q_{\mathrm{SC}=}^{\mathrm{ii}}\frac{n_{\mathrm{e}}(n_{\mathrm{e}}-1)Z^2}{4\pi\bar{r}^2}$$

$$\times\left(\int_{t=0}^{s-\frac{1}{4s}}\left\{\int_{u_{\mathrm{i}}}^{4su_{\mathrm{i}}(s-t)}A\alpha d(\Delta E)+\int_{4su_{\mathrm{i}}(s-t)}^{4su_{i}(s+t)}B\alpha d(\Delta E)\right\}f(t)u_{\mathrm{i}}^{\frac{1}{2}}dt\right.$$

$$\left.+\int_{t=s-\frac{1}{4s}}^{\infty}\int_{u_{\mathrm{i}}}^{4su_{\mathrm{i}}(s+t)}B\alpha f(t)u_{\mathrm{i}}^{\frac{1}{2}}d(\Delta E)dt\right)\pi a_0^2 \qquad (3.36)$$

when$\left(s-\frac{1}{4s}\right)$ is positive and

$$Q_{\mathrm{SC}}^{\mathrm{ii}}=\frac{n_{\mathrm{e}}(n_{\mathrm{e}}-1)Z^2}{4\pi\bar{r}^2}\times\left(\int_{t=\frac{1}{4s}-s}^{\infty}\int_{u_{\mathrm{i}}}^{4su_{\mathrm{i}}(s+t)}B\alpha f(t)u_{\mathrm{i}}^{\frac{1}{2}}\,d(\Delta E)dt\right)(\pi a_0^2) \qquad (3.37)$$

when $\left(s-\frac{1}{4s}\right)$ is negative. In the above expressions

$$\alpha=\int_0^{\infty}Q_{\mathrm{i}}(s,t)f(t)u_{\mathrm{ii}}^{\frac{1}{2}}\,dt\;(\pi a_0^2) \qquad (3.38)$$

and $s\,'$is dimensionless variable for second encounter with target electron defied as

$$s'^2=\begin{cases}\dfrac{E_q-\Delta E}{1836u_{\mathrm{ii}}}\\[2ex]\dfrac{E_q-\Delta E}{7344u_{\mathrm{ii}}}\end{cases} \qquad (3.39)$$

The upper equality is for H^+ impact and lower equality is for He^{2+} impact. Similarly, equations for ejected part are

$$Q_{\mathrm{ej}}^{\mathrm{ii}}=\frac{n_e(n_e-1)Z^2}{4\pi\bar{r}^2}\left(\int_{t=0}^{s-(1\pm\frac{u_{\mathrm{ii}}}{u_{\mathrm{i}}})/4s}\left\{\int_{u_{\mathrm{i}}+u_{\mathrm{ii}}}^{4su_{\mathrm{i}}(s-t)}A\alpha d+\int_{4su_{\mathrm{i}}(s-t)}^{4su_{\mathrm{i}}(s+t)}B\alpha d(\Delta E)\right\}f(t)u_{\mathrm{i}}^{\frac{1}{2}}dt\right.$$

$$\left.+\int_{t=s-(1+\frac{u_{\mathrm{ii}}}{u_{\mathrm{i}}})/4s}^{\infty}\int_{u_{\mathrm{i}}+u_{\mathrm{ii}}}^{4su_{\mathrm{i}}(s+t)}B\alpha f(t)u_{\mathrm{i}}^{\frac{1}{2}}d(\Delta E)dt\right)\pi a_0^2 \qquad (3.40)$$

when $s-\frac{\left(1+\frac{u_{\mathrm{ii}}}{u_{\mathrm{i}}}\right)}{4s}$ is positive and

$$Q_{\mathrm{ej}}^{\mathrm{ii}}=\frac{n_{\mathrm{e}}(n_{\mathrm{e}}-1)Z^2}{4\pi\bar{r}^2}\left(\int_{t=\frac{\left(1+\frac{u_{\mathrm{ii}}}{u_{\mathrm{i}}}\right)}{4s}-s}^{\infty}\int_{u_{\mathrm{i}}+u_{\mathrm{ii}}}^{4su_{\mathrm{i}}(s+t)}B\alpha' f(t)u_{\mathrm{i}}^{\frac{1}{2}}\,d(\Delta E)dt\right)(\pi a_0^2) \qquad (3.41)$$

when $s-\frac{\left(1+\frac{u_{\mathrm{ii}}}{u_{\mathrm{i}}}\right)}{4s}$ is negative with

$$\alpha'=\int_0^{\infty}Q_{\mathrm{i}}(s',t)f'(t)u_{\mathrm{ii}}^{\frac{1}{2}}\,dt\;(\pi a_0^2) \qquad (3.42)$$

Here $Q_i(s', t)$ is the expression for electron impact ionization cross section of atoms. (Jha and Roy, 2002) and s' is given by $s'^2 = (\Delta E - u_i)/u_{ii}$ for both H^+ and He^{2+} impact.

The above expression of Q_{SC}^{ii} and Q_{ej}^{ii} are Z^2 dependence in which the projectile knocks out two electrons successfully. In quantum mechanical approach this corresponds to a second order process, for which cross section scales as Z^4. In this connection it is pertinent to point out the observations made by Vriens (1969) that the two double binary encounter processes are linked with the quantum mechanical first and second order approximation. If one uses correlated many electron wave functions, DDICS will be finite even in the first Born approximation (FBA). This has been assumed to correspond to Q_{ej}^{ii} of the process of direct double ionization. There is also a contribution to DDI from the second Born approximation, which includes double processes like those represented by Q_{SC}^{ii}. In the present method the contributions of Q_{ej}^{ii} are found to be much smaller than those of Q_{SC}^{ii} (Kumar and Roy (1977, 1981). In the case of proton impact Z= 1 and therefore, Z^4 scaling for Q_{SC}^{ii} becomes essentially the same as Z^2 scaling and good agreement of calculated results with the experiment is achieved. However, in the case of alpha particle impact, calculation involves Z= 2 and Z^4 scaling of Q_{SC}^{ii} lead to much dominant contribution and produces adverse effect in results. Hence the processes represented by Q_{ej}^{ii} and Q_{SC}^{ii} to the first and the second Born approximations does not appear to be suitable (Minakshi et al., 2009). Beyond energy of 100 keV/amu the graphical representations of cross sections for Fe and Cu show approximate Z^2 dependence of H^+ and He^{2+} impact pure double ionization cross sections (Patton et al., 1995). From the experimental data of H^+ and He^{2+} ions incident on Fe and Cu targets, it is seen that the pure double ionization cross sections are smaller than the corresponding single ionization cross sections (SICS) which indicates usual trend of DDI. Keeping these observations in view, we have assumed Z^2 dependence of DDICS in the present calculations as no established dependence of DDICS on Z is available for this purpose. Therefor here we only consider Z^2 dependence of double ionization of Cu by alpha particle impact. The integral appearing in Q_{SC}^{ii} and Q_{ej}^{ii} have been evaluated numerically.

The functions $f(t)$and $f'(t)$ appearing in the above equations are momentum distributions corresponding to the first and the second ejected electron respectively and are constructed from HF radial wave functions. We have considered total direct double ionization cross section for heavy charged particle of Cu and Fe [when sub-shells 4s, 3d and 3p are only considered]. They are given by

$$Q_{\mathrm{D}}^{\mathrm{ii}} = Q_{\mathrm{D}}^{\mathrm{ii}}(4\mathrm{s}, 3\mathrm{d}) + Q_{\mathrm{D}}^{\mathrm{ii}}(4\mathrm{s}, 3\mathrm{p}) \tag{3.43}$$

and

$$Q_{\mathrm{D}}^{\mathrm{ii}} = Q_{\mathrm{D}}^{\mathrm{ii}}(4\mathrm{s}, 4\mathrm{s}) + Q_{\mathrm{D}}^{\mathrm{ii}}(4\mathrm{s}, 3\mathrm{d}) + Q_{\mathrm{D}}^{\mathrm{ii}}(4\mathrm{s}, 3\mathrm{p}) \tag{3.44}$$

where $Q_{\mathrm{D}}^{\mathrm{ii}}(4\mathrm{s}, 3\mathrm{d})$ and $Q_{\mathrm{D}}^{\mathrm{ii}}(4\mathrm{s}, 3\mathrm{p})$ stand for the direct double ionization cross sections corresponding to ejection of one electron from $4s$ shell and the other either from the $3\mathrm{p}$ shell or $3\mathrm{p}$ shell respectively. The factor$n_{\mathrm{e}}(n_{\mathrm{e}} - 1)/4\pi\bar{r}^2$ has been suitably modified for considering the mode of ionization in which the electrons are ejected from different shells. Here $n_{\mathrm{e}}(n_{\mathrm{e}} - 1)$has been replaced by $n_{\mathrm{e1}} \times n_{\mathrm{e2}}$ where these two stand for number of electrons in the two different sub shells under consideration. The binding energies, the expectation values of the shell radii and HF radial wave functions have been taken from the data reported by Clementi and Roetti (1974) and Desclanx (1973).

CHAPTER 4

4. RESULTS AND DISCUSSION

4.1 Electron impact single ionization of Kr and Xe

We have calculated electron impact single ionization cross sections for Kr and Xe using the equation (3.7), where Hatree-Fock momentum distribution function $f(t)$ is constructed from analytical expressions of equations (3.5) to (3.13) and detailed of which is mentioned in Section3.1.1. For shell radii, binding energies of orbing electron and quantum mechanical value of radial distance of maximum probability is given by Desclanx (1973) and quantum mechanical values of orbital energies given by Clementi and Roetti (1974) have been used in the calculations , respectively. The calculated results of electron impact of Kr and Xe along with experimental observations (Rejoub et al., 2002) have been plotted in the Figure 3 and 4 from data Table 1 and Table 2 as listed in Appendix-D.

4.1.1 Electron impact single ionization cross section of Kr

The theoretical calculations of single ionization cross section (SICS) of Kr have been carried out using equation (3.7) as discussed in Section 4.1.The computational calculation is carried in the energy region from threshold 15 eV to 1000 eV. We considered contribution of 4s, 4p and 3d sub shells only and inner shells contribution are not taken into account. In the threshold region the magnitude of the calculated cross sections are larger in comparison to the experimental data which is a usual feature of the model. Our calculated results come closer to the experimental data with increase of impact energy. The calculated peak has SICS of $4.83 \times 10^{-16}\text{cm}^2$ (45 eV) while the experimental peak has a magnitude $3.49 \times 10^{-16}\text{cm}^2$ (65 eV). The ratio of calculated cross section to the experimental cross section (ratio factor) is greater than two up to impact energy 24 eV. From impact energy of 26 eV to 1000 eV the ratio factor fall below 2 and it decreases gradually with increase of impact energy.

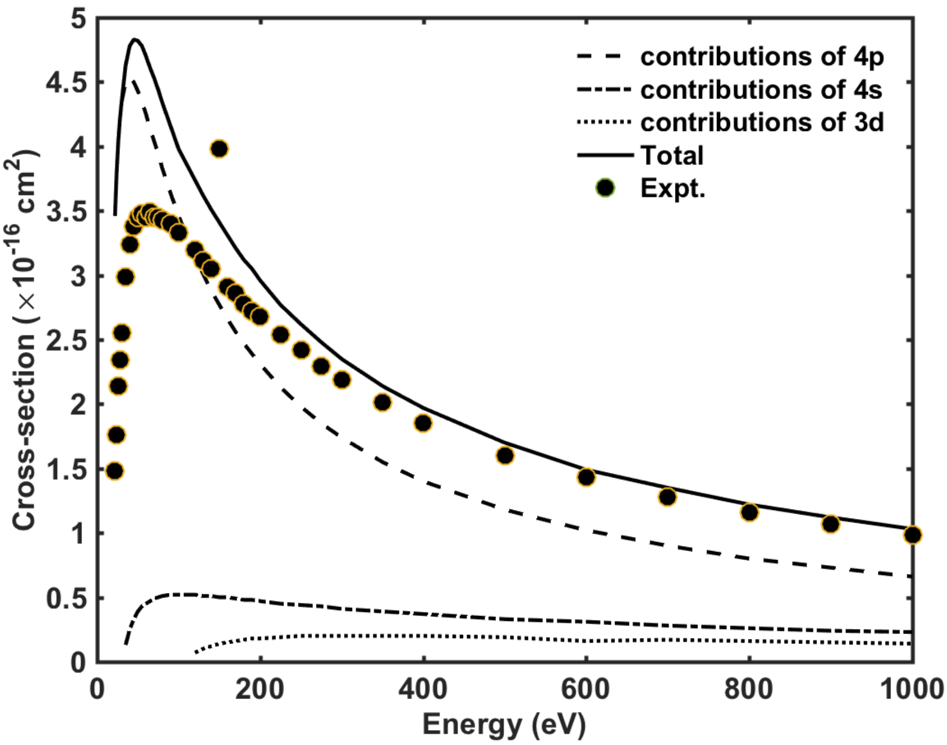

Figure 3: Electron impact single ionization cross section of Kr atom along with its experimental values of single ionization cross section (Rejob et al., 2002)] against respective impact energy.

About 97% of calculated results have ratio factor less than two and results are in agreement with the experimental data. Sub shell 4p has major contribution which varies from 97% to 64% to the total theoretical single ionization cross sections and 4s and 3d have small contribution which increases with impact energy up to 22% and 13% respectively. The total values of SICS at impact energies of 170 eV, 180 eV and 190 eV are 3.21×10^{-16} cm^2, 3.12×10^{-16} cm^2 and 3.05×10^{-16} cm^2 respectively and their corresponding experimental data are 2.86×10^{-16} cm^2, 2.78×10^{-16} cm^2 and 2.72×10^{-16} cm^2. Calculated results overestimate the experimental observations. He ratio factor fall below 1.1 from impact energy 200 eV to 1000 eV which is 34% of the total theoretical results and the results are very close to experimental data. From impact energy 700 eV to 1000 eV the ratio factor is almost same and about 1.05.The close inspection of the results revels that the calculated results are in excellent agreement with the experimental result in energy region 100 eV to 1000 eV.

4.1.2 Electron impact single ionization cross section of Xe

Electron impact single ionization cross sections (SICS) of Xe atom has been performed as mentioned in Section 4.1 from threshold energy of 14 eV to 1000 eV using BEA. The ratio factors is greater than 2 in energy range of 12 eV to 35 eV and beyond of 35 eV the ratio are within factor 2. About 71% of calculated results agree with experimental data. About 23.6% and 18.4% results have ratio factors less than 1.25 and 1.2 in energy range 250 eV - 1000 eV and 400 eV to 1000 eV respectively.

Here we considered contribution of 5p, 5s, 4d and 4p sub shells for the calculation of SICS. Major contribution is observed from 5p sub shell which varies from 97% to 77% and other sub shells have very small contribution. Variation of SICS of these subshells have been shown in Figure 5. The calculated peak value of Xe is $8.94 \times 10^{-16}\text{cm}^2$ (at 35 eV) while the experimental peak value is $4.67 \times 10^{-16}\text{cm}^2$ (at 70 eV). Calculated peak shifted towards the low energy region. The ratio of theoretical peak to the experimental peak is about 1.91.

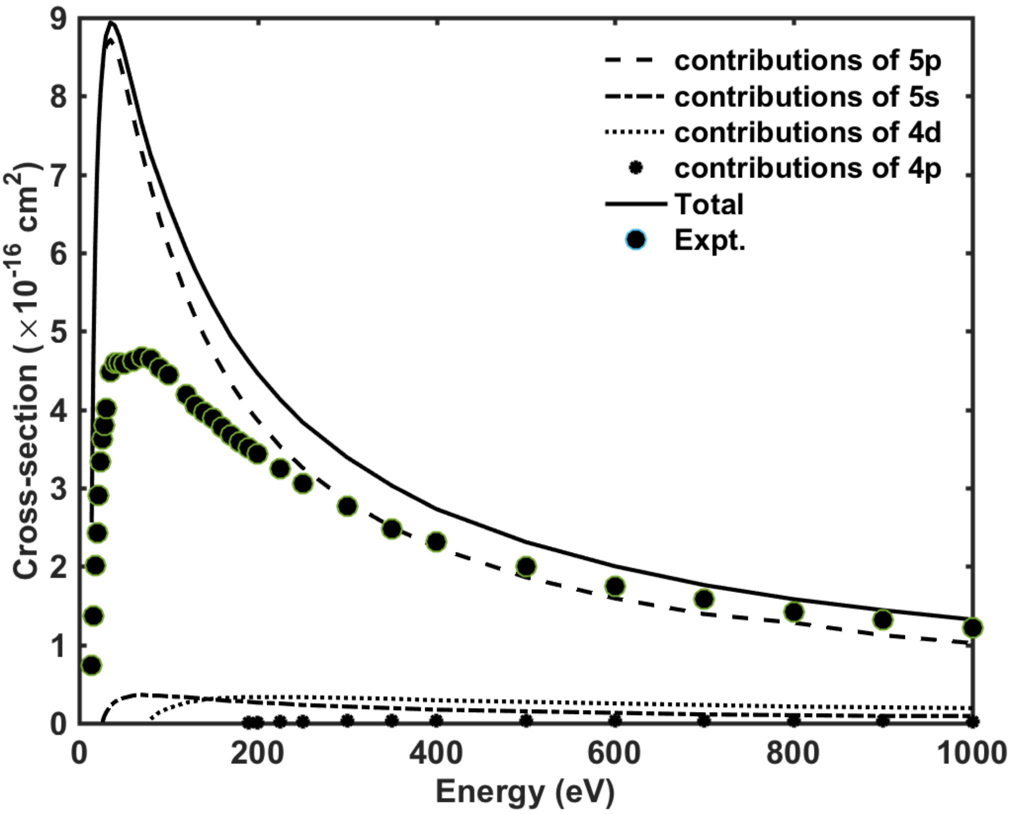

Figure 4: Electron impact single ionization cross section of Xe atom.along with its experimental values of single ionization cross section (Rejob et al., 2002)] against respective impact energy.

It is seen that the ratio factor gradually decreases with the increase of impact energies and the results come closer to the experimental data. At 900 eV and 1000 eV ratio factor is about 1.09 i.e. calculated result is almost equal to experimental data. The ratio factor in between energy range of 40 eV to 90 eV is greater than 1.5. Beyond impact energy of 90 eV the ratio factor falls below 1.5. Peak of the calculated results shifted towards the low energy region. Our calculated results overestimate the experimental values throughout the energy range. The calculated results show good agreement with the experiment in entire energy range.

4.2 Electron impact single ionization cross sections of Fe

The present theoretical investigation for single ionization cross section by electron impact of Fe has been carried out using equations mentioned in section 4.1 from the threshold energy range of 8.1 eV to 1250 eV (Shah et al.(1993). Theoretical results along with the experimental values have been reported in Table 3 and Figure 5.

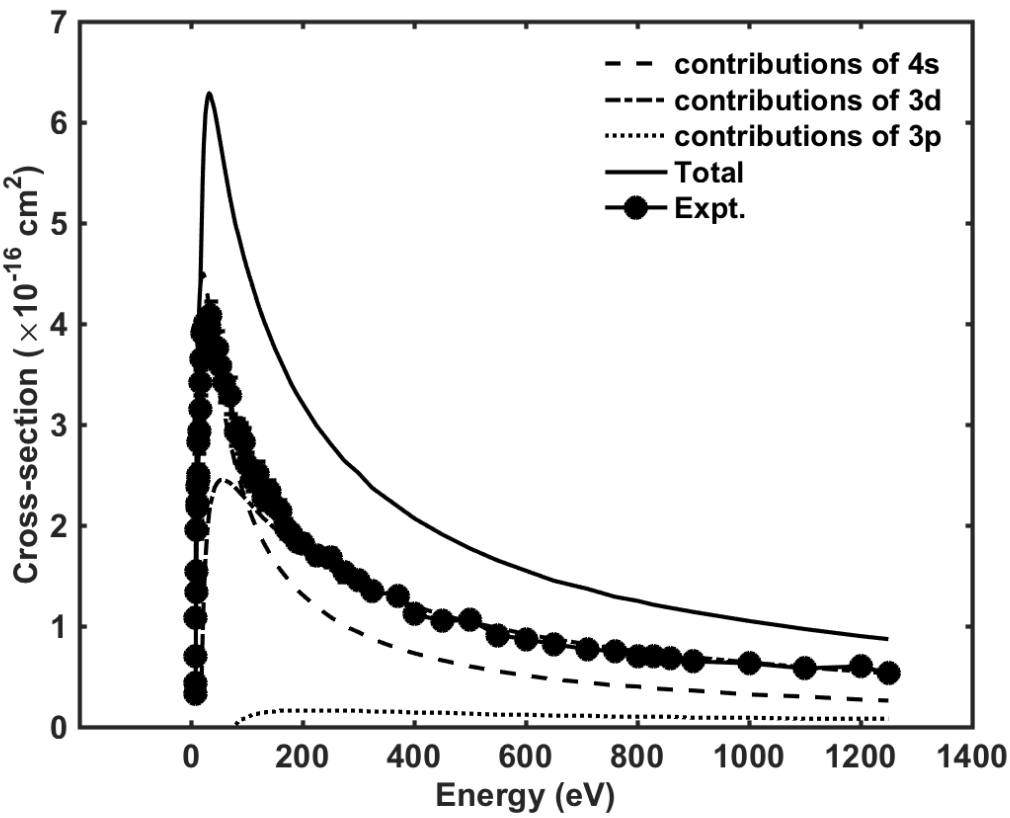

Figure 5: Electron impacts single ionization cross sections of Fe atom along with its experimental values of single ionization cross section (Shah et al., 1993)] against respective impact energy.

We considered contribution of 4s, 3d and 3p sub shells only for SICS of Fe. Our calculated results come closer to the experimental data with increase of impact energy from 8.6 eV to 1250 eV. The calculated peak has magnitude $6.29 \times 10^{-16}\mathrm{cm}^2$ (at 32.5 eV) while the peak measured by Shah et al.(1993) is $4.08 \times 10^{-16}\mathrm{cm}^2$ (at 35 eV). The ratio of the calculated peak to the experimental peak is 1.54. Below impact energy 8.8 eV the ratio factor is greater than 2. About 93.9% of calculated results have ratio factor less than 2 and about 85.4% results have ratio factor less than 1.5 in energy range from 26 eV to 1250 eV. The major contributions to the total calculated SICS are from 4s and 3d sub shells while the contribution of 3p shell is very small. There observed that the contributions of 4s shell falls sharply with the increase of impact energy while the contribution of 3d shells fall smoothly. Contribution from 4s varies from 90.8% to 29.8% and 3d increases from 9% to 61% to the total theoretical SICS of Fe. Thus theoretical results are valid both in the intermediate and high energy range. Nature of variation of calculated results and experimental results is nearly same. At 1250 eV both calculated and experimental cross sections have minimum values of $0.87 \times 10^{-16}\mathrm{cm}^2$ and $0.53 \times 10^{-16}\mathrm{cm}^2$ respectively.

4.3 H^+ impact single ionization cross section of Cu

Calculation of proton impact single ionization cross section has been performed using equation (3.15) with the inclusion of equations (3.14) where Hartree-Fock momentum distribution function $f(t)$ is constructed as mentioned in Section 4.1. Atonic data needed for the calculation are taken from Clementi and Roetii (1974) and Desclanx (1973). Our calculated results for single ionization along with experimental data (Patton et al.,1995) due to H^+ impact of Cu from impact energy of 80 keV/amu to 1440 keV/amu has been shown in Table 4 and Figure 6. In order to calculate SICS we considered ionization of 4s, 3d and 3p sub shells only. Ionization from inner shells (3s, 2p, 2s) has not been included in the present calculations because of their insignificant contribution to SICS. We have plotted the SICS considering ionization from 4s shell including contribution due to only one electron from 3d and 3p sub shells respectively. The single ionization cross section from 4s, 3d and 3p shells have been shown separately in the Table 4 and Figure 6. The ratio factor varies from 0.86 to 1.005 for energy range of 80 keV/amu to 1440 keV/amu and the ratio factors vary from 1.005 to 1.27 for energy range of 175 keV /amu to 1000 keV/amu. The calculated result is nearly identical at 175 keV/amu. At the highest energy of 1440 keV/amu the calculated and experimental values of SICS are $0.87 \times 10^{-16}\mathrm{cm}^2$ and$0.83 \times 10^{-16}\mathrm{cm}^2$ respectively and their ratio is 1.04.Variation of calculated results and experimental data is about six time i.e. almost similar features has been exhibited, For the total value (4s+3d+3p) all the calculated results have ratio factor $\leq$ 1.28 and 44.4% have ratio factor $\leq$ 1.12. For (4s + 3d) about 72% of results

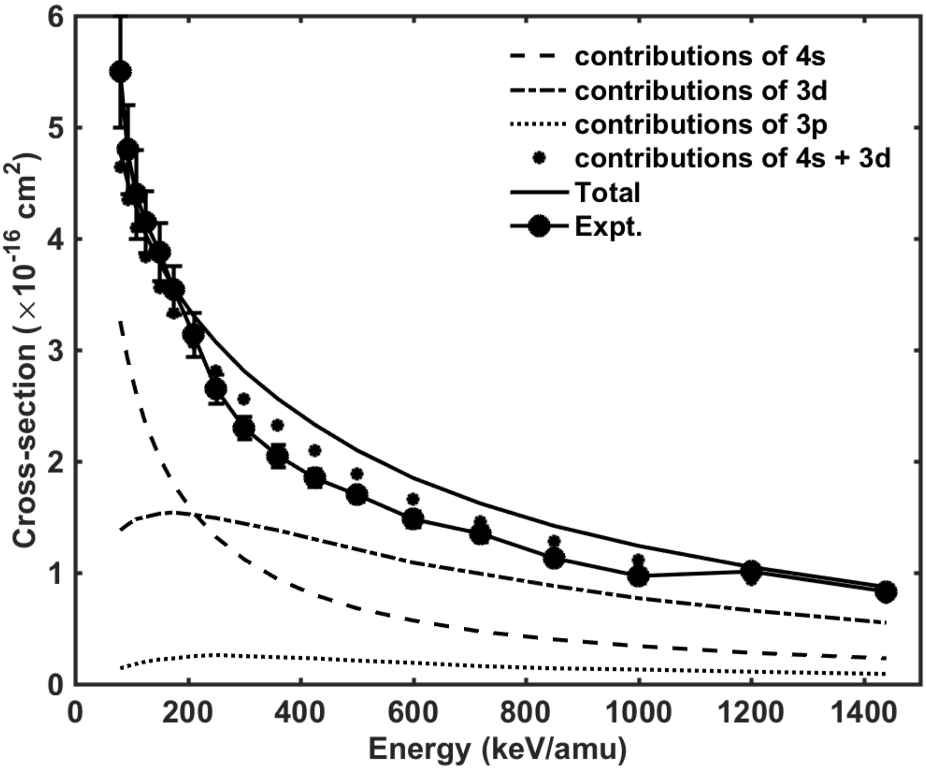

Figure 6: Proton impact single ionization cross sections of Cu atom along with its experimental values of single ionization cross section (Patton et al., 1995) against respective impact energy.

have ratio factor $\leq$ 1.12 and 50% have ratio factor 1.1. Contributions from sub shells 4s and 3d vary from 68% to 26% and 29% to 63% respectively. The theoretical results are in excellent agreement throughout the given energy range. In this connection, it may be mentioned that calculation of SICS in binary encounter approach shows good agreement with experimental data being always within a factor of two. Lotz (1970) calculated electron impact ionization cross section of the atoms with the help of empirical formula and 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 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 similar electronic configuration 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. The calculated results with the inclusion of 3d are in excellent agreement with the experimental data throughout the energy range. 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. Bell et al.(1993) and Jha and Roy (2000) 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. We would like to discuss the different physical processes consequent upon ionization of 3d electron in the case of Cu. After removal of one electron from 3d shell, the target is left in $3d^9$ 4s state. This is not an auto ionization state and hence auto ionization is not possible.

The discussion given above clearly explains why the inclusion of one 3d 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 3d shell of Cu. It is expected that this work will stimulates other theoretical workers. Further study of the problem needs more theoretical calculations to understand the dynamics of the system properly.

4.4 H^+ impact single ionization cross section of Fe

Calculation of proton impact single ionization cross section of Fe has been performed by using equation (3.15) and detailed is as mentioned in Section 4.1.3. In the present theoretical investigation we have carried out the calculation of H^+ impact single ionization cross section of Fe in the energy range 70 keV/amu to 1440 keV/amu. The results of calculated cross section along with experimental data of the single ionization have been shown in the Table 5 and Figure 7.

Here we have taken the contributions from 4s and 3d shells only. Our results have been compared with the experimental observations (Patton et al., 1995). The calculated cross sections over estimates the experimental results throughout the energy range. The experimental data are found to decreases gradually with the increase of impact energy in full given energy range (70 keV/amu to 1440 keV/amu).

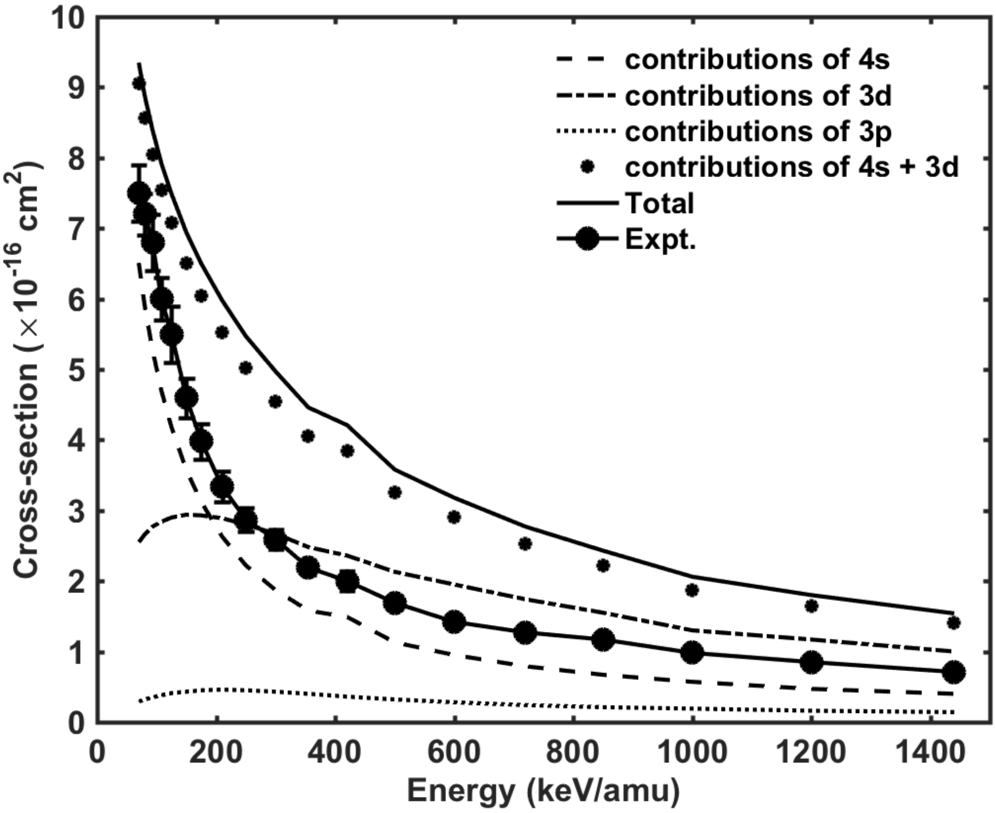

Figure 7: Proton impacts single ionization cross section of Fe atom along with total experimental values of single ionization cross section (Patton et al., 1995) against respective impact energy.

The calculated results also show similar variations with increase of impact energy. At 70keV/amu the ratio factor is 1.2. With the increase of impact energy from 70 keV to 500 keV the ratio factor increases but lies within factor 2. Beyond this energy the ratio factor falls within factor two. For (4s + 3d), about 94.7% calculated results have ratio factor less than 2, 31.5% have ratio factor less than 1.5 and 21% results have ratio factor less than 1.25. Contributions from 4s and 3d sub shells vary from 69% to 25% and 27% to 65% respectively. This tendency reflects that present results and the experimental data are in close agreement both qualitatively and qualitatively throughout the energy range investigated.

4.5 He^{2+} impact single ionization cross section of Cu

Alpha particle impact single ionization cross sections of Cu atom has been calculated by using equation (3.15) and detailed of which is mentioned in Section 3.1.4. We compared the result with experimental data. Theoretical calculations have been carried out in the energy range of 35 keV/amu to 425 keV/amu (Patton et al., 1995). There considered contribution of 4s, 3d and 3p sub shells only and results along with experimental data is presented in Table 6 and Figure 8.

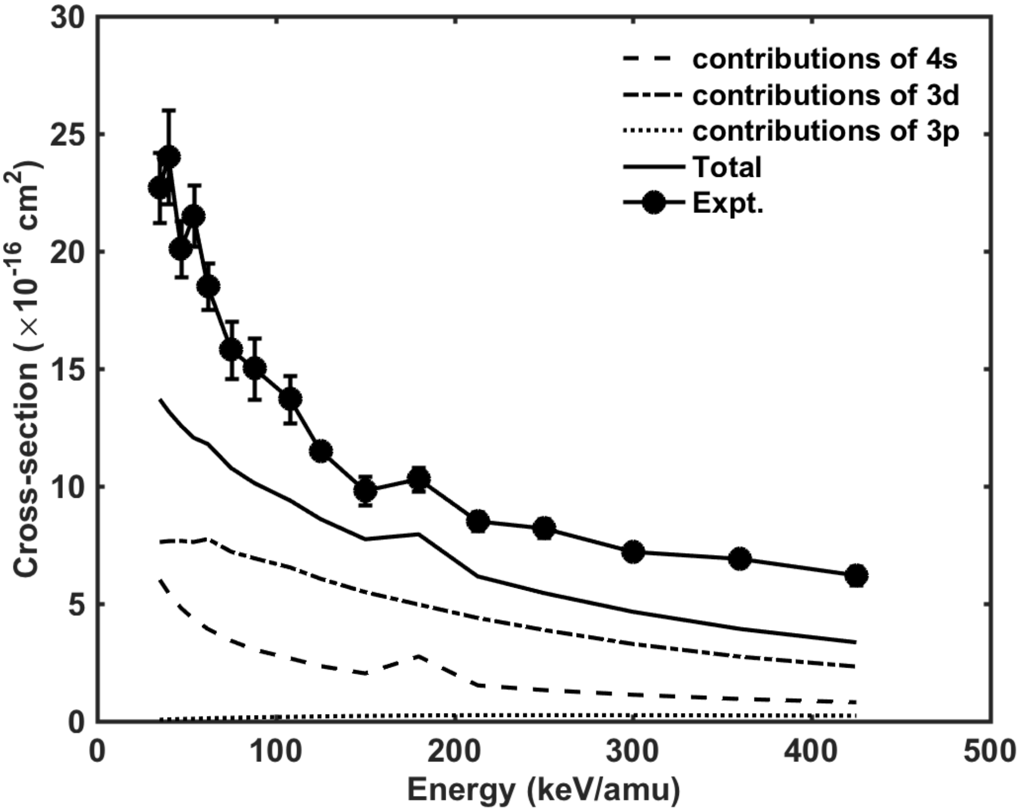

Figure 8: He^{2+} impact single ionization cross section of Cu atom along with its experimental values of single ionization cross section (Patton et al., 1995) against respective impact energy

The experimental and theoretical results show almost similar trend in variation of SICS of Cu with the increase of impact energy. The experimental results overestimate the calculated results of SICS of Cu throughout the energy range. The variations of the results in the both cases are almost 4 times. The calculated results decrease very slowly with the increase of impact energy. There observed major random fluctuations both in experimental and theoretical results in threshold and intermediate energies. The discrepancies observed at high energies might be possible due to some other physical process. For all values of theoretical results ratio factor is less than 2 and 50% results of total single ionization cross sections have ratio factor less than 1.5. Major contribution is from 3d orbital and then 4s orbital. Contributions from 3d and 4s orbitals vary from 55% to 71% and 43.7% to 23.8% respectively. The contribution of 3p shell is very small compared to the 4s and 3d shell.

4.6 He^{2+} impact single ionization cross section of Fe

Calculation of alpha particle impact single ionization cross section of Fe has been performed using equation (3.15) and detailed of which is mentioned in Section 3.1.4. The calculated results of single ionization cross section of Fe along with the experimental data have shown in the Table 7 and Figure 9. In the case of the alpha particle impact single ionization of Fe, we have considered the contributions of 4s, 3d, and 3p shells only. We have calculated the single ionization cross sections of these sub shells from energy range 35 keV/amu to 360 keV/amu and compared the results with experimental data (Patton et al., 1995).

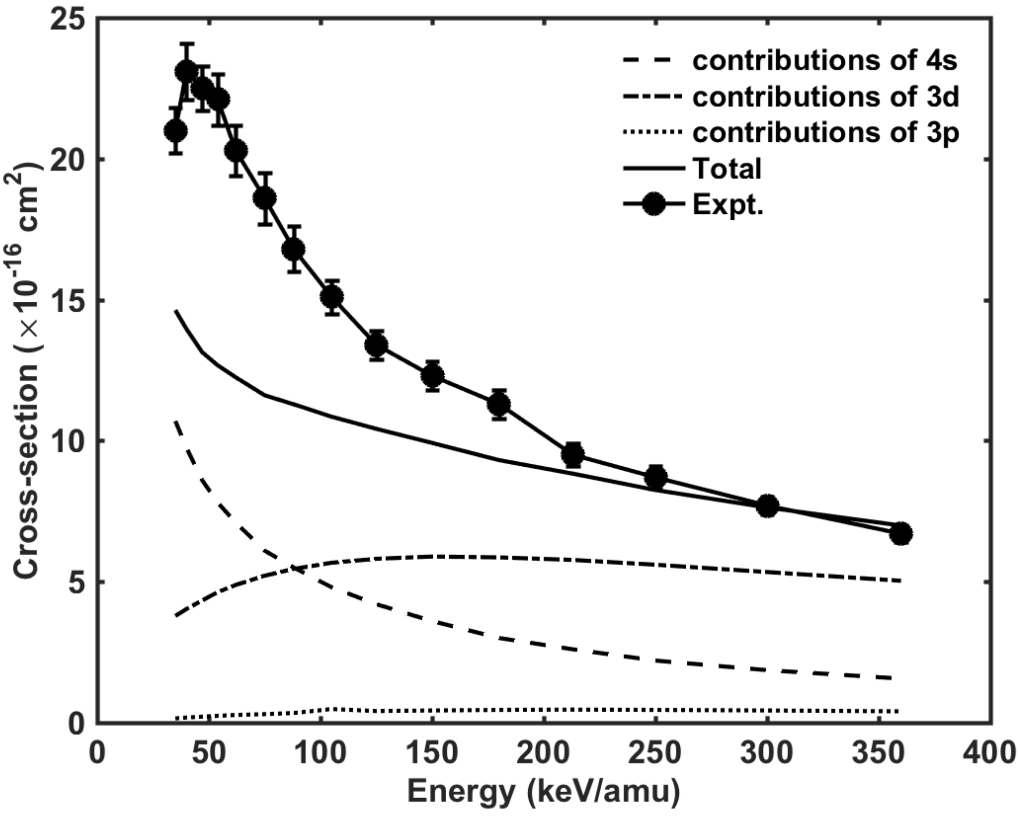

Figure 9: Alpha particles impact single ionization cross sections of Fe atom along with its experimental values of single ionization cross section (Patton et al., 1995) against respective impact energy.

The experimentally measured cross section overestimate throughout the calculated cross section except at energy 360 keV/amu. At impact energy 300 keV/amu and 360 keV/amu calculated results and experimental values are $7.63 \times 10^{-16}\mathrm{cm}^2$, $6.99 \times 10^{-16}\mathrm{cm}^2$ and $7.7 \times 10^{-16}\mathrm{cm}^2$, $6.7 \times 10^{-16}\mathrm{cm}^2$ respectively. The ratio factors at these energies are 1.009 and 1.04. It is surprising that the theoretical as well as experimental cross sections decreases slowly with the impact energy which is contrary to the results of proton impact single and double ionization of Fe . For the entire energy range calculated results gradually come closer to each other. For all values of impact energies the ratio factor is less than 2. About 66% results have ratio factors less than 1.5, 40% have ratio factor less than 1.25 and 20% have less than 1.05. Contribution to total SICS from sub shells 4s and 3d vary from 76% to 22% and 27% to 72% respectively. In high energy region results are very close to experimental values. Trend of variations in experimental cross sections and calculated cross sections shows that the experimental cross sections decrease very sharply and calculated cross sections decreases smoothly.

4.7 Electron impact double ionization cross section of Fe

Electron impact double ionization cross section has been performed using equation (3.18) with the inclusion of equations (3.21), (3.22) and (3.23). The factor $n_\mathrm{e}(n_\mathrm{e}-1)/4\pi\bar{r}^2$ has been suitably modified for considering the modes of ionization in which the electrons are ejected from same or different shells. Here n_e are number electrons in the shell under consideration. The factor $n_\mathrm{e}(n_\mathrm{e}-1)$ is used for pair of same subshells like ($4s^2$, $4s^2$) and the same expression is replaced by $n_{e1} \times n_{e2}$ for double ionization from different sub shells under consideration like ($4s^2$, $3d^6$) and $\bar{r}$ denotes the mean distance between the electrons in the shell such that $\bar{r} = R/n_\mathrm{e}^{1/3}$ (R being the radius of the shell of the target atom). For binding energies we have used the orbital energies of the shells of Fe given by Climenti and Roetti (1974) and expectation values of radii reported by Desclaux (1973). The calculated results along with experimental data in the energy region from 28.3 eV to 1200 eV have been presented in the Table 8 and Figure 10. It is quite surprising that the experimental data of electron impact double ionization measured by Shah et al. (1993) has eight peaks between energy range of 80 eV to 325 eV which indicates presence of large number of fluctuations in the results of experimental data. The Fe atom has an electronic structure with 6 electrons in 3d and 2 electrons in 4s orbitals. Direct double ionization of Fe is considered due to ejection of loosely bound electrons from 3d and 4s orbitals. In addition, we have considered ionization of 3s electrons to lead to an exited state which results double ionization through auto ionization. First we would like to discuss the degree of agreement of the calculated direct double ionization results with the

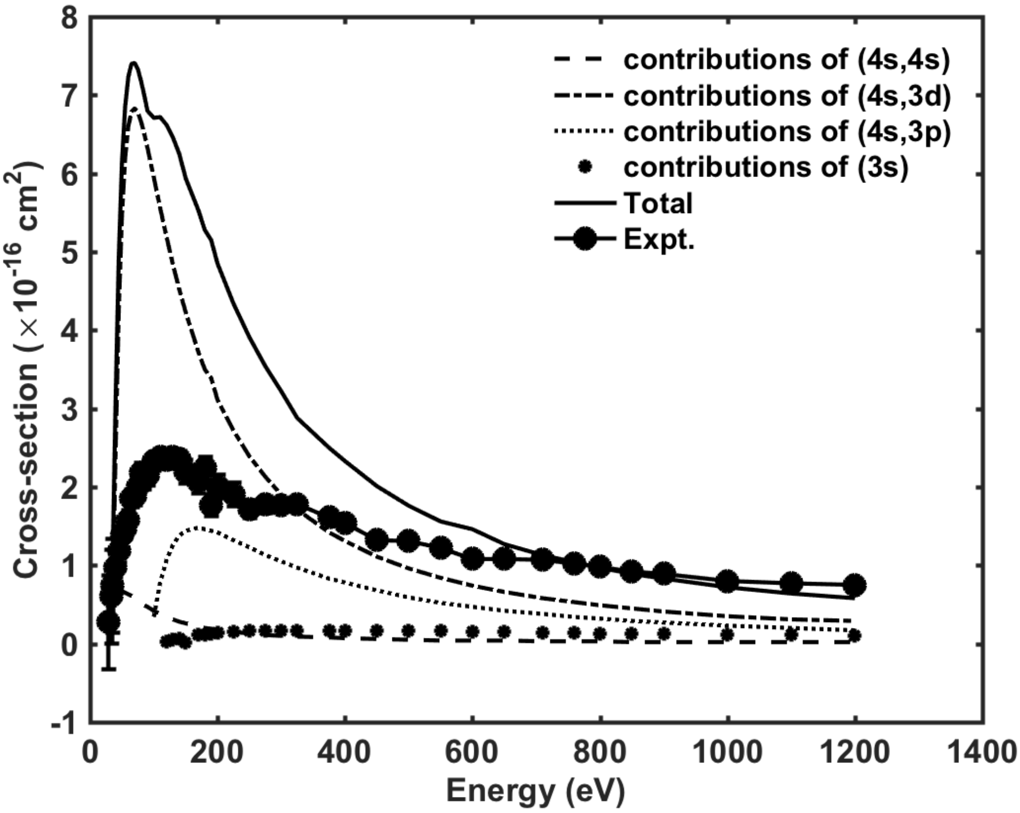

Figure 10: Electron impact double ionization cross section of Fe atom along with its experimental values of single ionization cross section (Shah et al., 1993) against respective impact energy

experimental data. In the threshold energy range of 28.3 eV to 250 eV the ratios factor are greater than 2. In the intermediate and high energy range of 275 eV to 1250 eV ratio factors are within 2. About 47% of calculated results have ratio factor less than 2. Closeness of results increases with impact energy and about 18% results have ratio factor of 1.2 and 11% have ratio factor 1.1. Major contribution is (4s, 3d) is from 60% to 50% and then from (4s, 3p) which vary from 32% to 29%. Major contribution is from (4s, 3d) and very insignificant contribution is from (4s, 4s) and (4s, 3p). At energy 760 eV the magnitude of the theoretical and experimental results are $1.04 \times 10^{-17}\text{cm}^2$ and $1.02 \times 10^{-17}\text{cm}^2$ (nearly same) and between energy 600 eV to 800 eV the experimental results are almost flat. Beyond the energy 760 eV the experimental results overestimate the calculated cross section at all impact energies up to 1250 eV. Indirect contributions from the inclusion of 3d shells play an important role at high impact energy regions. The position of the calculated peak is found to be shifted in lower energy side as compared to the experimental counterpart being. The calculated results above 250 eV shows a satisfactory agreement with experimental data. The discrepancy in experimental data reflects the possibility of some other physical processes contributing to double ionization. Structure in the experimental double ionization cross section- curves between energy 80 eV to 325 eV attributes to indirect ionization process arising from inner shells. But decrease in experimental cross section is rather slow in this energy region. This is not in accordance with the usual trend of direct double ionization cross section which shows a faster decrease in high energy region after attaining the maximum energy. This means variations of calculated results at energies 70 eV and 1200 eV is more than 12 times. Such a feature is not observed in the experimental data where variation is only 2.5 times. It is suggestion for the experimentalist to perform further experiments.

4.8 H^+ impact double ionization cross section of Cu

The calculation of proton impact double ionization cross section has been performed by using equation (3.30). The needed equations, approximations and atomic data are taken as discussed in Section 3.1.4. In the present work, an attempt has been made to obtain double ionization cross section of Cu by proton impact considering contributions of ejection of two electrons from pair of sub shells(4s,3d) and (4s,3p).

The theoretical calculations have been performed from impact energy 125 keV to 1440 keV/amu using BEA and HF velocity distribution function. The calculated results along with experimental data have been presented in the Table 9 and Figure 11. Major contribution is from pair of different sub shells (4s, 3d) for DICS of Cu. In the energy range 125 keV to 300 keV/amu, the calculated results have ratio factor more than 2. About 60% of results have ratio factor less than 2 in between impact energy 360 keV/amu to 1440 keV/amu; 33.3% have ratio factor less than 1.5 in between energy 500 keV/amu to 1000 keV/amu and 26.6% have ratio factor less than 1.25 in between energy of 600 keV/amu to 1000 keV/amu. Under the valid range of impact energy (4s, 3d) has major contribution of 95% to the total DICS of theoretical results. This shows good agreement with experimental data. It can be seen from the Table 9 that at impact energies 720 keV/amu and 850 keV/amu the calculated results agree well with the experimental data. With the increase of the impact energy both the results come closer to each other and at impact energy of 720 keV/amu it is almost similar. At these impact energies of 720 keV/amu and 850 keV/amu the magnitude of the calculated cross sections are $1.49 \times 10^{-17} \mathrm{cm}^2$ and $1.15 \times 10^{-17} \mathrm{cm}^2$ while the

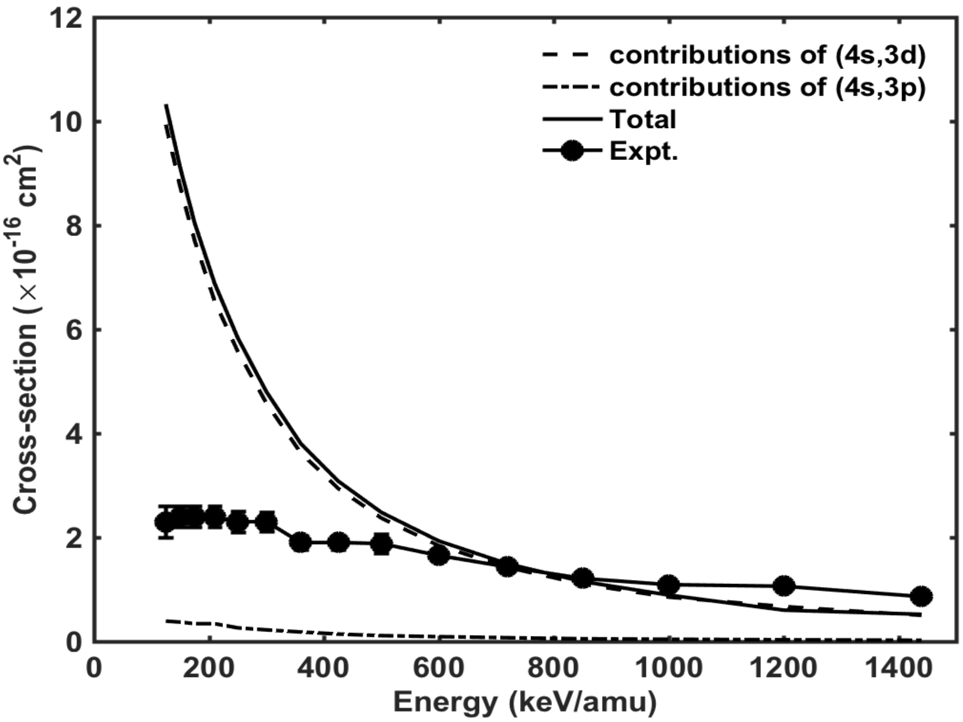

Figure 11: Proton impact double ionization cross sections of Cu atom along with its experimental values of single ionization cross section (Patton et al., 1995) against respective impact energy.

experimental data for these impact energies have cross sections of magnitudes and $1.21 \times 10^{-17} \mathrm{cm}^2$ respectively. The ratio factors of these two cross sections are 1.04 and 0.95. This shows that the theoretical value decreases very rapidly with the increase of the impact energies. The experimental data decreases very slowly with the increase of impact energy.

4.9 He^{2+} impact double ionization cross section of Cu

Alpha particle impact double ionization cross section has been computationally calculated by using equation (3.30). The needed equations, approximations and atomic data are taken as discussed in Section 3.1.4. The calculated result of double ionization cross sections of Cu atom along with experimental observations (Patton et al.1995) have been shown in Table 10 and Figure 12. The contribution of direct double ionization cross sections are considered from pair of sub shells (4s, 3d) and (4s, 3p). In the lower energy range from 54 keV to 88 keV/amu, the calculated cross sections overestimate the experimental data and ratio factor is greater than 2 . With the increase of impact energy, the calculated cross sections and experimental data

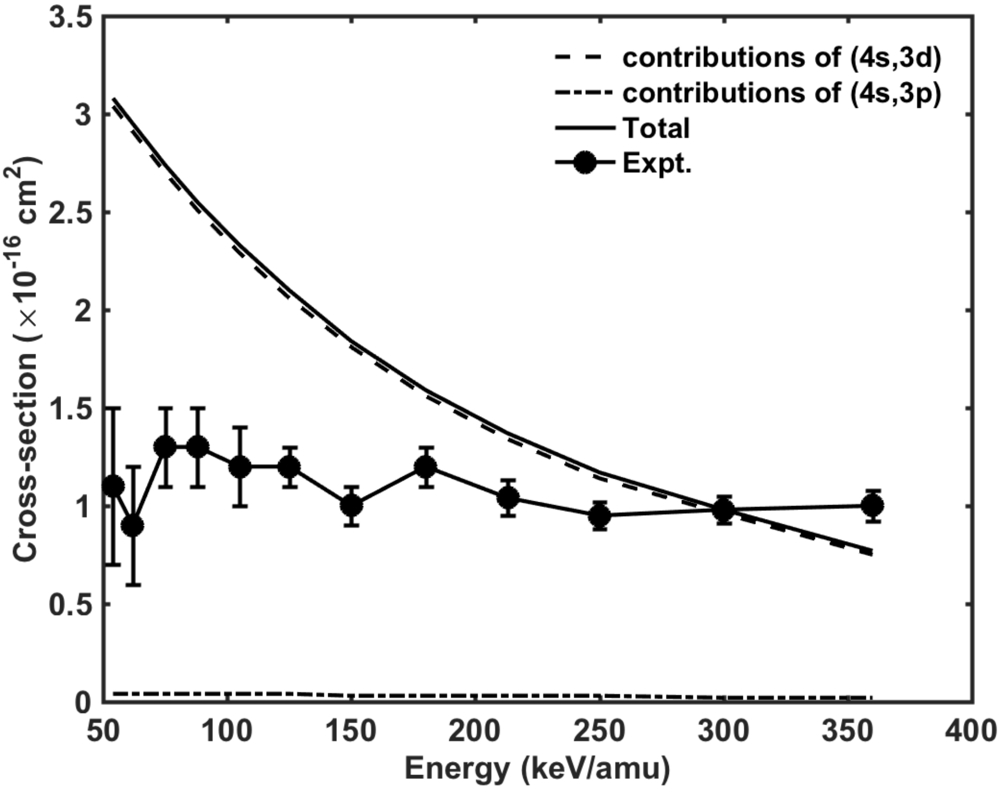

Figure 12: Alpha particle impact double ionization cross sections of Cu atom along with its experimental values of single ionization cross section (Patton et al., 1995) against respective impact.

closer to each other and identical at energy 300 keV/amu having magnitude of $0.98 \times 10^{-16}\text{cm}^2$. In threshold region the probability of ionization and capture should not be ignored due to the possibility of electron capture. The ratio factors are within 2 in between impact energies of 88 keV/amu to 360 keV/amu. About 75 % of total theoretical results are in agreement with experimental data. Major contribution is from (4s, 3d) which is about 98% to the total DICS of Cu. Overall our result revels success of BEA in the case of alpha particle impact double ionization of Cu.

4.10 H^+ impact double ionization cross section of Fe

As stated in Section 4.9, proton impact double ionization cross section of Fe has been calculated. The calculated result of double ionization cross sections of Cu atom by proton impact along with experimental observations (Patton et al.1995) have been shown in Table 11 and Figure 13. We have considered contribution of pair of orbitals (4s, 4s), (4s, 3d) and (4s, 3p). We have compared our results with the experimental data from energy range 93 keV/amu to 1440 keV/amu. Major contribution is from (4s, 3d) and it varies from 84% to 86%. Rest pairs of sub shells have insignificant contribution. In the threshold range the theoretical results dominates the experimental data while the calculated results decreases rapidly in comparison to the experimental measurements with the increase of energy. Both the results are coming closer to each other with the increase of energy and at 720 keV/amu it is almost similar. The calculated results and experimental data at 720 keV/amu are $1.84 \times 10^{-17}\mathrm{cm}^2$ and $1.81 \times 10^{-17}\mathrm{cm}^2$.In the threshold region of energy from 93 keV/amu to 250 keV /amu the ratio factor is greater than 2.

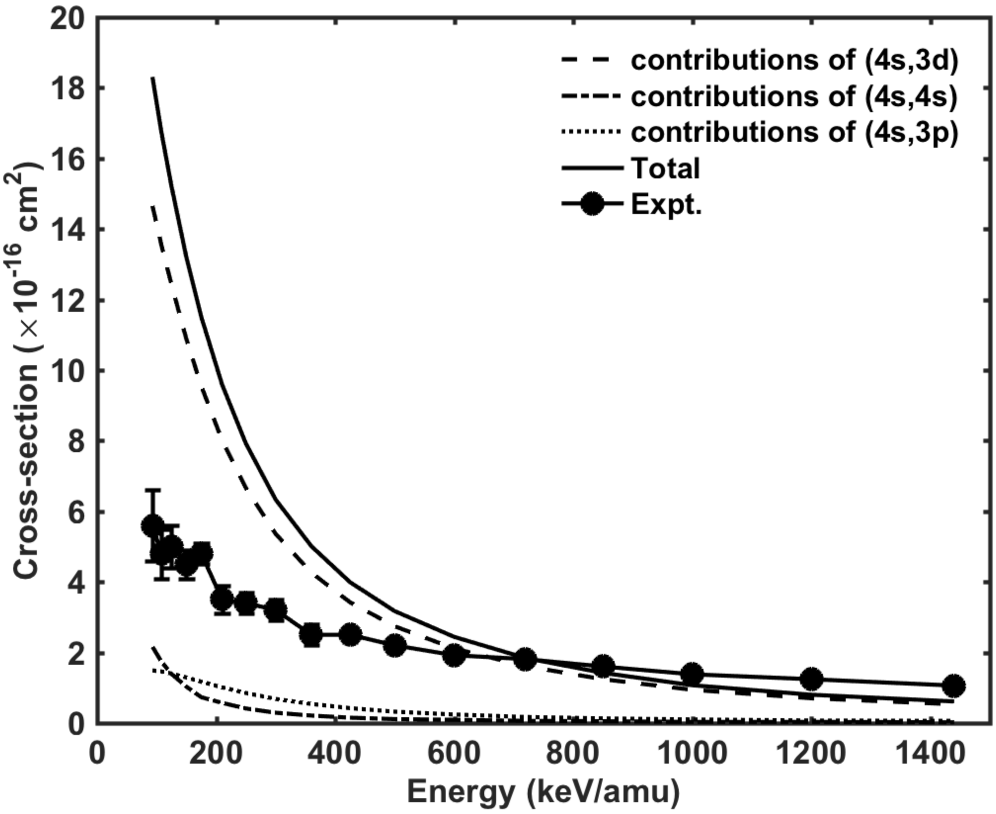

Figure 13: Proton impact double ionization cross section of Fe atom along with its experimental values of single ionization cross section (Patton et al., 1995) against respective impact energy.

All the calculated results above the impact energy 360 keV/amu are within ratio factor of 2. Both the results come closer to each other with the increase of energy. In between impact energy of 300 keV/amu to 1440 keV/amu 58.8% results are within ratio factor 2 and 29.4% total results have ratio factor ≤ 1.5. At 720 keV/amu both calculated and experimental cross section are $1.84 \times 10^{-17}\mathrm{cm}^2$ and $1.81 \times 10^{-17}\mathrm{cm}^2$ respectively. Figure.13 shows that the experimental data have random fluctuation from threshold energy range. Magnitude of experimental data decreases smoothly with slight fluctuation in threshold region. The over estimation of the calculated results at low energy range is the usual feature of our BEA. The ratio factor are 1.44, 1.01, 0.88, 0.64, 0.57 at impact energies 500 keV/amu, 720 keV/amu, 850 keV/amu, 1200 keV/amu, and 1440 keV/amu respectively. From the above discussion it is seen that with the increase of impact energy the theoretical results are coming closer to each other. Results are supposed to be in good agreement with the experimental results.The discrepancies observed in experimental results in threshold range might be due to quantum nature of interaction and probability of electron capture process which have not included in our present model of BEA.

4.11 He^{2+} impact double ionization cross section of Fe

Alpha particle impact double ionization of Fe has been computationally calculated by using equation (3.30).The needed equations, approximations and atomic data are taken as discussed in Section 3.1.4.

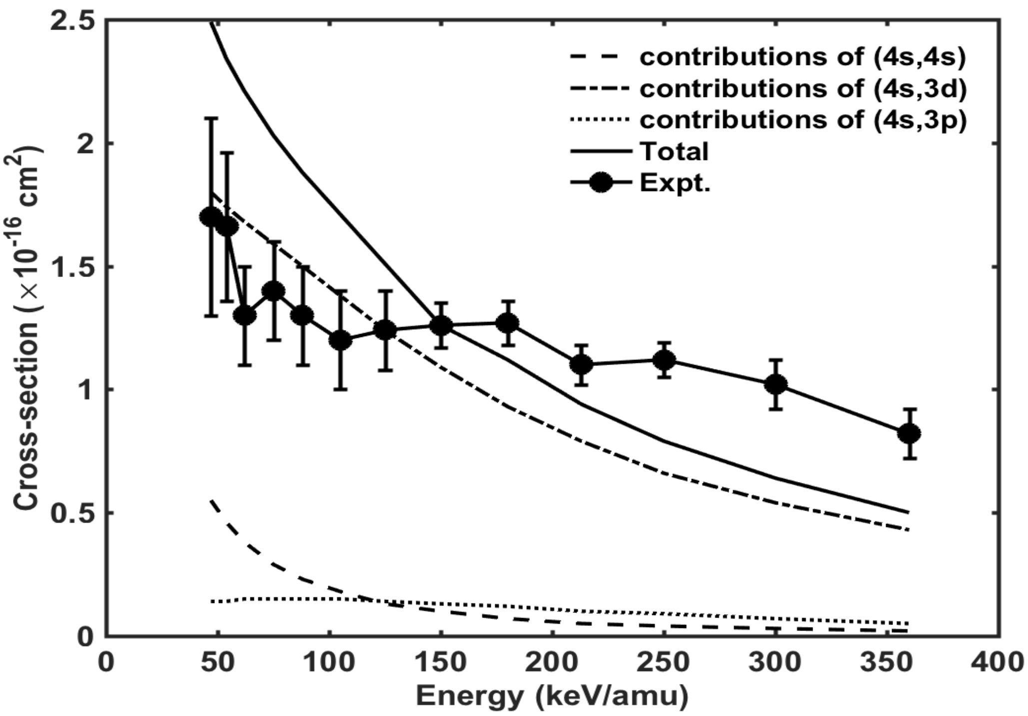

Figure 14: Alpha particles impact double ionization cross sections of Fe atom along with its experimental values of single ionization cross section (Patton et al., 1995) against respective impact energy.

We have calculated alpha particle impact direct DICS of Fe from impact energy of 47 keV/amu to 360 keV/amu and analyzed with the experimental data (Patton et al., 1995) as shown in Table 12 and Figure 14. All theoretical results have ratio factor less than 2. About 76.9% results have ratio factor less than 1.5 and 38.4% have ratio factor 1.25. So, the results are in good agreement with experimental data. We considered the contribution of pair of sub shells (4s, 4s), (4s,3d) and (4s, 3p) only. Major contribution to the total DICS is from (4s, 3d) which is of 72% to 86%. The overestimation of the calculated DICS at low energy range is usual trend of binary encounter approximation. The ratio of the calculated cross sections to the experimental data is almost within the factor 2 for all impact energies. However there is randomness in the experimental data especially in low energy range. Our model does not include process of pure quantum effect of indirect ionization occurring in the threshold region. So, the results are in good agreement with experimental data. The variations in the calculated results and experimental data are five and two times respectively.

CHAPTER 5

5. CONCLUSION AND RECOMMENDATIONS

5.1 CONCLUSION

Theoretical investigation of electron impact single ionization cross sections of Kr, Xe and Fe, electron impact double ionization of Fe, proton and alpha particles impact single and double ionization of Cu and Fe have been performed. The binary encounter approximation is used in above mentioned calculations. Accurate expression of $\sigma_{\Delta E}$ including exchange and interference effects given by Vriens and Hartree-Fock velocity distribution function for the target electrons have been used in the calculations.

In the case of Kr, the ionization cross section from threshold 15 eV to 1000 eV impact energy has been calculated. Such calculation over a wide energy range has never been reported earlier. In case of Kr, we have taken the contribution of 4p, 4s and 3d shells respectively; the remaining inner shell contributions are almost negligible and hence not taken into account. Near the threshold energy range the magnitude of calculated cross sections are higher in comparison to experimental data which is a usual feature of model used. Present model is valid for intermediate and high energy range. With the increase of energy the calculated results come closer to the experimental data. The peak is observed in the present calculations at impact energy 45 eV while the experimental peak is observed at impact energy of 65 eV. The ratio of the calculated peak to experimental peak is 1.38 and calculated peak shifted towards low energy side. Collectively about 94.7% of theoretical results have ratio factor less than two, 84.2% have less than 1.5 and 60% have less than 1.25.Major contribution to total single ionization cross section is from 4p sub shell which vary from 97% to 64%. Beyond energy 700 eV the ratio of theoretical to experimental values are almost same and ratio factor is 1.05. Calculated results are in excellent agreement with the experimental findings in the energy range 102 eV to 1000 eV.

In the case of Xe, the electron impact ionization cross section from the threshold 14 eV to 1000 eV of impact energy. The contribution of 5p, 5s, 4d and 4p shells are considered for the calculation of single ionization cross sections. The ratio of theoretical peak to the experimental peak is about 1.91. Ratio factor in threshold region below 35 eV is greater than 2 and increase with decreases of impact energy. In general, about 71% theoretical results have ratio factor less than 2, 55% have less than 1.5. With the increase of the impact energy, the ratio gradually decreases. Beyond impact energy of 90eV, the ratio factor becomes less than 1.5. Major contribution to the total SICS is from 5p which varies from 97% to 77%. It is because of the high energy state of the 5p. The calculated results are higher than the experimental data throughout the energy range considered. The calculated results show reasonably good agreement with experiment in the entire energy range. Beside this the electron impact single ionization cross section of Fe has also been calculated from 8.1 eV to 1250 eV of impact energy. In this calculation we have taken the contribution of 4s, 3d and 3p shells only. The calculated results come closer to the experimental results with increase of impact energy from 8.6 eV to 1250 eV. The calculated peak and the peak measured by Shah et al. (1993) have the ratio above 1.54. Similar to the case of Kr and Xe the magnitude of the calculated peak is shifted slightly towards lower energy side compared to the experimental peak. About 93.9% of results have ratio factor less than 2 and 16% have less than 1.5. The major contribution to the total SICS are from 4s and 3d sub shells while the contributions of 3p sub shell is almost negligible. Here Fe has an electronic structure with 6 electrons in 3d shell and 2 electrons in 4s shell. It is quite surprising that the experimental data of electron impact double ionization Fe measured by Shah et al. (1993) has eight peaks in between energy range of 80 eV to 325 eV. It indicates that there are large fluctuations in the results of experimental measurement. Experimental data attain maximum at 80 eV and slow decrease in DICS in energy range of 80 eV to 325 eV indicating significant contribution from direct process. Obviously direct double ionization of Fe is considered from ejection of loosely bound electrons from pair of orbitals (3d, 4s) ionization of 3s electron alone which lead to an excited state which results double ionization through auto ionization. One more sticking feature that observed in the experiment is indirect ionization process arising from inner shell in between the energy of 80 eV to 320 eV. However, there is no indication of structure in the theoretical double ionization curve. This is not in accordance with the usual trend of direct double ionization cross section which shows a faster decrease of ICS in high energy region after attaining maximum value $7.4 \times 10^{-17} \mathrm{cm}^2$ at impact energy at 74 eV. Beyond this energy the contribution of direct double ionization falls rapidly. In the case of proton impact single ionization cross section of Cu and Fe in given range of impact energy, the ratio factor for former case vary from 1.27 to 1.005 for energy range of 175 keV /amu to 1000 keV/amu. All the calculated result have ratio factor less than 1.28 and about 88% of the results have ratio factor less than 1.25 and 44% of data have ratio factor less than 1.12. The results are excellent agreement with experimental data. Major contributions to the total value are from 4s and 3d that varies from 68.2% to 20.4% and 28.8% to 63.2% respectively. In the latter case of SICS of Fe by proton impact 58% of results have ratio factor less than 2 where major contribution to total SICS from 4s and 3d having contributions of 69% to 25% and 27% to 64% respectively. About 94% of results have ratio factor less than 2 for (4s+3d) and 31% have ratio factor less than 1.5. The theoretical results are in excellent agreement throughout the given energy range. The binary encounter approximation approach shows good agreement with the experimental data at high energy region lying within factor two. At this point it is worth mentioning that the observation made by Lotz (1970) on calculated electron impact ionization cross section of atoms and ions with the help of empirical formula and found reasonable agreement with experimental data in most of the cases. In the case of electron impact single ionization of Cu, Lotz has pointed out that it is necessary 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 Ag ($4d^{10}$ $5s^1$) 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 that the result so obtained is in excellent agreement with the experimental data throughout the energy range investigated. The discussion given above clearly explains why the inclusion of one 3d electron brings calculated result in excellent agreement with the experiment. More theoretical investigation is required for quantitively understanding of the processes of single ionization from 3d shell of Cu. It is hoped that this work will stimulate other theoretical workers to take up further study of the problem. In the case of double ionization cross sections of Cu by H^+ impact we considered contributions from the ejection of two electrons from pairs of sub shells (4s, 3d) and (4s, 3p) only in the energy range 125 keV/amu to 1440 keV/amu. About 60% of theoretical results have ratio factor ≤ 2 from energy range 360 keV/amu to 1440 keV/amu and in threshold range our model fails to account. Under valid range (4s, 3d) has major contribution of 95% to 96%. At 720 keV/amu ratio factor is 1.04. In the case of H^+ impact single ionization of Fe in energy range 70 keV/amu to 1440 keV/amu about 94.7% of theoretical results of (4s+3d) have ratio factor ≤ 2 and 31% has ratio factor ≤ 1.5. The results in excellent agreement to experiment Major contributions are from sub shell 4s and 3d. Theoretical results overestimate the experimental data throughout the energy range. In the case of proton impact double ionization of Fe 58% of total results have ratio factor ≤ 2 and major contribution is from (4s, 3d) which is 84% to 86% of total DICS of Fe. Results are in satisfactory agreement to experimental results. At low energy the theoretical results dominate to the experimental data and falls sharply with the increase of impact energy. With the increase of impact energy, the results are coming close to each other and are within the factor of 2. In the case of alpha particle impact single ionization of Cu and Fe experimental curve dominates theoretical curve. Here in the first case all results have ratio factor less than 2 and major contribution are from 3d and 4s. About 50% of results have ratio factor less than 1.5. These results are in good agreement to experimental data for respective impact energy. Variation in theoretical results and experimental data are nearly same. In the case of SICS of Fe all results have ratio factor less than 2 and about 66% results have ratio factor less than 1.5, 40% have ratio factor less than 1.25 and 20% have ratio factor less than 1.05. The theoretical and experimental data converge with impact energy and come closer to each other. These results and nature of the results of two different atoms revels good agreement to the experimental data. Similar features in the case of alpha particle single and double ionization of Fe atom have been observed.

5.2 RECOMMENDATIONS

In this work heavy charged particles impact single and double ionization cross section for Cu and Fe atoms has been calculated in binary encounter approximation using Hartree-Fock momentum distribution for the target electrons. Electron impact single ionization cross sections for Kr, Xe and single and double ionization cross sections for Fe has been carried out. The findings of direct single and double ionization cross sections are compared and analyzed with the corresponding experimental data for given impact energies.

In the present calculation we have used the Hartree-Fock wave functions for the target electrons. It does not take proper account for the correlation between the electrons in the atom. The Hartree-Fock method is a form of the central field approximation. A better account of correlation between electrons can be taken into the wave functions by configuration interaction approach based of Slater-Condon theory and the multi configuration Hartree-Fock approach used by Fischer. It is expected that the cross sections calculated using wave function which take an account of configuration interaction would lead to improve the agreement between theoretical results and experimental data (Deb and Crothers, 1991).

It has been found that the binary encounter theory give reasonable estimates of ionization and electron capture cross sections in a variety of ion-atom collision processes. At high impact energies the processes may take place from inner-shells of the target. In the case of heavier targets, the inner shell electrons have velocities comparable to the velocity of light. In such cases relativistic effects becomes important. Contribution from the inner shells has to be taken for high atomic number systems where electrons have relativistic nature. Hence effect of relatively on the motion of electrons must be considered. It has been reported that the effect of relativity enhances the ion cross sections when ionization takes place from inner shells. In the case of binary encounter calculation for ion impact inner shell ionization cross section, the effect of polarization of atomic orbital due to passage of projectile and the effect of finite energy loss of the projectile are usually neglected. Several workers (Brandt et al., 1979; Mukoyama et al.,1982) have proposed on the basis of quantal and semi-classical approximations, some simple correction factors to account for the relativistic effects of the bound electron. This correction factor may be used in the BE calculations. The relativistic effects can also be approximately taken into account by using the relativistic expressions of mass and kinetic energy of the bound electron in the cross section formula (Hansen, 1973). Inclusion of the contribution of these effects may improve the results of ionization cross sections under binary encounter approximation. This can be done by using the correction factor proposed on the basis of quantal calculation (Brandt and Lapicki, 1979).

CHAPTER 6

6. SUMMARY

It is observed that the binary encounter theory gives reliable values of cross sections for variety of charged particle-atom collision processes with varying amount of success at intermediate and high impact energy. In general, it is observed that the calculated cross sections overestimate the experimental cross sections at low impact energy region whereas these cross sections fall below the experimental values at high impact energy. The above facts is true in the case of alpha particle impact double ionization of Fe, H^+ impact double ionization of Fe, Cu and electron impact double ionization of Fe. In the case of alpha particle impact single ionization of Fe and Cu, experimental results overestimate the calculated results throughout the energy region. In some cases, there are some uncertainties in experimentally observed data because of the presence of significant fluctuations and more experiments as well as theoretical analysis are required. In the case of Cu, percentage contribution of 3d relative to 4s are found more than twice compared to 4s in in the intermediate and higher energy regions. Maximum and minimum contribution of 3d are 71.2662% and 63.184% whereas maximum and minimum contribution of 4s are 35.655% and 22.959% above impact energy of 54 keV/amu. Contribution of 4s decreases with increase of impact energy. On the other hand 3d contribution increases with the rise of impact energy. Ionization of orbitals depends on the electronic energy states. Orbital electrons take part in the process of ionization that possesses relatively high energy. Collision interaction at low energy is purely of quantum effect and phenomenon of electron capture dominant. The Model does not include all physical insight of ionization at low energy range. The sharp fall in cross sections of 4s in low energy range is due to lack of suitability of our semi-classical model of BEA. Overestimation of cross section at low incident energies is be due to the neglect of the presence of other electron in the target atom and some other process happening during ionization. The binary encounter approximation fails to take proper account of distant encounters. On the basis of results it is concluded that the present approach of binary encounter approximation provides suitable theoretical description of electron and heavy particle impact single and double ionization cross sections and results are in overall good and satisfactory agreement with the experimental observations for wide range of impact energy.

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APPENDEX

A. Wave function approach

(i) Hartree`s approximation

The Hartree method (1968) is one of the first approximations that tried to deal problem of many particles system. It does not account the anti-symmetric characteristic of all electron wave functions. As a result, the exchange term is missing. According to this theory the many- body wave function can be expressed as a product of independent single electron functions $\phi_i(r_i)$ .The wave function of the system will be of form

$$\psi_H(r_1, r_2 \dots r_n) = \phi_1(r_1)\phi_2(r_2) \dots \phi_n(r_n) \quad (1)$$

The total energy of the system becomes

$$H\psi(r_1, r_2, \dots, r_n) = E\psi(r_1, r_2, \dots, r_n) \quad (2)$$

$$E = \langle\psi|H|\psi\rangle = \int d^3\, r_1 \int d^3\, r_2 \dots \int d^3\, r_n(\phi_1^*\phi_2^* \dots \phi_n^* H \phi_1\phi_2 \dots \phi_n)$$

$$= \sum_{i=1}^{n} \int d^3\, r\phi_i^*(r)\left\{-\frac{\nabla^2}{2}\ (r)\right\}\phi_{\mathrm{i}}(r)$$

$$\times \sum_{ij, i\neq j} \int d^3\,(r) \int d^3\,(r')\phi_i^*\,(r)\frac{1}{|r-r'|}\phi_j^*(r')\phi_j(r') \quad (3)$$

To obtain electron wave function ψ_i(r) we we must minimize the total energy subjecting to normalization condition:

$$I = \int \phi_i^*\ \phi_i(r)dr = 1 \quad (4)$$

One may replace the Schrodinger equation with the Variational principle. By variational method, wave function $\psi_i(r)$ and total energy E satisfy

$$\delta\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = 0 \quad (5)$$

$$\delta(E-\lambda I) = \int d^3(r)\delta\phi_i^*\,(r)\left\{\left(-\frac{\nabla^2}{2} + V_{\mathrm{ext}}\right)\psi_i + \left(\int d^3\,(r')\right)\frac{1}{|r-r'|}\sum_{j\neq i}\phi_i^*(r')\phi_i(r') - \lambda\phi_i\right\}$$

$$+ \int d^3 r\delta\phi_i\,(r)\left\{\left(-\frac{\nabla^2}{2} + V_{\mathrm{ext}}\right)\phi_i^* + \left(d^3(r')\frac{e^2}{|r-r'|}\sum_{j\neq i}\phi_i^*(r')\phi_j(r')\right)\psi_i^* - \lambda\phi_i^*\right\} = 0 \quad (6)$$

Now the equation of Hamiltonian in terms of $\phi_i(r)$ can be written as,

$$\left(-\frac{\nabla^2}{2}+V_{\text{ext}}+\int d^3\,r'\,\frac{1}{|r-r'|}\sum_{i\neq j}\phi_j^*\,(r')\phi_j(r')\right)=\lambda\phi_i(r) \tag{7}$$

$$\left(-\frac{\nabla^2}{2}+V_{\text{ext}}+V_{\text{SC}}\right)\phi_i=\varepsilon_i\phi_i(i=1,2,3,\ldots,n,\lambda\rightarrow\varepsilon_i) \tag{8}$$

where

$$V_{\text{SC}}=V_{\text{H}}=\int d^3r'\,\frac{1}{|r-r'|}\sum_{i\neq j}\phi_j^*\,(r')\phi_j(r')=\sum_{j\neq i}\left|\phi_j^*(r')\right|^2 \tag{9}$$

This is called the Hartree`s potential which only includes Coulomb repulsion between electrons. Potential is different for each particle. It is a mean field approximation to electron-electron interaction, considering elctronic charge only. It is also called self-consistent field approximation. This is an equation that satisfies single particle wave function for the i^{th} electron. It is an eigen value equation for a single electron moving in Coulomb potential of the nucleus plus a potential due to all the other electrons. The potential due to the other electrons depends on the charge density $\left|\phi_{(rj)}\right|^2$.Self-consistent field approximation is an iterative procedure for solving the above set of equations. A trial function is used to calculate the initial charge density. New single particle wave function is found by solving the above equations. These wave functions now yield new charge density and hence yield new wave function. The procedure is repeated until the single particle wave functions ϕ_i and the single particle energy ε_i no longer change, i.e., until self-consistency is reached.

The Hartree approximation is a staightforward task to calculate the variational lowest energy. Since the simple product of wave equations doesn`t change when the posions of any two electrons are changed i.e. the Hartree equation neglects the spin direction of electrons. So, to account spin direction of an electron we have to go through Hartree-Fock approximation. In order to satisfy the anti-symmetry condition and to include exchange and corelation part, a more sophisticated form of the Hartree wave function is requried.

(ii) Hartree-Fock approximation

Hartree-Fock theory (1930) is one of the simplest approximate theories for solving the mainy-body Hamiltonain. This approximation includes the anti-symmetric character of electronic wave function in terms of single Slater (1937) determinant of n spin-orbitals as,

$$\psi_{HF} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(r_1, s_1) & \phi_2(r_1, s_2) & \cdots & \cdots & \phi_n(r_1, s_n) \\ \phi_2(r_2, s_1) & \phi_i(r_2, s_2) & \cdots & \cdots & \phi_2(r_2, s_n) \\ \cdots & \cdots & \cdots & \cdots & \cdots\cdots \\ \phi_n(r_n, s_1) & \phi_n(r_n, s_2) & \ldots & \ldots & \phi_n(r_n, s_n) \end{vmatrix} \tag{10}$$

Now the Hamiltonian in the form of ϕ (r) can be expressed as,

$$\left(-\frac{\nabla^2}{2} + V_{\text{ext}}\right) + \int d^3 r' \frac{1}{|r - r'|} \sum_{\mathrm{j \neq i}} \phi_j^*(r')\phi_j(r')\phi_i(r)$$
$$- \sum_{\mathrm{j \neq i}} \phi_j^*(r')\phi_i(r')\phi_j(r)\delta_{\delta_i \delta_j} = \varepsilon_i \phi_i(r) \tag{11}$$

where the exchange potential can be expressed as

$$V_{\mathrm{x}} = -\sum_{\mathrm{j \neq i}} \frac{1}{|r - r'|} \phi_j^*(r')\phi_j(r')\phi_i(r) = \varepsilon_i \phi_i(r) \tag{12}$$

This indicates that the screening potential includes both Hartree and exchange terms, the equation of Hartree-Fock approximation will be

$$\left(-\frac{\nabla^2}{2} + V_{\text{ext}} + V_{\text{SC}}\right)\phi_i = \varepsilon_i \phi_i \tag{13}$$

$$V_{\text{SC}} = V_{\text{H}} + V_{\text{x}} \tag{14}$$

The left-hand side of the equation 11 consists of four terms. The first and second are the kinetic energy contribution and the electron–ion potential, third term or Hartree term, is the simply electrostatic potential arising from the charge distribution of N electrons. Inclusion of an in physical self-interaction of an electron term (when $j = i$) is canceled in the fourth exchange term. The exchange term results from our inclusion of the Pauli principle and the determinantal form of wave function. The Hartree-Fock energy E_{HF}^0 is higher than the exact ground state energy E_{exact}^0 of the many body system and the difference ($E_{\text{exact}}^0 - E_{\text{HF}}^0$) is called the correlation energy. Hartree-Fock approximation does not include the electron correlation part to the multi-electron wave function, which plays an important role in the electronic structure and binding of many solid.

In spite of the importance and achievements of the Hartree-Fock approximation, corrections beyond it are often considered due to the fact that a single determinant state, even with the best possible orbitals, remains in general a rather poor representation of the complicated ground state wave function of many-body system. This leads to the development of the density functional theory.

B. Electron correlation and correlation energy

It is very difficult to know with certainty what is going to happen in the atomic scale in matter or molecules.

Correlation may be regarded as a conceptual bridge from properties of individual to properties of groups. In atoms and molecules correlation occurs because electrons interact with one another and electrons are interdependent. This electron correlation determines structure and dynamics of many electron systems. The dynamics of electron correlation may affect single electron transition. However, this effect is sometimes difficult to separate from other effects. Correlation is usually dominant in multiple electron transitions for fast collisions. This means that multiple electron transitions in fast collisions provides an unobstructed view the dynamics of electron correlation.

First, a review of uncorrelated classical probabilities and then extends these concepts to correlated quantum systems. A transition occurs in an atom when one or more electron jumps from their initial state to a different final state in the atom. The outcome of such an atomic transition is specified by the final state of the atom after the interaction. Within the Hartree-Fock method of Quantum chemistry, the antisymmetric wave function is approximated by a single Slater-determinant. Exact wave function, however, cannot, generally, be expressed as a single determinant. The single determinant approximation does not consider Coulomb correlation, leading to a total electronic energy different from the exact solution of the no relativistic Schrodinger equation within Born-Oppenheimer approximation.

The concept of the correlation energy has been studied earlier by Winger. A certain amount of electron correlation found in the electron exchange term describing the correlation between electrons with parallel spin, is already considered within the HF approximation. The basic correlation prevents two parallel spin electrons from being found at the same point in space.

C. Density functional theory

Hartree-Fock method considers the interaction between electrons only in an average way, but motion of electrons of opposite spins remains uncorrelated. The H-F approximation can be improved by considering the electron correlation which is mainly caused by the instantaneous interaction between electrons.

The first attempt to use the electron density rather than the wave function for obtaining information about atomic and molecular systems is the method of Thomas and Fermi proposed in 1927. Although their approximation is not accurate enough for present day electronic calculations, the approach illustrates the way density functional theory (DFT) work.

The modern formulation of the density function theory originated by P. Hohenberg and W. Kohn in 1964. Later on, Kohm and L. Sham (1965) developed with the introduction of atomic orbitals which is the foundation of current application of DFT in computational approach.

Density function theory (DFT) is one of the most useful and fundamental approach to consider of electron correlation. It is a quantum mechanical theory of correlated many body systems and is used to investigate the electronic structure of systems. The DFT is most popular and versatile methods available in condensed matter physics. As the name density functional suggests, it is a many body theory based on the idea of using only the density as basic variable for describing many electrons system. All of this is done by promoting the particles density n(r) from just one among observables to the status of key variable, on which the calculation of all other observables can be based. This approach forms the basis of the large majority of electronic structure calculations in the physics and chemistry. The electrical, magnetic and structural properties of atoms and materials have been calculated using DFT.

The DF approach can be summarized by the sequence

$$(r) \rightarrow \psi(\mathrm{r}_1, \mathrm{r}_2, \ldots, \mathrm{r}_\mathrm{n}) \rightarrow \mathrm{V(r)} \qquad (15)$$

This relation implies that if one has knowledge of *n(r)* also has knowledge of the wave function and the potential and hence of all other observables. The electron density is related to total electron number by the relation

$$N = \int n(r)dr \qquad (16)$$

D. Tables

Table 1: Electron impact single ionization cross section of Kr in the units of 10^{-16} cm^2.

E(eV)	Contribution of			Total	Experiment
	4p	4s	3d		
22	3.46	-	-	3.46	1.48
24	3.80	-	-	3.80	1.76
26	4.04	-	-	4.04	2.14
28	4.21	-	-	4.21	2.34
30	4.34	-	-	4.34	2.55
35	4.5	0.13	-	4.63	2.99
40	4.53	0.25	-	4.78	3.24
45	4.50	0.33	-	4.83	3.38
50	4.43	0.39	-	4.82	3.45
55	4.35	0.43	-	4.78	3.48
60	4.25	0.45	-	4.70	3.45
65	4.14	0.47	-	4.61	3.49
70	4.04	0.49	-	4.53	3.45
75	3.94	0.50	-	4.44	3.45
80	3.83	0.51	-	4.34	3.43
90	3.64	0.52	-	4.16	3.40
100	3.46	0.52	-	3.98	3.33
120	3.15	0.52	0.07	3.74	3.20
130	3.01	0.51	0.10	3.62	3.11
140	2.88	0.51	0.12	3.51	3.05
150	2.77	0.50	0.14	3.41	3.98
160	2.66	0.50	0.15	3.31	2.91
170	2.56	0.49	0.16	3.21	2.86
180	2.47	0.48	0.17	3.12	2.78
190	2.39	0.48	0.18	3.05	2.72
200	2.31	0.47	0.18	2.96	2.68
225	2.13	0.45	0.19	2.77	2.54
250	1.98	0.44	0.20	2.62	2.42
275	1.85	0.43	0.20	2.48	2.29
300	1.74	0.41	0.20	2.35	2.19
350	1.55	0.39	0.20	2.14	2.01
400	1.40	0.37	0.20	1.97	1.85
500	1.18	0.33	0.19	1.70	1.60
600	1.02	0.31	0.16	1.49	1.43
700	0.90	0.28	0.17	1.35	1.28
800	0.80	0.26	0.16	1.22	1.16

900	0.73	0.24	0.15	1.12	1.07
1000	0.66	0.23	0.14	1.03	0.98

Table 2: Electron impact single ionization cross-sections of Xe in the units of 10^{-16} cm^2.

E (eV)	Contribution of				Total	Experiment
	5p	5s	4d	4p		
14	2.56	-	-	-	2.56	0.73
16	4.70	-	-	-	4.70	1.37
18	6.08	-	-	-	6.08	2.01
20	7.00	-	-	-	7.00	2.43
22	7.63	-	-	-	7.63	2.90
24	8.05	-	-	-	8.05	3.33
26	8.34	0.01	-	-	8.35	3.62
28	8.52	0.08	-	-	8.60	3.80
30	8.64	0.13	-	-	8.77	4.01
35	8.72	0.22	-	-	8.94	4.48
40	8.63	0.27	-	-	8.90	4.59
45	8.46	0.30	-	-	8.76	4.60
50	8.24	0.32	-	-	8.56	4.58
60	7.76	0.35	-	-	8.11	4.62
70	7.29	0.36	-	-	7.65	4.67
80	6.85	0.35	0.05	-	7.25	4.64
90	6.44	0.35	0.14	-	6.93	4.53
100	6.08	0.34	0.19	-	6.61	4.44
120	5.45	0.33	0.26	-	6.04	4.19
130	5.18	0.32	0.28	-	5.78	4.05
140	4.94	0.31	0.30	-	5.55	3.97
150	4.72	0.30	0.31	-	5.33	3.89
160	4.52	0.29	0.32	-	5.13	3.78
170	4.33	0.28	0.32	-	4.93	3.67
180	4.16	0.28	0.33	-	4.77	3.58
190	4.00	0.27	0.33	0.01	4.61	3.51
200	3.86	0.26	0.33	0.01	4.46	3.44
225	3.53	0.25	0.33	0.02	4.13	3.25
250	3.26	0.23	0.33	0.02	3.84	3.06
300	2.83	0.21	0.32	0.03	3.39	2.77
350	2.50	0.19	0.31	0.03	3.03	2.48
400	2.24	0.17	0.29	0.03	2.73	2.31
500	1.86	0.15	0.27	0.03	2.31	2.00
600	1.59	0.13	0.25	0.03	2.00	1.75
700	1.39	0.11	0.23	0.03	1.76	1.58
800	1.28	0.10	0.21	0.03	1.58	1.42

900	1.12	0.09	0.20	0.03	1.44	1.32
1000	1.02	0.09	0.19	0.02	1.32	1.21

Table 3: Electron impact single ionization cross section of Fe in the unit of $\times 10^{-16}$ cm^2.

E(eV)	Contribution of			Total	Experiment .
	4s	3d	3p		
8.10	1.26	-	-	1.26	0.33 ± 0.05
8.30	1.47	-	-	1.47	0.44 ± 0.06
8.60	1.76	-	-	1.76	0.70 ± 0.06
8.80	1.93	-	-	1.93	1.08 ± 0.07
9.40	2.38	-	-	2.38	1.34 ± 0.08
9.90	2.70	-	-	2.70	1.54 ± 0.08
10.40	2.96	-	-	2.96	1.96 ± 0.09
11.00	3.23	-	-	2.23	2.18 ± 0.08
11.60	3.46	-	-	3.46	2.22 ± 0.07
12.00	3.59	-	-	3.59	2.39 ± 0.10
12.60	3.76	-	-	3.76	2.46 ± 0.01
13	3.85	-	-	3.55	2.50 ± 0.11
14	4.05	-	-	4.05	2.83 ± 0.11
15	4.20	-	-	4.20	2.94 ± 0.11
16.10	4.32	-	-	4.32	3.15 ± 0.14
16.80	4.38	-	-	4.38	3.42 ± 0.13
19	4.48	0.45	-	4.93	3.65 ± 0.17
21	4.50	0.93	-	5.43	3.91 ± 0.17
23	4.49	1.29	-	5.78	3.95 ± 0.13
26	4.42	1.67	-	6.09	4.01 ± 0.13
29	4.30	1.92	-	6.22	3.80 ± 0.16
30	4.27	1.98	-	6.25	3.92 ± 0.13
32.5	4.17	2.12	-	6.29	3.98 ± 0.12
35	4.06	2.21	-	6.27	4.08 ± 0.15
42	3.76	2.37	-	6.13	3.77 ± 0.15
47	3.56	2.42	-	5.98	3.76 ± 0.17
52	3.37	2.45	-	5.82	3.58 ± 0.14
60	3.11	2.45	-	5.56	3.42 ± 0.19
70	2.83	2.42	-	5.25	3.29 ± 0.18
80	2.59	2.37	0.02	4.98	2.93 ± 0.14
85	2.49	2.34	0.05	4.88	2.93 ± 0.13
90	2.39	2.31	0.07	4.77	2.87 ± 0.15
95	2.30	2.28	0.08	4.66	2.83 ± 0.14
100	2.22	2.25	0.09	4.56	2.60 ± 0.13
110	2.07	2.19	0.12	4.38	2.46 ± 0.12

120	1.94	2.13	0.13	4.20	2.51 ± 0.13
130	1.83	2.07	0.14	4.04	2.27 ± 0.11
140	1.73	2.02	0.15	3.90	2.34 ± 0.11
150	1.64	1.97	0.15	3.76	2.19 ± 0.04
160	1.56	1.92	0.16	3.64	2.14 ± 0.11
170	1.49	1.87	0.16	3.52	1.97 ± 0.10
180	1.42	1.82	0.16	3.40	1.92 ± 0.08
190	1.36	1.78	0.16	3.30	1.84 ± 0.07
200	1.31	1.74	0.16	3.21	1.82 ± 0.09
225	1.19	1.64	0.16	2.99	1.70 ± 0.08
250	1.09	1.56	0.16	2.81	1.68 ± 0.09
275	1.00	1.48	0.16	2.64	1.53 ± 0.09
300	0.94	1.42	0.16	2.52	1.46 ± 0.05
325	0.87	1.35	0.15	2.37	1.35 ± 0.07
370	0.78	1.26	0.15	2.19	1.30 ± 0.07
400	0.73	1.20	0.14	2.07	1.12 ± 0.05
450	0.66	1.11	0.14	1.91	1.05 ± 0.05
500	0.60	1.04	0.13	1.77	1.06 ± 0.05
550	0.55	0.98	0.12	1.65	0.91 ± 0.04
600	0.51	0.92	0.12	1.55	0.87 ± 0.03
650	0.47	0.87	0.11	1.45	0.82 ± 0.04
710	0.44	0.82	0.11	1.37	0.77 ± 0.03
760	0.41	0.78	0.10	1.29	0.75 ± 0.04
800	0.40	0.75	0.10	1.25	0.70 ± 0.04
830	0.38	0.73	0.10	1.21	0.70 ± 0.04
860	0.37	0.71	0.10	1.18	0.68 ± 0.04
900	0.36	0.69	0.09	1.14	0.65 ± 0.04
1000	0.32	0.64	0.09	1.05	0.63 ± 0.05
1100	0.30	0.59	0.08	0.97	0.58 ± 0.05
1200	0.27	0.55	0.08	0.9	0.60 ± 0.05
1250	0.26	0.53	0.08	0.87	0.53 ± 0.05

Table 4 : Proton impact single ionization of Cu in the unit of 10^{-16} cm^2.

E(keV/amu)	Contribution of				Total	Experiment.
	4s	3d	3p	4s+3d		
80	3.26	1.38	0.14	4.64	4.78	5.50 ± 0.50
93	2.92	1.43	0.16	4.35	4.51	4.80 ± 0.40
108	2.62	1.48	0.18	4.10	4.28	4.40 ± 0.40
125	2.34	1.50	0.2	3.84	4.04	4.15 ± 0.28
150	2.03	1.53	0.22	3.56	3.78	3.88 ± 0.26
175	1.79	1.54	0.23	3.33	3.56	3.54 ± 0.22

210	1.54	1.52	0.25	3.06	3.31	3.14 ± 0.20
250	1.32	1.49	0.26	2.81	3.07	2.65 ± 0.13
300	1.12	1.44	0.25	2.56	2.81	2.30 ± 0.10
360	0.94	1.38	0.24	2.32	2.56	2.05 ± 0.10
425	0.80	1.30	0.23	2.10	2.33	1.85 ± 0.08
500	0.68	1.21	0.21	1.89	2.10	1.70 ± 0.06
600	0.57	1.09	0.19	1.66	1.85	1.48 ± 0.07
720	0.47	0.99	0.16	1.46	1.62	1.35 ± 0.07
850	0.40	0.88	0.14	1.28	1.42	1.13 ± 0.06
1000	0.34	0.77	0.13	1.11	1.24	0.97 ± 0.06
1200	0.28	0.66	0.11	0.94	1.05	1.01 ± 0.06
1440	0.23	0.55	0.09	0.78	0.87	0.83 ± 0.06

Table 5:.Proton impact single ionization cross section of Fe in the unit of 10^{-16} cm^2.

E (keV)	Contribution of				Total	Experiment
	4s	3d	3p	4s+3d		
70	6.51	2.55	0.29	9.06	9.35	7.5 ± 0.40
80	5.90	2.66	0.32	8.56	8.88	7.2 ± 0.30
93	5.28	2.77	0.35	8.05	8.40	6.8 ± 0.40
108	4.70	2.84	0.38	7.54	7.92	6.0 ± 0.30
125	4.18	2.90	0.41	7.08	7.49	5.5 ± 0.40
150	3.57	2.94	0.43	6.51	6.94	4.6 ± 0.28
175	3.12	2.93	0.45	6.05	6.50	3.9 ± 0.25
210	2.63	2.89	0.46	5.52	5.98	3.3 ± 0.22
250	2.22	2.80	0.45	5.02	5.47	2.8 ± 0.17
300	1.87	2.67	0.43	4.54	4.97	2.5 ± 0.14
355	1.58	2.48	0.40	4.06	4.46	2.1 ± 0.10
420	1.49	2.36	0.36	3.85	4.21	2.0 ± 0.14
500	1.13	2.13	0.32	3.26	3.58	1.6 ± 0.10
600	0.95	1.95	0.28	2.90	3.18	1.4 ± 0.07
720	0.79	1.74	0.24	2.53	2.77	1.2 ± 0.05
850	0.67	1.55	0.21	2.22	2.43	1.1 ± 0.05
1000	0.57	1.30	0.19	1.87	2.06	0.9 ± 0.05
1200	0.47	1.17	0.16	1.64	1.80	0.8 ± 0.06
1440	0.40	1.00	0.14	1.40	1.54	0.7 ± 0.05

Table 6: He^{2+} impact single ionization cross sections of Cu in the unit of 10^{-16} cm^2.

E (keV/amu)	Contribution of			Total	Experiment
	4s	3d	3p		
35	6.0	7.62	0.06	13.70	22.7 ± 1.5
40	5.4	7.66	0.07	13.18	24.0 ± 2.0
47	4.8	7.67	0.09	12.57	20.1 ± 1.2
54	4.3	7.62	0.10	12.06	21.5 ± 1.3
62	3.9	7.75	0.12	11.79	18.5 ± 1.0
75	3.4	7.21	0.14	10.77	15.8 ± 1.2
88	3.0	6.93	0.16	10.13	15.0 ± 1.3
108	2.6	6.54	0.18	9.39	13.7 ± 1.0
125	2.3	6.06	0.20	8.60	11.5 ± 0.2
150	2.0	5.49	0.22	7.74	9.8 ± 0.6
180	2.7	4.96	0.24	7.95	10.3 ± 0.5
213	1.5	4.39	0.25	6.16	8.5 ± 0.4
250	1.3	3.88	0.25	5.45	8.2 ± 0.4
300	1.1	3.28	0.25	4.65	7.2 ± 0.3
360	0.9	2.74	0.24	3.92	6.9 ± 0.3
425	0.8	2.32	0.23	3.35	6.2 ± 0.4

Table 7: Alpha impact single ionization cross section of Fe in the unit of $10^{-16}cm^2$.

Energy (keV)	Contribution of			Total	Experiment.
	4s	3d	3p		
35	10.70	3.78	0.15	14.63	21.0 ± 0.8
40	9.75	4.03	0.18	13.96	23.1 ± 1.0
47	8.60	4.33	0.21	13.14	22.5 ± 0.8
54	7.80	4.63	0.24	12.67	22.1 ± 0.9
62	7.10	4.88	0.27	12.25	20.3 ± 0.9
75	6.10	5.21	0.30	11.61	18.6 ± 0.9
88	5.50	5.45	0.34	11.29	16.8 ± 0.8
105	4.80	5.67	0.48	10.85	15.1 ± 0.6
125	4.20	5.81	0.41	10.42	13.4 ± 0.5
150	3.60	5.89	0.43	9.92	12.3 ± 0.5
180	3.00	5.86	0.45	9.31	11.3 ± 0.5
213	2.60	5.77	0.46	8.83	9.5 ± 0.4
250	2.20	5.60	0.45	8.25	8.7 ± 0.4
300	1.86	5.34	0.43	7.63	7.7 ± 0.3
360	1.56	5.03	0.40	6.99	6.7 ± 0.3

Table 8: Electrons impact double ionization cross section of Fe in the unit of $10^{-17}cm^2$.

E (eV)	Contribution of				Total	Experiment
	(4s,4s)	(4s,3d)	(4s,3p)	3s		
28.3	0.27	-	-	-	0.27	0.28 ± 0.06
33.3	0.48	-	-	-	0.48	0.61 ± 0.06
35.3	0.54	0.49	-	-	1.03	0.74 ± 0.06
40	0.62	2.45	-	-	3.07	0.97 ± 0.15
45	0.66	4.26	-	-	4.92	1.19 ± 0.09
50	0.67	5.47	-	-	6.14	1.39 ± 0.12
55	0.65	6.2	-	-	6.85	1.46 ± 0.13
60	0.63	6.6	-	-	7.23	1.58 ± 0.11
65	0.61	6.79	-	-	7.40	1.86 ± 0.11
70	0.58	6.83	-	-	7.41	1.88 ± 0.11
75	0.55	6.78	-	-	7.33	2.01 ± 0.12
80	0.52	6.66	-	-	7.18	2.18 ± 0.13
85	0.49	6.51	-	-	7.00	2.11 ± 0.13
90	0.47	6.33	-	-	6.80	2.15 ± 0.12
100	0.42	5.95	0.34	-	6.71	2.33 ± 0.11
110	0.38	5.56	0.78	-	6.72	2.38 ± 0.11
120	0.34	5.19	1.07	0.02	6.62	2.35 ± 0.11
130	0.31	4.84	1.26	0.05	6.46	2.38 ± 0.11
140	0.28	4.52	1.38	0.07	6.25	2.36 ± 0.11
150	0.26	4.23	1.44	0.01	5.94	2.20 ± 0.15
170	0.22	3.72	1.48	0.11	5.53	2.07 ± 0.15
180	0.20	3.50	1.46	0.12	5.28	2.24 ± 0.15
190	0.19	3.39	1.44	0.13	5.15	1.77 ± 0.15
200	0.18	3.11	1.42	0.14	4.85	2.01 ± 0.11
225	0.15	2.72	1.32	0.15	4.34	1.91 ± 0.11
250	0.13	2.39	1.23	0.16	3.91	1.72 ± 0.11
275	0.11	2.13	1.13	0.17	3.54	1.78 ± 0.09
300	0.10	1.90	1.05	0.17	3.22	1.77 ± 0.09
325	0.09	1.71	0.97	0.17	2.88	1.78 ± 0.09
375	0.08	1.42	0.83	0.17	2.50	1.61 ± 0.06
400	0.07	1.31	0.78	0.17	2.33	1.54 ± 0.08
450	0.06	1.11	0.68	0.16	2.01	1.32 ± 0.05
500	0.05	0.96	0.59	0.16	1.76	1.31 ± 0.05
550	0.04	0.84	0.52	0.16	1.56	1.22 ± 0.05
600	0.04	0.74	0.47	0.15	1.46	1.08 ± 0.04
650	0.04	0.66	0.42	0.15	1.27	1.08 ± 0.05
710	0.03	0.58	0.38	0.14	1.13	1.07 ± 0.04
760	0.03	0.53	0.34	0.14	1.04	1.02 ± 0.04

800	0.03	0.49	0.32	0.13	0.97	0.98 ± 0.04
850	0.02	0.45	0.29	0.13	0.89	0.92 ± 0.05
900	0.02	0.41	0.27	0.13	0.83	0.89 ± 0.04
1000	0.02	0.35	0.23	0.12	0.72	0.80 ± 0.04
1100	0.02	0.31	0.2	0.11	0.64	0.77 ± 0.04
1200	0.02	0.29	0.17	0.1	0.58	0.75 ± 0,04

Table 9: Proton impact double ionization cross sections of Cu in the unit of $10^{-17}cm^2$.

E (keV/amu)	Contributions of		Total	Experiment
	(4s, 3d)	(4s,3p)		
125	9.94	0.39	10.33	2.30 ± 0.30
150	8.74	0.37	9.11	2.40 ± 0.20
175	7.71	0.34	8.05	2.40 ± 0.20
210	6.54	0.34	6.88	2.40 ± 0.20
250	5.58	0.26	5.84	2.30 ± 0.20
300	4.58	0.22	4.80	2.30 ± 0.18
360	3.62	0.18	3.80	1.90 ± 0.14
425	2.94	0.14	3.08	1.90 ± 0.14
500	2.37	0.11	2.48	1.88 ± 0.18
600	1.84	0.09	1.93	1.65 ± 0.11
720	1.42	0.07	1.49	1.43 ± 0.08
850	1.10	0.05	1.15	1.21 ± 0.09
1000	0.85	0.04	0.89	1.09 ± 0.09
1200	0.67	0.03	0.60	1.06 ± 0.10
1440	0.50	0.02	0.52	0.86 ± 0.09

Table 10: He^{2+}impct double ionization cross section of Cu in the unit of $10^{-16}cm^2$.

E(KeV/amu)	Contribution of		Total	Experiment.
	(4s,3d)	(4s,3p)		
54	3.04	0.04	3.08	1.10 ± 0.40
62	2.91	0.04	2.95	0.90 ± 0.30
75	2.70	0.04	2.74	1.30 ± 0.20
88	2.51	0.04	2.55	1.30 ± 0.20
105	2.29	0.04	2.33	1.20 ± 0.20
125	2.06	0.04	2.10	1.20 ± 0.10
150	1.81	0.03	1.84	1.00 ± 0.10
180	1.56	0.03	1.59	1.20 ± 0.10
213	1.34	0.03	1.37	1,04 ± 0.09
250	1.14	0.03	1.17	0.95 ± 0.07

300	0.96	0.02	0.98	0.98 ± 0.07
360	0.75	0.02	0.77	1.00 ± 0.08

Table 11: Proton impact double ionization cross sections of Fe in the unit of 10^{-17} cm^2.

E (keV/amu)	Contribution of			Total	Experiment.
	(4s,3d)	(4s,4s)	(4s,3p)		
93	14.66	2.16	1.49	18.31	5.60 ± 1.00
108	13.55	1.74	1.46	16.75	4.80 ± 0.70
125	12.42	1.39	1.40	15.21	5.00 ± 0.60
150	10.88	1.03	1.29	13.2	4.50 ± 0.40
175	9.55	0.73	1.17	11.51	4.80± 0.30
210	8.01	0.57	1.01	9.59	3.50 ± 0.40
250	6.66	0.41	0.85	7.92	3.40 ± 0.30
300	5.36	0.29	0.68	6.33	3.20 ± 0.30
360	4.26	0.21	0.54	5.01	2.50 ± 0.30
425	3.42	0.15	0.42	3.99	2.50 ± 0.20
500	2.74	0.11	0.32	3.17	2.20 ± 0.20
600	2.11	0.09	0.24	2.44	1.92 ± 0.16
720	1.61	0.06	0.17	1.84	1.81 ± 0.12
850	1.24	0.05	0.13	1.42	1.60 ± 0.15
1000	0.94	0.03	0.10	1.07	1.38 ± 0.12
1200	0.70	0.03	0.07	0.80	1.24 ± 0.12
1440	0.53	0.02	0.06	0.61	1.00 ± 0.10

Table 12: Alpha particle impact double ionization cross section of Fe in the unit of 10^{-16} cm^2.

E (keV/amu)	Contribution of			Total	Experiment
	(4s,4s)	(4s,3d)	(4s,3p)		
47	0.55	1.80	0.14	2.49	1.70 ± 0.40
54	0.46	1.74	0.14	2.34	1.60 ± 0.30
62	0.38	1.68	0.15	2.21	1.30 ± 0.20
75	0.29	1.59	0.15	2.03	1.40 ± 0.20
88	0.23	1.50	0.15	1.88	1.30 ± 0.20
105	0.18	1.38	0.15	1.71	1.20 ± 0.20
125	0.13	1.24	0.14	1.51	1.24 ± 0.16
150	0.10	1.09	0.13	1.26	1.26 ± 0.09
180	0.07	0.93	0.12	1.12	1.27 ± 0.09
213	0.05	0.79	0.10	0.94	1.10 ± 0.08
250	0.04	0.66	0.09	0.79	1.12 ± 0.07
300	0.03	0.54	0.07	0.64	1.02 ± 0.10
360	0.02	0.43	0.05	0.50	0.82 ± 0.10

PAPER PUBLISHED

Gupta, S. P., Jha, L. K., and Khanal, R. (2017).Study of proton and alpha particle impact double ionization of Fe. *Bulletin of Pure and Applied science. Vol.* 36 D (1), 43 - 52

Gupta, S. P., Jha, L. K., and Khanal, R. (2017). Electron impact single and double ionization of Fe atom. *Bulletin of Pure and Applied science. Vol.* 36 D (1), 53 - 62

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Original Article

Bulletin of Pure and Applied Sciences.
Vol.36 D (Physics), Issue (No.1) 2017: P.43-52
Print version ISSN 0970 6569
Online version ISSN 2320 3218
DOI 10.5958/2320-3218.2017.00006.9

Study of proton and alpha particle impact double ionization of Fe

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Received on 31.03.2017,
Accepted on 26.05.2017

Abstract

Theoretical calculations of H^+ and He^{2+} impact double ionization cross sections for ground state Fe atoms have been performed in the binary encounter approximation(BEA) in the energies region ranging from 80 to 1440 keV/amu for proton impact and from 47 to 360 keV/amu in the case of alpha particle impact. 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^+ and He^{2+} impact double ionization cross sections are in good agreement with the experimental data throughout the given energy range.

INTRODUCTION

Among different multiple ionization processes the double ionization is most important. These calculations are considered to be much significance because contribution from different physical process can be separately estimated at various impact energies. The rigorous theoretical calculation of direct double ionization becomes extremely difficult as it needs consideration of four charged particles in the final channel interacting through the long range coulomb potential[1]. Hence, sophisticated calculations of the integrated double ionization cross sections of many electron- atoms by ion impact are not available in the literature.

However, in the past the BEA has been used successfully in the calculation of the charged particle impact single and double ionization cross section for several atoms and ions.
Gryzinski reasonably considered two processes in a double BE model to describe direct double ionization[2].In the first process the two electrons may be ejected from the system by two successive interactions 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 idea of above mentioned two step interactions has been supported by number of workers[3, 4]. Roy and Rai modified Gryzinski`s theory of electron impact double ionization cross section suitably. In these calculations Hartree-Fock (HF) and hydrogenic velocity distribution were used while considering ejection of the first and second target electrons separately. Later on Jha and Roy used HF velocity distribution while considering the ejection of both electrons of the target in the single and double ionization cross sections of Mg and Ar [5, 6]. The calculated results in BEA are in good agreement with the experimental data. Calculation of double ionization cross sections of titanium-ion by electron impact also shows satisfactory agreement with the experimental observation[6].

In the case of heavy charged particle impact the BE calculations of double ionization cross section of atoms are very few in the literature. Kumar and Roy[7] pointed out some error in the Gryzinski`s theory for calculation of the above mentioned processes and modified the mathematical frame work suitably incorporating the necessary corrections using the accurate expression of $\sigma_{\Delta E}$ as given by Vriens[8], they calculated proton impact double ionization cross section of He, Ne, Ar, and Kr, which were found to be satisfactory agreement with the experimental observation[7, 9]. In these calculations hydrogenic and HF velocity distribution were used for considering the ejection of the first and second target electrons respectively. From comparison of two distribution functions they have concluded that the use of HF velocity distribution for the ejection of both electrons in calculations of direct double ionization would lead to better agreement with the experimental data. Singh et al. has calculated proton and alpha particle impact single and double ionization cross sections of Mg atom and found reasonably good agreement with the experiment[10]. Keeping the above mentioned facts in view, we have considered it worthwhile to carry out calculations of H^+ and He^{2+} double ionization cross sections for iron atoms in BE using HF velocity distribution for both the ejected electrons. This work will encourage us to critically analyze direct double ionization cross sections and to verify the contribution to double ionization from indirect physical processes.

THEORETICAL DETAILS

In accordance with the prediction of the first Born approximation, the single ionization cross section depends on the 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 binding energy of the atomic electron[11]. Here we have assumed Z^2 dependence also in calculation of direct double ionization cross sections in the present double binary encounter model, justifications of which will be after the presentation of the mathematical expression.

In the present work we have used the accurate expression of $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) as given by Vriens for heavy charged particles incident on atoms[8]. Following Catlow and McDowell we have introduced two dimensionless variables *s* and *t* defined by $s^2 = v_1^2 / v_0^2$ 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[11]. All other energies involved are also expressed in rydbergs. In terms of these variables, the expressions of ionization cross section due to a projectile of unit charge for a particular incident energy and a particular velocity of bound electron are given by (see Kumar and Roy[7])

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

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

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

(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.

Heavy charged particle impact double ionization cross section Q_D^{ii} is given by

$$Q_D^{ii} = Q_{sc}^{ii} + Q_{ej}^{ii} \tag{2}$$

In accordance of the idea given by Gryzinski[2] in double binary encounter model, these cross sections involving integrals over energy transfer are given by

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

(3)

and

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

(4)

where n_e is number of electrons in a shell and $f(t)$ is the momentum distribution function of the target electrons and defined as

$$f(t) = 4\pi t^2\rho_{nl}(u_i^{1/2}t)u_i$$

where

$$\rho_{nl} = \frac{1}{2l+1}\sum_{m=-1}^{m=+1}\left|\psi_{nlm}(x)\right|^2$$

and

$\psi_{nlm}(x) = \frac{1}{(2\pi)^{3/2}}\int\Phi_{nlm}(r)e^{ix.r}dr$ is the Fourier transform of the one electron orbit and

$$\Phi_{nlm}(r) = N_{nl}R_{nl}(r)Y_{lm}(\Omega)$$

where $R_{nl}(r)$ is the analytical Hartree-Fock radial function which has been taken from Roothaan et al.[12].

The symbols used in the above expressions have been defined by Gryzinski[2]. 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.

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[7])

$$\sigma_{\Delta E} d(\Delta E) = \begin{Bmatrix} Ad(\Delta E); & \Delta E \le 4su(s-t) \\ Bd(\Delta E); & 4su(s-t) \le \Delta E \le 4su(s+t) \\ 0; & \Delta E > 4su(s+t) \end{Bmatrix} \tag{5}$$

where

$$A = \frac{4}{s^2 u}\left(\frac{1}{(\Delta E)^2} + \frac{4t^2 u}{3(\Delta E)^3}\right) \quad \text{and} \quad B = \frac{2}{3t(\Delta E)^3}\left(8s - \frac{\left|(\Delta E + t^2 u)^{1/2} - tu^{1/2}\right|^3}{s^2 u^{3/2}}\right) \tag{6}$$

The expressions of the scattered 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.

$$Q_{sc}^{ii} = \frac{n_e(n_e-1)Z^2}{4\pi\bar{r}^2} \times \left(\int_{t=0}^{s-\frac{1}{4s}} \left\{ \int_{u_i}^{4su_i(s-t)} A\alpha d(\Delta E) + \int_{4su_i(s-t)}^{4su_i(s+t)} B\alpha d(\Delta E) \right\} f(t) u_i^{1/2} dt + \int_{t=s-\frac{1}{4s}}^{\infty} \int_{u_i}^{4su_i(s+t)} B\alpha f(t) u_i^{1/2} d(\Delta E) dt \right) (\pi a_0^2) \tag{7}$$

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

$$Q_{sc}^{ii} = \frac{n_e(n_e-1)Z^2}{4\pi\bar{r}^2} \times \left(\int_{t=\frac{1}{4s}-s}^{\infty} \int_{u_i}^{4su_i(s+t)} B\alpha f(t) u_i^{1/2} d(\Delta E) dt \right) (\pi a_0^2) \quad \text{when } (s-1/4s) \text{ is negative} \tag{8}$$

In the above expressions $\alpha = \int_0^{\infty} Q_i(s', t) f'(t) u_{ii}^{1/2} dt (\pi a_0^2)$ (9)

Here s' is given by

$$s'^2 = \begin{Bmatrix} \frac{E_q - \Delta E}{1836 u_{ii}} \; for \quad H^+ \quad impact \\ \frac{E_q - \Delta E}{7344 u_{ii}} \; for \quad He^{2+} \quad impact \end{Bmatrix} \tag{10}$$

Similarly equations for ejected part are

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

(11)

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

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

(12)

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

$$\alpha^{'}=\int\limits_0^{\infty}q_i(s^{'},t)f^{'}(t)u_{ii}^{1/2}dt(\pi a_0^2)$$

(13)

Here $q_i(s^{'},t)$ is the expression for electron impact ionization cross section of atoms (see Jha and Roy[5]) and $s^{\backslash}$ is given by $s^{'2}=\dfrac{\Delta E-u_i}{u_{ii}}$ for both H^+ and He^{2+} impact.

Now we discuss the Z^2 dependence of the expression of Q_{sc}^{ii} which denote a process in which the projectile knock out two electrons successively. In a quantum mechanical approach this corresponds to a second order process, for which cross section scales as Z^4 .In this connection it is pertinent to point out the observations made by Vriens[3] and the two double binary encounter processes are linked with the quantum mechanical first and second order approximations. If one uses correlated many electron wave functions, direct double ionization cross section will be finite even in the first Born approximation. This has been assumed to correspond to Q_{ej}^{ii} of the process of direct double ionization. There is also a contribution to direct double ionization from the second Born approximation, which includes double processes like those represented by Q_{sc}^{ii}. In the present method the contribution of Q_{ej}^{ii} are found to be much smaller than those of Q_{sc}^{ii} (see Kumar and Roy[7,9]). In case of proton impact $Z=1$ and therefore Z^4 scaling for Q_{sc}^{ii} become essentially the same as Z^2 scaling and good agreement of calculated results with the experiment is achieved. However, in the case of alpha particle impact calculation involves $Z=2$ and a Z^4 scaling of Q_{sc}^{ii} lead to much dominant contribution of the process adversely affecting the results. Hence the correspondence of the processes represented by Q_{ej}^{ii} and the Q_{sc}^{ii} to the first and the second Born approximation does not appear to be suitable. In this contest the experimental results of H^+ and He^{2+} impact pure double ionization cross sections are noteworthy.

The integral appearing in Q_{sc}^{ii} and Q_{ej}^{ii} have been evaluated numerically. The functions $f(t)$ and $f^{'}(t)$ appearing in the above equations are momentum distributions corresponding to the first and the second ejected electron respectively. These have been constructed from HF radial wave functions (see Catlow and McDowell[13], Jha and Roy[5]). We have considered total cross section for heavy charged particle impact direct double ionization of Fe as given by

$$Q_D^{ii} = Q_D^{ii}(4s,4s) + Q_D^{ii}(4s,3d) + Q_D^{ii}(4s,3p) \tag{14}$$

The factor $\frac{n_e(n_e-1)}{4\pi\bar{r}^2}$ has been suitably modified for 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 these two 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[14].

RESULT AND DISCUSSION

Fe+ H^+ impact Double ionization

In the case of H^+ impact double ionization of Fe we have considered contribution of (4s,4s), (4s,3d) and (4s,3p) shells. In this case we have compared our calculated results with the experimental data of Patton et al.[15]. We have calculated the cross sections from energy range 93 to 1440 keV/amu. In our calculated results we found that the contributions of (4s,4s), (4s,3d) and (4s.3p) having magnitudes 2.16×10^{-17} cm^2, 14.66×10^{-17} $cm^2$and 1.49×10^{-17} cm^2 at impact energies 93 keV/amu. At this energy range the experimental results having magnitude $5.60 \times 10^{-17}cm^2$ while the calculated results having magnitude 18.31×10^{-17} cm^2 respectively. The ratio of the theoretical calculation to the experimental data is 3.26 at the lowest energy. Both the experimental data and the calculated cross sections is highest at the lowest energy while it gradually decreases with the increase of energies considered. A low energy the theoretical results dominates to the experimental data while with the increase of energy the calculated results decreases rapidly as compared to the experimental measurements. With the increase of energy both the results are coming closer to each other and at the energy 720 keV/amu it is almost similar. At this energy the calculated result is of magnitude1.84×10^{-17} cm^2 and the experimental data is of the magnitude $1.81\times10^{-17}cm^2$. Beyond this energy the magnitude of the calculated results gradually decreases as compaired to the magnitude of experimental data. At the highest energy 1440 keV/amu the magnitude of calculated result is 0.61×10^{-17} cm^2 while the experimental data is of magnitude $1.06\times10^{-17}cm^2$. At this energy the ratio of calculated results to the experimental data is 0.57.From the energy range 93 keV/amu to 250 keV /amu he results are beyond the factor of 2. But with the increase of energy both the results are coming close to each other. From the energy range 360 keV/amu to 1440 keV/amu the results are within the factor of 2. From the close inspection the magnitude of experimental measurement decreases slowly while the magnitudes of theoretical results are decreasing very rapidly i.e. the ratio of the lowest to highest energies cross sections in the case of theoretical to experimental are more than thirty times and and more than five times respectively. The overestimation of the calculated results at low energy range is the usual feature of our calculation (i.e. following BEA) The ratio of the calculated cross section to the experimental measurements are 2.0, 1.44, 1.01, 0.88, 0.64, 0.57 at impact energies 360, 500, 720, 850, 1200, and 1440 keV respectively. At the energies 360, 500, 720, 850, 1200 and 1440 keV/amu the magnitudes of the calculated results are 5.01×10^{-17} cm^2, 3.17×10^{-17} cm^2, 1.84×10^{-17} cm^2, 1.4×10^{-17} cm^2 0.80×10^{-17} cm^2 and 0.61×10^{-17} cm^2 while the experimental results having magnitudes $2.5\times10^{-17}cm^2$, $2.2\times10^{-17}cm^2$, $1.81\times10^{-17}cm^2$, $1.6\times10^{-17}cm^2$, 1.24×10^{-17} cm^2 and 1.06×10^{-17} cm^2 respectively. From the discussion given above it clearly indicates that with the increase of energy the results are coming close to each other and are within the factor of 2 and supposed to be in good agreement with the experimental results

Table 1: Proton impact double ionization cross sections of Fe in unit of 10^{-17} cm^2

Energy(keV/amu)	Contribution of (4s,3d)	Contribution of (4s,4s)	Contribution of (4s,3p)	Total	Expt.[15]
93	14.66	2.16	1.49	18.31	5.6
108	13.55	1.74	1.46	16.75	4.8
125	12.42	1.39	1.40	15.21	5
150	10.88	1.03	1.29	13.2	4.5
175	9.55	0.73	1.17	11.51	4.8
210	8.01	0.57	1.01	9.59	3.5
250	6.66	0.41	0.85	7.92	3.4
300	5.36	0.29	0.68	6.33	3.2
360	4.26	0.21	0.54	5.01	2.5
425	3.42	0.15	0.42	3.99	2.5
500	2.74	0.11	0.32	3.17	2.2
600	2.11	0.09	0.24	2.44	1.92
720	1.61	0.06	0.17	1.84	1.81
850	1.24	0.05	0.13	1.42	1.6
1000	0.94	0.03	0.10	1.07	1.38
1200	0.70	0.03	0.07	0.80	1.24
1440	0.53	0.02	0.06	0.61	1.06

Table 2: Alpha particle impact double ionization cross section of Fe in unit of 10^{-16} cm^2

E(keV/amu)	Contribution of (4s,4s)	Contribution of (4s,3d)	Contribution of (4s,3p)	Total	Expt.[15]
47	0.55	1.80	0.14	2.49	1.7
54	0.46	1.74	0.14	2.34	1.66
62	0.38	1.68	0.15	2.21	1.3
75	0.29	1.59	0.15	2.03	1.4
88	0.23	1.50	0.15	1.88	1.3
105	0.18	1.38	0.15	1.71	1.2
125	0.13	1.24	0.14	1.51	1.24
150	0.10	1.09	0.13	1.26	1.26
180	0.07	0.93	0.12	1.12	1.27
213	0.05	0.79	0.10	0.94	1.1
250	0.04	0.66	0.09	0.79	1.12
300	0.03	0.54	0.07	0.64	1.02
360	0.02	0.43	0.05	0.50	0.82

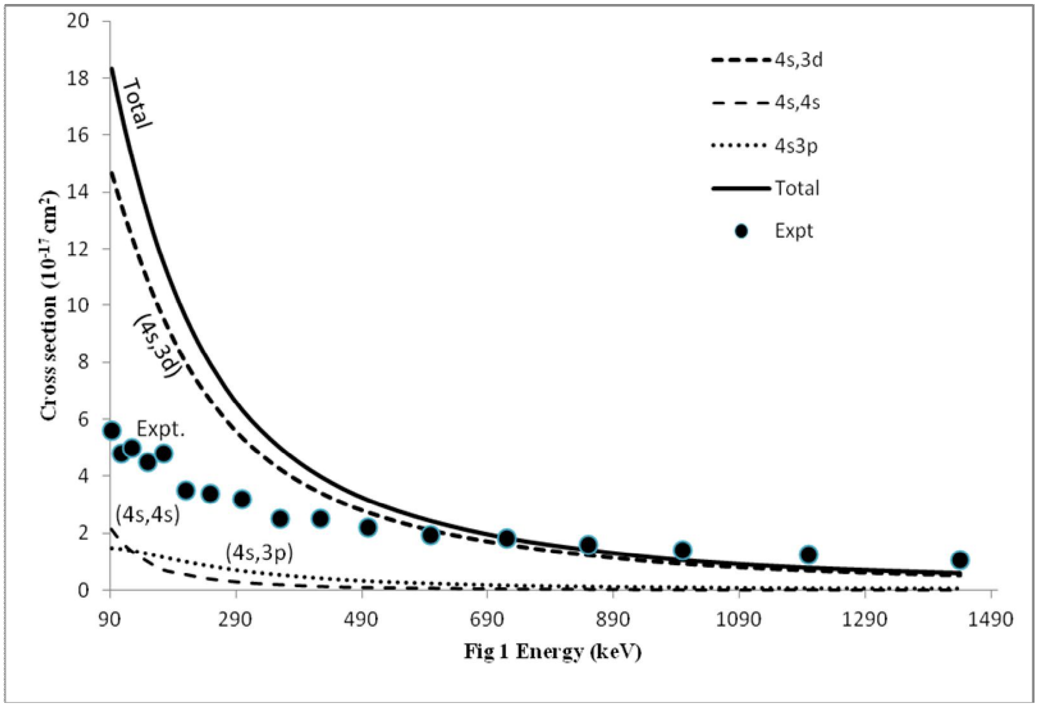

Figure 1: Proton impact double ionization cross section of Fe:
The (4s,4s), (4s,3d) and (4s, 3p) stand for partial contribution to the proton impact direct double ionization and Total stands for the total theoretical double ionization cross section of Fe and experimental data as Expt.[15]

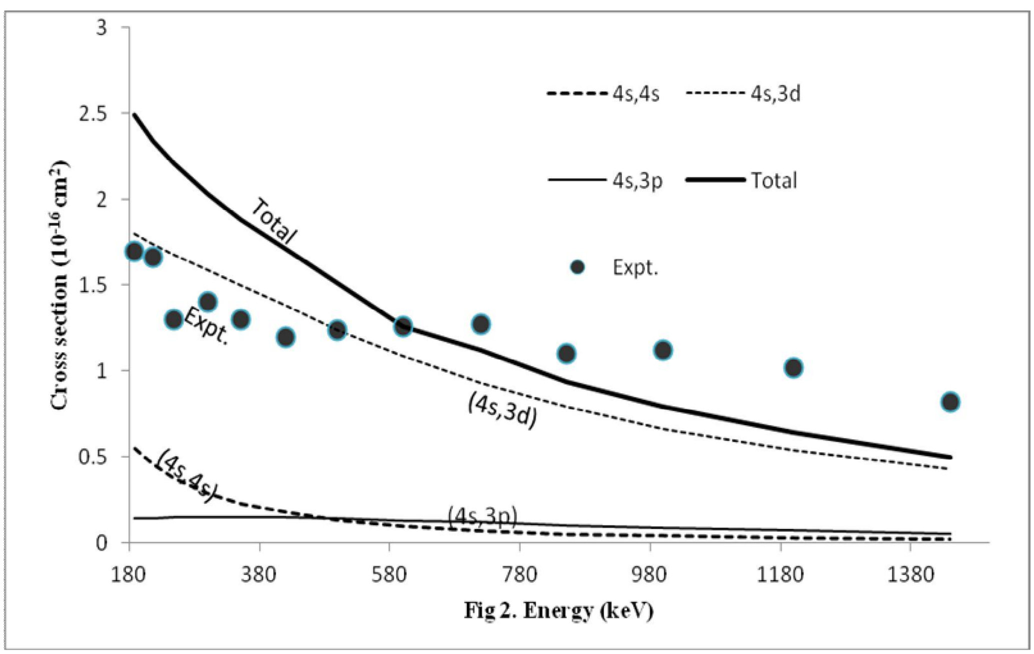

Figure 2: Alpha particle impact double ionization cross section of Fe:

The (4s,4s), (4s,3d) and (4s, 3p) stand for partial contribution to the electron impact direct double ionization of Fe and Total stands for the total theoretical double ionization cross section of Fe and experimental data as Expt.[15]

He^{2+} impact Double Ionization of Fe

In the calculation of He^{2+} impact double ionization of Fe we have calculated the cross sections from the energy range 47 keV/amu to 360 keV/amu and compared with the experimental data of Patton et al.[15]. In this calculation we have taken the contribution of (4s,4s), (4s,3d) and (4s,3p) shells only. In this calculation from the lower energy range to 125 keV/amu the calculated cross sections overestimate the measured data. Beyond this energy the calculated cross sections underestimates the contributions of the experimental cross sections up to the highest energy which we have considered, except at 150 keV/amu. The overestimation of the calculated cross sections at low energy range is the usual trend of BEA. The ratio of the calculated cross sections to the experimental measured data is almost within the factor of 2 and it becomes identical at energy of 150 keV/amu. At the lower energies 47 keV/amu, 54 keV/amu, 75 keV/amu the ratios of calculated to experimental cross sections are 1.46, 1.40 and 1.45 respectively. But the increase of the energies at 150, 213, 300 and 360KeV/amu the ratio of the calculated cross sections to the experimental data are 1.0, 0.85, 0.62 and 0.60 respectively. The experimental cross sections at lowest energy 47 keV/amu is of magnitude 1.7×10^{-16} cm^2 while at the highest energy of 360 keV/amu it becomes 0.82×10^{-16} cm^2. The ratio of the lowest cross section to the highest cross section is almost doubled while the ratio of the lowest calculated cross section to the highest cross section is all most five times greater which indicates that the fall in magnitude of the experimental cross sections decrease slowly while the calculated cross sections fall rapidly with the increase of energy as compared to the experimental findings.

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Original Article

Bulletin of Pure and Applied Sciences.
Vol.36 D (Physics), Issue (No.1) 2017: P.53-62
Print version ISSN 0970 6569
Online version ISSN 2320 3218
DOI 10.5958/2320-3218.2017.00007.0

Electron impact single and double ionization of Fe atom: PACS. 34.80 Dp Atomic excitation and ionization by electron impact

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Received on 08.01.2017,
Accepted on 28.03.2017

Abstract:

Theoretical calculations of electron impact single and double ionization cross sections for ground state Fe atoms have been performed in the binary encounter approximation(BEA) in the energy region ranging from threshold to 1250 eV and 1200eV respectively. The accurate expression for $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) including exchange and interference as given by Vriens and Hartree – Fock velocity distributions for the target electrons have been used throughout the calculations.

INTRODUCTION

Various processes can contribute to electron impact double ionization of atoms and ions depending on the incident electron energy and on the structure of parent and intermediate atomic states. For direct ejection of two outer shell electrons, two different types of mechanism are identified: shake off and two state mechanism. In addition, many indirect double ionization processes are associated with the formation of auto ionizing states following inner shells ionization or excitation.

In the case of direct double ionization (DDI) via shake off the incident electron interacts with a bound electron and ejects it with outer bound electrons being left in the state which is not an Eigen state of the residual ion. In the subsequent relaxation process there is finite probability of a second ionization. Electron impact double ionization of atoms and ions is a four particle (one ion and three electrons) problem. In the final channel, these four charged particles interacts with each other via long range Coulomb potential, making the correct treatment of this many body problem extremely difficult. For this reason, it is still impossible to carry out exact calculations for these processes, both full theoretical calculation and detail experimental investigations remain scare. On the other hand, the most detailed description of the process is given by means of full differential cross sections allowing the analysis of angular and energy distributions for each one of the ejected or scattered electrons. On the other hand the total double ionization cross sections describe the global importance of non charge state. Electron impact ionization of ions is a fundamental process in any discharge or plasma so that measurement of absolute total ionization cross section of various ions have long been performed , including the case of double ionization where a number of reports are available.

Electron impact ionization of atoms and ions is one of the most fundamental collision processes in atomic and molecular physics. Knowledge of ionization cross section for these processes finds wide application in plasma kinematics problems, mass spectroscopy, gas laser, upper atmospheric physics and astrophysics. Ionization rate of various atomic species found in astronomical plasma are also a great interest. From an applied view point multiple ionization process are important in moderate and high temperature plasma in all gaseous environment with an abundant energetic electrons [1].

Experimental investigation of ionization cross section for metals lead to several difficulties and have been carried out by only very few experimental groups for limited number of elements. Accurate experimental measurement of multiple ionization of iron by electron impact have been carried out by Shah et al.[2] using pulse cross beam technique incorporating time - of –flight spectroscopy of the collision products to study the electron impact ionization of ground state Fe atom within the energy range from respective thresholds to 1250eV . Experimental data obtained by Shah et al. [2] would not be compared with previous theoretical calculation of double ionization cross section due to non availability of the data in the literature.

Individual cross sections have been obtained by normalization to lower energy values of σ_2 . Previously measured by Freund et al. [3] using a fast crossed beam experiment analysis was complicated by the presence of metastable atom in Fe-beam. Measured cross sections exhibit evidence of contribution from inner shell electrons. The high energy values of single ionizations are in good agreement with theoretical predictions based on the first Born approximation.

Sophisticated theoretical calculations of single and double ionization cross section of Fe are not available in the literature. Rigorous theoretical calculation of double ionization cross section becomes very complicated as it is related with the consideration of the four charged particles in the final channel interacting through the long range Coulomb potential [4]. Quantal calculation of the integrated double ionization cross sections of atoms/ions by electron impact have not been reported so far. Recently Belenger et al. [5] have reported a semi empirical formula for evaluation of double ionization cross section of neutral atoms, and positive and negative ions by electron impact and also presented results for Cu-target. In this approach the shape of the cross section is described by analytical expression and approximation -parameters are estimated by fitting the model cross sections to reliable experimental data. Besides this, similar methods have been reported by Fisher el al. [6] and Deutsch et al. [1]

A few attempts have been made to calculate electron impact double ionization cross section for light target e.g. H^+, He and Li^+ is the Born approximation (see Tweed [7, 8] and Mc Guire [9]. In a promising approach the time dependent close coupling method was used by Pindzola et al.[10] in the calculation of electron impact double ionization of cross section of He. Afterward Pindzola and his coworkers carried out calculations of electron impact double ionization cross section of Mg [11] , Be [12] and B^+ ion [13] using a non perturbative time dependent close coupling method. However, such calculations are restricted so far to essentially two electrons system. Using classical binary encounter approximation (BEA), Gryzinski and Kun [14] have derived general analytical expression for electron impact double ionization cross section of atoms with atomic number Z ≥20 and *s* or *d* outer shell with two electrons. They have compared their calculations only with experimental data for Ca, Sr, Ba and Hg atoms and found satisfactory agreement. Although, this model is consistent and convenient but it treats processes of double ionization in statistical ways. However, this model is not applicable in case of Fe. Here we would like to mention that the wave functions representing the bound electrons are characteristic of the target atoms but there is no consideration of wave function in above mentioned calculation.

Keeping in view the above mentioned fact, we have used the symmetrical collision model of Vriens including exchange and interference in the present work and used Hartree-Fock velocity distribution for the target electrons. We have also taken into consideration of inner shells. In the past, the BE approximation has been found successful in the calculation of electron impact single and double ionization of atoms [15-17].

THEORETICAL METHODS

We have used the accurate expression for $\sigma_{\Delta E}$ including exchange and interference as given by Vriens [18] for calculating electron impact single ionization cross sections. The expression used in the calculation has been discussed in detail by Roy and Rai [19]. A brief presentation of the expression in final form used in the calculations is given below. Using dimension less variables introduced by Catlow and McDowell [20], the expression for cross section for particular incident energy and a particular velocity of the bound electron can be written as in the form

$$Q^i(s,t) = \frac{4}{(s^2+t^2+1)u^2}\left[\frac{s^2-1}{s^2} + \frac{2t^2}{3}\left(\frac{s^4-1}{s^4}\right) - \frac{\phi \ln s^2}{(s^2+1)}\right](\pi a_0^2)$$

$$where \qquad \phi = \cos\left\{\left(\frac{1}{s^2u+u}\right)^{1/2} \ln s^2\right\} \tag{1}$$

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 for electron impact single ionization cross section for a particular shell of the target is given by

$$Q^i(s) = n_e \int_0^\infty Q^i(s,t) f(t) u^{1/2} dt \tag{2}$$

The method of calculating electron impact double ionization cross section of atoms in double binary encounter model has been discussed in detail in earlier publications [21, 22, 15]. However, it is desirable to give a brief discussion of the expression which has been used in present calculations. Electron impact double ionization cross sections including contribution from Auger emission can be written as

$$Q^{ii}(T) = Q_D^{ii} + Q_A^{ii} \qquad (3)$$

where Q_D^{ii} denotes the contribution from direct ejection of two electron and Q_A^{ii} that from Auger emission. The expressions for cross sections corresponding to the two processes of the double binary encounter model leading to direct double ionization are given by (see Jha and Roy [15]).

$$Q_{SC}^{ii} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int_{t=0}^{\propto}\int_{U_i}^{E_q-U_{ii}}\sigma_{\Delta E}\left[\int_{t=0}^{\propto}\int_{U_{ii}}^{E_q-\Delta E}\sigma_{\Delta E'} f(t)U_{ii}^{1/2}d(\Delta E^i)dt\right]\times f(t)U_i^{1/2}d(\Delta E)dt\times 8.797\times10^{-17}(\pi a_0^2) \qquad (4)$$

and

$$Q_{ej}^{ii} = \frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int_{t=0}^{\propto}\int_{U_i+U_{ii}}^{E_q}\sigma_{\Delta E}\times\left[\int_{t=0}^{\propto}\int_{U_{ii}}^{\Delta E-U_i}\sigma_{\Delta E'} f(t)U_{ii}^{1/2}d(\Delta E^i)dt\right]\times f(t)U_i^{1/2}d(\Delta E)dt\times 8.797\times10^{-17}(\pi a_0^2) \qquad (5)$$

In the case of single ionization, we have used the accurate expression for $\sigma_{\Delta E}$ as given by Vriens [18]in the above expression also. Using dimensionless variables introduced by Catlow and McDowell [20] $\sigma_{\Delta E}$ is given by (see Kumar and Roy [23])

$$\sigma_{\Delta E} = \frac{2}{(s^2+t^2+1)u}\left[\left(\frac{1}{\Delta E^2}+\frac{4t^2u}{3\Delta E^3}\right)+\left(\frac{1}{(s^2u+u-\Delta E)^2}+\frac{4t^2u}{3(s^2u+u-\Delta E)^3}\right)-\frac{\phi}{\Delta E(s^2u+u-\Delta E)}\right] \qquad (6)$$

where $\phi = \cos\left\{\left(\frac{1}{s^2u+u}\right)^{1/2}\ln s^2\right\}$

Due to indistinguishability of electron in the symmetrical model of Vriens the cross sections corresponding to the two process are exactly equal at all incident energies (see Kumar and Roy [23]) and hence in order to obtain the direct double ionization cross section, either of the cross sections should be multiplied by two. In equation (4) u and s^2 have been replaced by U_i and E_q/U_i in the expression for $\sigma_{\Delta E}$ and by U_{ii} and $(E_q-\Delta E)/U_{ii}$ in the case of $\sigma_{\Delta E'}$. The only difference in the equation (5) is that s^2 assumes the value $(\Delta E-U_i)/U_{ii}$ in the expression for $\sigma_{\Delta E'}$.The function $f(t)$ appearing in equations (2), (4) and (5) is the momentum distribution function (see Catlow and McDowell [20]) and Jha and Roy[15].In case of double ionization $f(t)$ has been constructed replacing u by U_i and U_{ii} for ejection of first and the second electron respectively. In order to obtain Q_A^{ii} (contribution to the double ionization from Auger emission), the single ionization cross section should be multiplied by Auger yield of the shell under consideration.

We have considered total cross section for electron impact direct double ionization of Fe as given by

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

where $Q_D^{ii}(4s,3d)$ stands for the double ionization cross section corresponding to one electron ejected from 4s shell and the other from the 3d shell. The factor $n_e(n_e-1)/4\pi\bar{r}^2$ has been suitably modified for considering the modes of ionization in which the electrons are ejected from different shells. $n_e(n_e-1)$ has been replaced by $n_e1\times n_e2$ where these two stand for number of the electrons in the shell under consideration. In order to obtain the value of $\bar{r}$, the atomic radius has been replaced by the mean of the expectation value of radii of the shell (see Jha and Roy[15]). For binding energies we have used the magnitude of orbital energies of the shells of Fe given by Climenti and Roetti [24] and Hartree-Fock radial wave functions have been used to construct momentum distribution functions for the target electron in the present calculation. The expectation values of radii reported by Desclaux [25] have been used as shell radii.

RESULTS AND DISCUSSION

Electron Impact Single Ionization cross sections of Fe

We have calculated the electron impact single ionization cross sections of Fe from 8.1 eV to 1250 eV impact energies. Such calculations over a wide energy range with an experiment [2] have been reported in Table1 and Figure1. In this calculation we have calculated single ionization cross sections of 4s, 3d and 3p shells. The remaining inner shells contributions are almost negligible and hence contribution of inner shells has not taken into account. Near the threshold the magnitude of the calculated cross sections are greater in compared to the experimental results which is a usual feature of this model. The present model is valid for high energy ranges. Our calculated results come closer to the experimental data with increase of impact energy from 8.6 eV to 1250 eV. The calculated peak has magnitude 6.29 x 10^{-16} cm^2 at 32.5 eV while the peak measured by M B Shah et al. is 4.08 x 10^{-16} cm^2 at 35 eV. The ratio of the calculated peak to the experimental peak is 1.54.The magnitude of the calculated peak is shifted slightly towards lower energy side compared to the experimental peak. The ratio of calculated cross sections to the experimental cross sections becomes greater than 2 above impact energy 8.8 eV. One of the important and noticeable thing is that both calculated cross section 0.87 x 10^{-16} cm^2 and experimental cross section 0.53 x 10^{-16} cm^2 respectively have minimum value at same impact energy 1250 eV. From the close inspection of the curves it is found that the major contributions to the calculated cross sections comes from 4s and 3d sub shells while the contribution of 3p shell is very small. In the calculated results it is found that the contributions of *4s* shell falls sharply with the increase of energy up to 275 eV while the contribution of 3d shells fall smoothly with the increase of energy up to 170 eV. At the impact energy 110 eV the magnitudes of 3d shells and 4s shells are almost similar.

Table 1: Electron impact single ionization cross section of Fe in the unit of 10^{-16} cm^2

E(eV)	Contribution of 4s	Contribution of 3d	Contribution of 3p	Total	Expt[2]
8.10	1.26			1.26	0.33
8.30	1.47			1.47	0.44
8.60	1.76			1.76	0.70
8.80	1.93			1.93	1.08
9.40	2.38			2.38	1.34
9.90	2.70			2.70	1.54
10.40	2.96			2.96	1.96
11	3.23			2.23	2.18
11.60	3.46			3.46	2.22
12	3.59			3.59	2.39
12.60	3.76			3.76	2.46
13	3.85			3.55	2.50
14	4.05			4.05	2.83
15	4.20			4.20	2.94
16.10	4.32			4.32	3.15
16.80	4.38			4.38	3.42
19	4.48	0.45		4.93	3.65
21	4.50	0.93		5.43	3.91

23	4.49	1.29		5.78	3.95
26	4.42	1.67		6.09	4.01
29	4.30	1.92		6.22	3.80
30	4.27	1.98		6.25	3.92
32.50	4.17	2.12		6.29	3.98
35	4.06	2.21		6.27	4.08
42	3.76	2.37		6.13	3.77
47	3.56	2.42		5.98	3.76
52	3.37	2.45		5.82	3.58
60	3.11	2.45		5.56	3.42
70	2.83	2.42		5.25	3.29
80	2.59	2.37	0.02	4.98	2.93
85	2.49	2.34	0.05	4.88	2.93
90	2.39	2.31	0.07	4.77	2.87
95	2.30	2.28	0.08	4.66	2.83
100	2.22	2.25	0.09	4.56	2.60
110	2.07	2.19	0.12	4.38	2.46
120	1.94	2.13	0.13	4.20	2.51
130	1.83	2.07	0.14	4.04	2.27
140	1.73	2.02	0.15	3.90	2.34
150	1.64	1.97	0.15	3.76	2.19
160	1.56	1.92	0.16	3.64	2.14
170	1.49	1.87	0.16	3.52	1.97
180	1.42	1.82	0.16	3.40	1.92
190	1.36	1.78	0.16	3.30	1.84
200	1.31	1.74	0.16	3.21	1.82
225	1.19	1.64	0.16	2.99	1.70
250	1.09	1.56	0.16	2.81	1.68
275	1.00	1.48	0.16	2.64	1.53
300	0.94	1.42	0.16	2.52	1.46
325	0.87	1.35	0.15	2.37	1.35
370	0.78	1.26	0.15	2.19	1.30
400	0.73	1.20	0.14	2.07	1.12
450	0.66	1.11	0.14	1.91	1.05
500	0.60	1.04	0.13	1.77	1.06
550	0.55	0.98	0.12	1.65	0.91
600	0.51	0.92	0.12	1.55	0.87
650	0.47	0.87	0.11	1.45	0.82
710	0.44	0.82	0.11	1.37	0.77
760	0.41	0.78	0.10	1.29	0.75
800	0.40	0.75	0.10	1.25	0.70
830	0.38	0.73	0.10	1.21	0.70
860	0.37	0.71	0.10	1.18	0.68
900	0.36	0.69	0.09	1.14	0.65
1000	0.32	0.64	0.09	1.05	0.63
1100	0.30	0.59	0.08	0.97	0.58
1200	0.27	0.55	0.08	0.9	0.60
1250	0.26	0.53	0.08	0.87	0.53

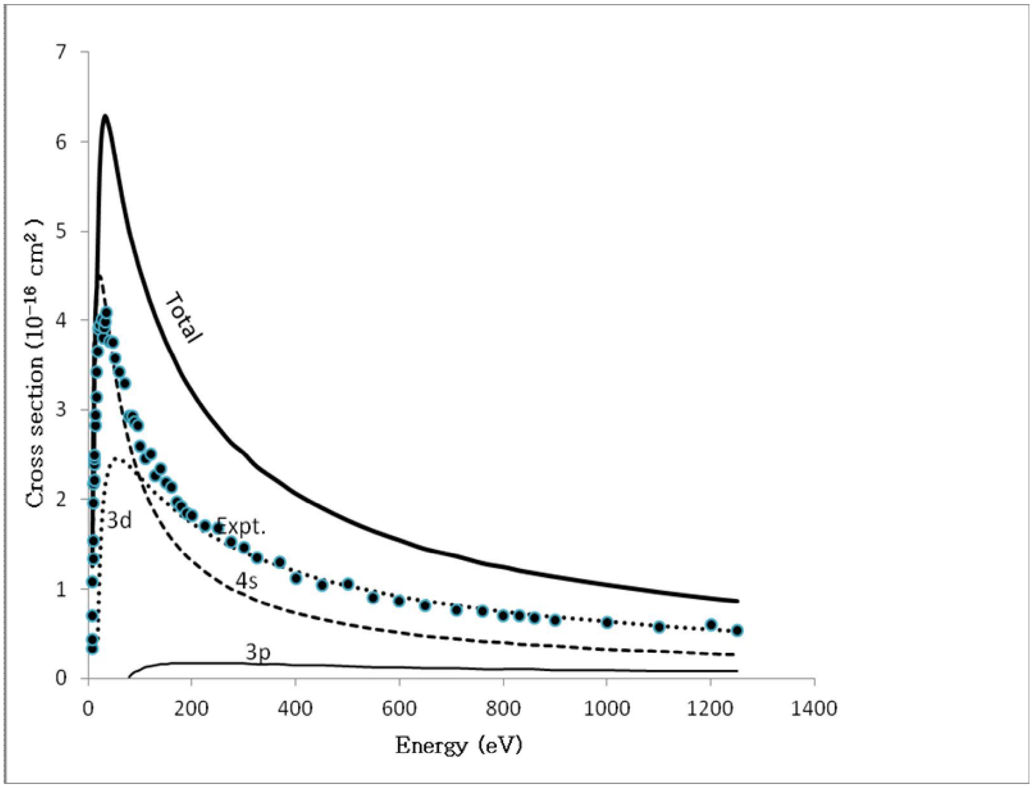

Figure 1: Electron impact single ionization cross section of Fe:
The 4s, 3d and 3p stand for the ionization cross sections for the respective shells and **Total** stands for total theoretical single ionization cross section and experimental data as **Expt.[2]**

Electron impact double ionization of Fe

The Fe has an electronic structure with 6 electrons in 3d and 2 electrons in 4s outside the close core. The experimental double ionization cross sections after attaining maxima at energies 80 eV, 90 eV, 110 eV, 140 eV,170 eV, 200eV, 250 eV and 325 eV respectively it is quite surprising that the experimental data of electron impact double ionization measured by Shah et al. [2] has eight peaks between the energy range 80 eV to 325 eV.It indicates that there are large fluctuations in the results of experimental measurements. When experimental results attains maxima at 80 eV there is slow decrease in energy in the region 80 – 325 eV indicating significant contribution from direct process. Obviously direct double ionization of Fe is considered to the result from ejection of loosely bound 3d and 4s electrons. In addition we have considered ionization of 3s electrons to lead to an exited state which results double ionization through auto ionization. The theoretical results of double ionization cross sections along with experimental data in the energy region from threshold to 1200 eV have been presented in the Table2 and Figure 2. First we would like to discuss the degree of agreement of the calculated direct double ionization results with the experimental data. Near to the threshold at impact energies 18.3 to 35.3 eV the ratios of calculated cross sections to the experimental data are always within the factor 2. After the inclusion of (4s,3d) contribution beyond the energy 40 eV the calculated cross sections and the experimental data are diverging very rapidly and the theoretical results are 4.13, 4.65, 3.97 and 3.64 times at impact energies 45 eV, 55 eV, 65 eV, and 75 eV respectively. The diversity of the calculated results along with the experimental findings might be due to the inclusion of contribution of (4s, 3d) shells in the calculations. Beyond the energy 75 – 225 eV impact energies our calculated results are more than three times and 4 times compared to the experimental data. After the impact energy 275 eV the result comes closer to each other. At this energy 760 eV the magnitude of the theoretical and experimental results are 1.04 x 10^{-17} $cm^2$and 1.02 x 10^{-17} $cm^2$and between the energy 600 eV to 800 eV the experimental results are almost flat. Beyond the energy760 eV the experimental results overestimates the calculated cross section at all impact energies up to 1200 eV. The variations of the theoretical as well as experimental results are almost similar in nature except for a few energy regions.

Table 2: Electron impact double ionization cross section of Fe in the unit of $10^{-17}cm^2$

E (eV)	Contribution of (4s,4s)	Contribution of (4s,3d)	Contribution of (4s,3p)	Contribution of 3s	Total	Expt[2]
28.3	0.27				0.27	0.28
33.3	0.48				0.48	0.61
35.3	0.54	0.49			1.03	0.74
40	0.62	2.45			3.07	0.97
45	0.66	4.26			4.92	1.19
50	0.67	5.47			6.14	1.39
55	0.65	6.2			6.85	1.46
60	0.63	6.6			7.23	1.58
65	0.61	6.79			7.40	1.86
70	0.58	6.83			7.41	1.88
75	0.55	6.78			7.33	2.01
80	0.52	6.66			7.18	2.18
85	0.49	6.51			7.00	2.11
90	0.47	6.33			6.80	2.15
100	0.42	5.95	0.34		6.71	2.33
110	0.38	5.56	0.78		6.72	2.38
120	0.34	5.19	1.07	0.02	6.62	2.35
130	0.31	4.84	1.26	0.05	6.46	2.38
140	0.28	4.52	1.38	0.07	6.25	2.36
150	0.26	4.23	1.44	0.01	5.94	2.20
170	0.22	3.72	1.48	0.11	5.53	2.07
180	0.2	3.5	1.46	0.12	5.28	2.24
190	0.19	3.39	1.44	0.13	5.15	1.77
200	0.18	3.11	1.42	0.14	4.85	2.01
225	0.15	2.72	1.32	0.15	4.34	1.91
250	0.13	2.39	1.23	0.16	3.91	1.72
275	0.11	2.13	1.13	0.17	3.54	1.78
300	0.1	1.9	1.05	0.17	3.22	1.77
325	0.09	1.71	0.97	0.17	2.88	1.78
375	0.08	1.42	0.83	0.17	2.50	1.61
400	0.07	1.31	0.78	0.17	2.33	1.54

450	0.06	1.11	0.68	0.16	2.01	1.32
500	0.05	0.96	0.59	0.16	1.76	1.31
550	0.04	0.84	0.52	0.16	1.56	1.22
600	0.04	0.74	0.47	0.15	1.46	1.08
650	0.04	0.66	0.42	0.15	1.27	1.08
710	0.03	0.58	0.38	0.14	1.13	1.07
760	0.03	0.53	0.34	0.14	1.04	1.02
800	0.03	0.49	0.32	0.13	0.97	0.98
850	0.02	0.45	0.29	0.13	0.89	0.92
900	0.02	0.41	0.27	0.13	0.83	0.89
1000	0.02	0.35	0.23	0.12	0.72	0.8
1100	0.02	0.31	0.2	0.11	0.64	0.77
1200	0.02	0.29	0.17	0.1	0.58	0.75

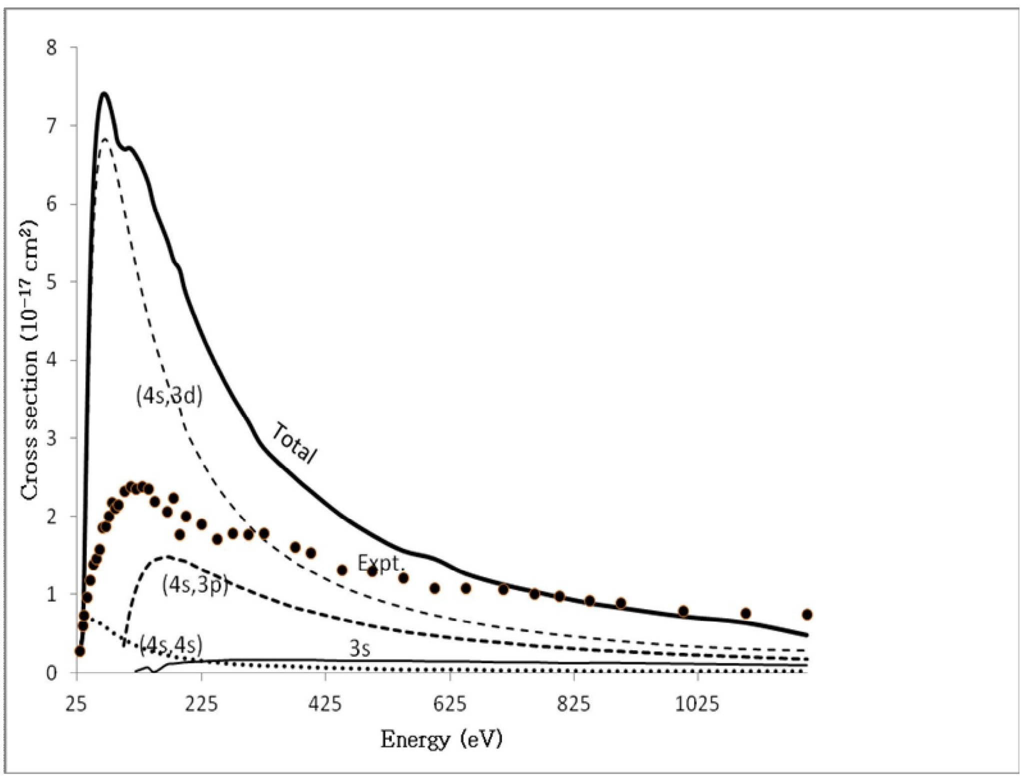

Figure 2: Electron impact double ionization cross section of Fe:

The (4s,4s), (4s,3d) and (4s, 3p) stand for partial contribution to the electron impact direct double ionization of Fe and 3s is included as an additional contribution and **Total** stands for the total theoretical double ionization cross section of Fe and experimental data as **Expt.[2]**

Our calculated results exhibits only one pick at the impact energy 70 eV having magnitude 7.41 x 10^{-17} cm^2 and indirect contributions from the inclusion of shells play an important role at high energy regions. The position of the calculated peak is found to be shifted in lower energy side as compared to the experimental counterpart. Magnitudes of cross sections above 140 eV shows a satisfactory agreement with experimental data but there is same discrepancies in the high energy regions where the calculated cross sections are found to be smaller and smaller as compared to the experiment with increase of energy. This discrepancy reflects the possibility of some other physical process contributing double ionization. Structure in the experimental double ionization cross section- curves between energy 80 eV to 325 eV attributes to indirect ionization process arising from inner shells. However, there is no indication of structure in the double ionization curve. But decrease in experimental cross section is rather slow in this energy region. This is not in accordance with the usual trend of direct double ionization cross section which shows a faster decrease in high energy region after attaining the maximum energy. Such a trend exhibits in the calculated cross section when attaining the maximum value 7.41×10^{-17} cm^2 at impact energy 70 eV, but beyond this energy the contribution of direct double ionization falls rapidly and it is observed that at the highest energy of 1200 eV the magnitude of the cross section is 0.58×10^{-17} cm^2. This means the ratio of these two calculated results of cross sections at energies 70 eV and 1200 eV is more than 12 times. Such a feature is not observed in the double ionization cross section in the measured data. Further it is suggestion for the experimentalist that there needs further experiment to perform.

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STUDY OF H^+ IMPACT SINGLE IONIZATION OF FE

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Abstract

Theoretical calculations of proton impact single ionization cross sections for ground state Fe atoms have been performed in the binary encounter approximation (BEA) within the energy range 70 - 1440 keVamu^{-1}. The accurate expression for $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) including exchange and interference as given by Vriens and Hartree –Fock velocity distributions for the target electrons have been used throughout the calculations. Our calculated values at lower energies are in close agreement with the experimental findings both in magnitude and position.

Key words: Proton impact, Single ionization cross section of Fe, Binary encounter approximation,

1. Introduction

Understanding of collision phenomena by charged particle is of considerable interest in many branches of physics e.g. plasma physics, fusion, upper atmospheric studies and astrophysics. It is also fundamental in the case of irradiation of biological matter when it is necessary to know how the projectile beam deposits energy on the target. Electron can be ejected during the collision as the result of the direct interaction of the projectile with the target electron or as the result of a post-collision relaxation of the residual target. Processes of direct target ionization with or without electron capture can contribute to multiple ionization. In the second case, inner shell vacancies produced in the first state of the reaction can be followed by inner shell Auger or intra shell Coster-kronig electron emission[1].

Studies of ionization of metallic atoms are considered to be valuable. It is because a detailed understanding of collision processes involving many stages of ionization of such species is important in astrophysics and in the physics of controlled thermo nuclear plasma[2]. Unfortunately studies in this field are limited because of several difficulties in experimental determination of ionization cross section. In one of the early investigation of metal, Shah et al.[3] used a crossed beam technique incorporating time- of- flight analysis and coincidence counting of the collision product to carry out an interesting work on electron capture, transfer ionization in collision as fast proton ions with atomic magnesium which is important in astrophysics since its emission spectra have recorded by several ground based and space craft based instruments.

In the past BEA has been used successfully to calculate charge particle impact single ionization cross sections of several atoms and ions[4]. There used accurate

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expression for $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) as given by Vriens[5] and Hertree-fock velocity distribution in present work. Recently Minakshi et al.[6] has calculated H^{+} and He^{2+} impact single and double ionization of lead and satisfactory results were obtained[6]. Keeping the above mentioned facts in view we have considered it worthwhile to carryout calculation of proton impact single ionization cross section for Fe atoms in the BEA. This work enabled to analyze single ionization cross sections and to identify the ionization from inner shells.

2. Theoretical Method

In the present work we have used the accurate expression of $\sigma_{\Delta E}$ (cross section for energy transfer ΔE) as given by Vriens[5] for heavy charged particles incident on atoms. Following Catlow and McDowell[7] we have introduced two dimensionless variables s and t 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. In terms of these variables, the expressions of ionization cross section due to a projectile of unit charge for a particular incident energy and particular velocity of bound electron are given by (see Kumar and Roy[8])

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

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

$$t = 0, \qquad 1 > 4s(s+t) \tag{1}$$

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 for heavy charged particle impact single ionization cross section for a particular shell of the target is given by

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

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

$$f(t) = 4\pi t^2 U \rho_{nl}(U^{1/2} t) \tag{3}$$

where $$\rho_{nl} = \frac{1}{2l+1}\sum_{-1}^{+1}\left|\psi_{nlm}(x)\right|^2$$

(4)

and

$$\psi_{nlm}(x) = \frac{1}{(2\pi)^{3/2}}\int \Phi_{nlm}(r)e^{ix.r}dr$$

(5)

is the Fourier transform of the one electron orbit and

$$\Phi_{nlm}(r) = N_{nl}R_{nl}(r)Y_{lm}(\Omega)$$

(6)

in which $R_{nl}(r)$ is the analytical Hatree-Fock radial function which has been taken from Roothaan et al[9].

In the present calculations, momentum distribution functions for the bound electrons have been constructed using Hartree-Forck radial functions reported by Clementi and Roetti[10]. For shell radii and binding energies of electrons, quantum mechanical value of radial distance of maximum probability given by Desclaux[11] and quantum mechanical values of orbital energies given by Clementi and Roetti have been used respectively in the calculations.

3. Result and discussion

In the present theoretical investigation we have carried out the calculation of H^+ impact single ionization of Fe in the energy range 70 keV/amu to 1440 keV/amu. The results of calculated cross section along with experimental results of the single ionization have been shown in the Table 1 and Figure 1. In the case of H^+ impact single ionization of Fe we have taken the contributions of 4s and 3d shells only. As shown in table contribution from 3p is very small and its contribution has been ignored. Our calculated results are compared with the experimental investigation of Patton et al [12]. The experimental observation clearly indicate that the lowest energy 70 keV/amu at which single ionization cross section has been measured is higher than the energy corresponding to the experimental maximum cross section. The experimental cross sections are found to decreases gradually with the increase of energy in the energy range 70 keV/amu to 1440 keV/amu. The calculated results show similar decrease in cross section with increase in energy. At 70 keV/amu, the ratio of the theoretical to experimental cross section is 1.2. With the increase of the energy from 70 keV to 500 keV the ratio increase but within factor 2 and at energies 600 keV/amu and 720 keV/amu ratios are 2.02 and 2 respectively. Beyond this energy range the theoretical to the experimental results again falls within factor 2. From the close inspection of the calculated results, it is found that 4s sub shell contribution dominates at lower energy region while the 3d contribution is dominant at the higher energy region. The lowest energy considered in this calculation shows the value 9.06×10^{-16} cm^2 while at this energy the experimental measured data shows the value

7.5×10^{-16} cm^2. Thus our calculated value at lowest energy is in close agreement with the experimental findings both in magnitude and position. This tendency reflects that present results and the experimental cross sections are in close agreement both qualitatively and quantitatively throughout the energy range investigated.

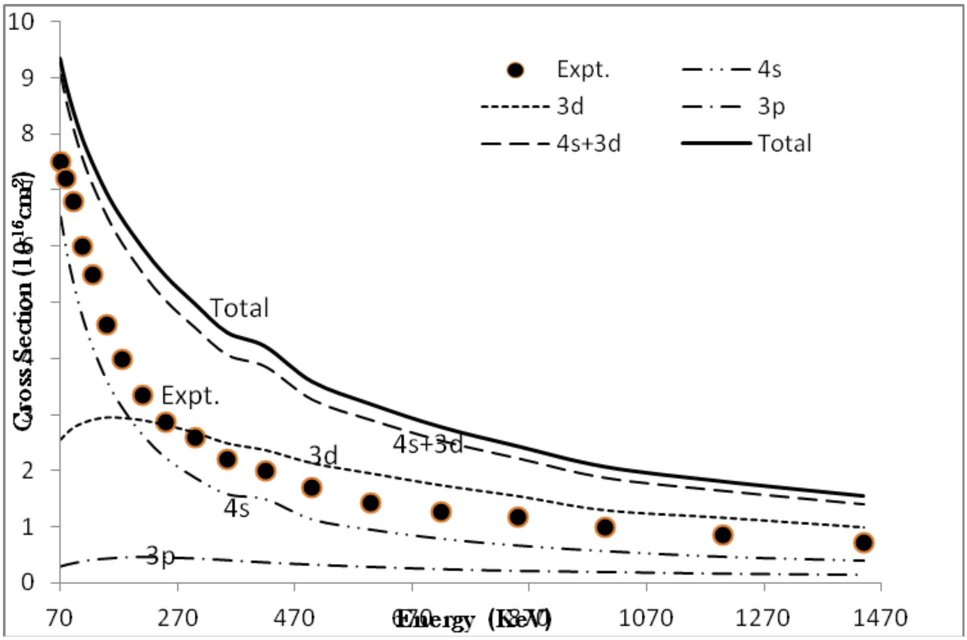

Figure1. Proton impact single ionization cross section of Fe where the 4s, 3d and 3p stand for the ionization cross sections for the respective shells and **Total** stands for total theoretical single ionization cross section and experimental data as **Expt.**

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

Energy(keV)	4s	3d	3p	4s+3d	Total	Expt.(Source)[12]
70	6.51	2.55	0.29	9.06	9.35	7.5
80	5.90	2.66	0.32	8.56	8.88	7.2
93	5.28	2.77	0.35	8.05	8.40	6.8
108	4.70	2.84	0.38	7.54	7.92	6
125	4.18	2.90	0.41	7.08	7.49	5.5
150	3.57	2.94	0.43	6.51	6.94	4.6
175	3.12	2.93	0.45	6.05	6.50	3.98
21	2.63	2.89	0.46	5.52	5.98	3.34
250	2.22	2.80	0.45	5.02	5.47	2.87
300	1.87	2.67	0.43	4.54	4.97	2.59
355	1.58	2.48	0.40	4.06	4.46	2.19
420	1.49	2.36	0.36	3.85	4.21	2
500	1.13	2.13	0.32	3.26	3.58	1.69
600	0.95	1.95	0.28	2.90	3.18	1.42
720	0.79	1.74	0.24	2.53	2.77	1.27
850	0.67	1.55	0.21	2.22	2.43	1.17
1000	0.57	1.30	0.19	1.87	2.06	0.98
1200	0.47	1.17	0.16	1.64	1.80	0.85
1440	0.40	1.00	0.14	1.40	1.54	0.71

Conclusion

It is concluded on the basis of present calculations that the proton impact single ionization cross sections of Fe in energy range 70-1440 keV/amu are well explained by considering 4s and 3d shells only. The 4s contributions dominates at lower energy regions and 3d contributions dominate at the higher energy regions.

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Bulletin of Pure and Applied Science
Vol. 34 D (Physics) Issue (No.2) 2015:P.71-80
Print version ISSN 0970 6569 Online version ISSN 2320 3218
www.bpas.in DOI

ELECTRON IMPACT SINGLE IONIZATION OF Kr AND Xe

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Received on : Accepted on 2015

ABSTRACT

Theoretical studies of electron impact single ionization cross sections of Kr and Xe atoms have been performed in the Binary Encounter Approximation (BEA). Accurate expression of $\sigma_{\Delta E}$ (cross-section for energy transferΔE) and the Hartree-Fock (HF) velocity distributions for the target electrons have been used throughout the calculations. The present results of single ionization cross sections are in good agreement with the experimental observations.

Key Word: Single Ionization, Binary Encounter Approximation, Kr Atoms, Xe Atoms

1.INTRODUCTION

Cross section for ionization of atoms by electron impact finds wide applications in various branches of science and technology. The cross sections are widely used in applications such as the modelling of plasmas in tokomaks, modelling of radiation effects for both material and medical research as well as in basic research in astrophysics.

Ionization cross sections at all energies are needed to follow the history of an incident particle and its products. Proper understanding of the role of ejected electrons is crucial because a large number of them mostly slow electrons are generated in the course of an energetic incident particle penetrating through matter. These electrons in turn interact with other targets until the electrons are thermalised. Electron-atom collision can be divided into two broad types: soft or distant collisions with large impact parameters and hard or close collision with small impact parameters. The Mott theory [1] which describes the collision of two free electrons, accounts for hard collisions well but not for soft collision. Bethe [2] has shown that soft collision takes place essentially through the dipole interaction between the incident particle and the target electron. The symmetric form of the Binary Encounter theory described by Vriens [3] is for electron impact ionization.

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A large number of investigations dealing with electron impact single ionization of atoms have been carried out and a number of reviews covering the developments in this field in recent years are available. The various quantum mechanical methods employed for electron impact ionization have been discussed by Younger [4]. To obtain total ionization cross-sections for complex targets over a wide range, a number of semi classical and semi-empirical formulae have also been developed by Younger [5]. An elegant discussion on electron impact ionization of alkali metals have been given by McDowell [6] (see also Roy and Rai [7]). McGuire [8] applied Plane Wave Born Approximation (PWBA) to calculate electron impact ionization cross sections for atoms. Also, exchange has been included in quantal calculation. In spite of all these successes, the difficulty still lies in the calculation of electron impact single ionization cross sections for heavy atoms in quantal approximations due to mathematical complexities.

On the other hand, a Binary encounter theory for the investigation of electron mpact ionization cross sections of atoms has been found to be suitable as it gives reliable results consistent with the experiments. The earlier classical model did not take into account the indistinguishability of the incident and the bound electron (unsymmetrical collision model) and is not reliable at low impact energies. At low incident energies, exchange plays an important role. To remove these difficulties, a more reliable classical formalism of electron impact ionization including the effect of exchange and interference, has been given by Vriens [9] (symmetrical collision model).

Various experimental observations have clearly indicated the presence of structures in the ionization curves of atoms especially in the alkali metals, the alkaline earths and in most of the heavy atoms. The structures observed in the experiments have been clearly explained by different theoretical approaches. In case of electron impact ionization of the alkaline earths, Peach [10a, 10b] has performed a quantal calculation for Mg. Vainshtein et al. [11] also used the Born Approximation and the classical Binary Encounter theory to explain the experimentally observed structures. Though, these calculations have shown good agreement between theory and experiment, the calculations suffer from two deficiencies. First, the Born Approximation is not well suited for low incident energy in which the structures are present. Secondly, in case of Binary Encounter calculations, Vainshtein et al. has modified Stabler's [12] expression by considering the acceleration of the incident electron by the field of neutral atom but have used a δ function velocity distribution for the bound electron and has not taken exchange into consideration. Some calculations on electron impact ionization have been reported by McFarland [13], Tripathi et al. [14] and Mann [15] for the alkaline earths. Roy and Rai [7] have used symmetrical collision model including exchange and interference given by Vriens [9] to investigate the structures observed in the ionization curves of heavier alkali atoms and alkaline earths. They have used the correct Hartree-Fock velocity distribution for the bound electron to obtain single ionization cross-sections. The contribution of inner cell as well as excitation auto ionization has been explicitly included. The results obtained are in fairly good agreement with the experimental observations.

Keeping in view the above mentioned facts, we have used the symmetrical collision model of Vriens including exchange and interference in the present work and used Hartree-Fock velocity distribution for the target electron. We have also taken into consideration the contributions of inner shells. In the past, the BEA has been found successful in the calculations of electron impact single ionization cross sections of atoms [16,17].

2.2. Theoretical methods

Vriens expression [9] in symmetrical model including exchange and interference has been used for calculating electron impact single ionization cross sections. A brief outline of the method of calculation is given below. Expression for electron impact ionization and excitation- auto ionization, including exchange and interference due to Vriens are given by

$$Q^i = \frac{\pi e^4}{E_1 + E_2 + U}\left[\frac{\left(\frac{1}{U} - \frac{1}{E_1}\right) + \frac{3E_2}{2}\left(\frac{1}{U^2} - \frac{1}{E_1{}^2}\right) - \phi'}{E_1 + U}\; In\left(\frac{E_1}{U}\right)\right] \tag{1}$$

With

$$\phi' = cos\left[\left(\frac{R}{E_1 + U}\right)^{1/2}\; In\left(\frac{E_1}{U}\right)\right] \tag{2}$$

Here E_2 and R are the kinetic energy and Rydberg constant of the target electrons respectively.

Following Catlow and McDowell [18], we now introduce two dimensionless variables s and t defined as

$$s^2 = \frac{V_1^2}{V_0^2} \quad and \quad t^2 = \frac{V_2^2}{V_0^2} \tag{3}$$

$$Q^i(s,t) = \frac{4}{s^2 + t^2 + 1}\left[\frac{s^2 - 1}{s^2 U} + \frac{2}{3}t^2\left(\frac{s^4 - 1}{s^4 U^2}\right) - \frac{\phi Ins^2}{U^2(s^2 + 1)}\right](\pi a_0^2) \tag{4}$$

With $$\phi' = COS\left[\left(\frac{1}{s^2U + U}\right)^{\frac{1}{2}} Ins^2\right] \tag{5}$$

where V_1 and V_2 are the velocities of the incident and bound electrons respectively and are expressed in atomic units; $V_0^2 = U_i$ is the ionization potential of the target atom in Rydbergs. All other energies involved have also been expressed in Rydbergs.

The above expression for $Q^i(s, t)$ has been integrated over the Hartree-Fock velocity distribution for the target electron to obtain the ionization as well as excitation cross sections. Hence, the final forms of expression for these cross sections become

$$(s) = n_e \int_0^\infty Q^i(s,t) f(t) U^{1/2} dt \, \pi a_0^2 \qquad (6)$$

where n_e is the number of equivalent electrons in the shell under consideration and f(t) is the momentum distribution function for the bound electron which is given by

$$f(t) = 4\pi t^2 U \rho_{nl}(U^{1/2} t) \qquad (7)$$

Where

$$\rho_{nl} = \frac{1}{2l+1} \sum_{-1}^{+1} |\psi_{nlm}(\mathbf{x})|^2 \qquad (8)$$

Where

$$\psi_{nlm}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int \phi_{nlm}(\mathbf{r}) \exp(i\mathbf{x}.\mathbf{r}) \, d\mathbf{r} \qquad (9)$$

is the Fourier transform of the one electron orbital.

$$\varphi_{nlm}(r) = N_{nl} R_{nl}(r) Y_{lm}(\Omega) \qquad (10)$$

in which R_{nl} (**r**) is the analytical Hartree-Fock radial function.

In the present calculations, momentum distribution functions for the bound electrons have been constructed using Hartree-Forck radial functions reported by Clementi and Roetti [19]. For shell radii and binding energies of electrons, quantum mechanical value of radial distance of maximum probability given by Desclanx [20] and quantum mechanical values of orbital energies given by Clementi and Roetti have, respectively, been used in the calculations.

3. RESULTS AND DISCUSSION

In the present work we have calculated electron impact single ionization cross sections for Kr and Xe using the method described in section 2. The calculated electron impact ionization cross sections of Kr and Xe along with experimental observations of Rejoub et al. [21] have been presented in the figures (1 & 2) and tables (1 & 2) respectively.

Table 1. Electron impact single ionization cross-sections Kr in units of 10^{-16} cm^2

Energy (eV)	Contributions of 4p	Contributions of 4s	Contributions of 3d	Total	Expt. [21]
22	3.46	-	-	3.46	1.48
24	3.80	-	-	3.80	1.76
26	4.04	-	-	4.04	2.14
28	4.21	-	-	4.21	2.34
30	4.34	-	-	4.34	2.55
35	4.50	0.13	-	4.63	2.99
40	4.53	0.25	-	4.78	3.24
45	4.50	0.33	-	4.83	3.38
50	4.43	0.39	-	4.82	3.45
55	4.35	0.43	-	4.78	3.48
60	4.25	0.45	-	4.70	3.45
65	4.14	0.47	-	4.61	3.49
70	4.04	0.49	-	4.53	3.45
75	3.94	0.50	-	4.44	3.45
80	3.83	0.51	-	4.34	3.43
90	3.64	0.52	-	4.16	3.40
100	3.46	0.52	-	3.98	3.33
120	3.15	0.52	0.07	3.74	3.20
130	3.01	0.51	0.10	3.62	3.11
140	2.88	0.51	0.12	3.51	3.05
150	2.77	0.50	0.14	3.41	2.98
160	2.66	0.50	0.15	3.31	2.91
170	2.56	0.49	0.16	3.21	2.86
180	2.47	0.48	0.17	3.12	2.78
190	2.39	0.48	0.18	3.05	2.72
200	2.31	0.47	0.18	2.96	2.68
225	2.13	0.45	0.19	2.77	2.54
250	1.98	0.44	0.20	2.62	2.42
275	1.85	0.43	0.20	2.48	2.29
300	1.74	0.41	0.20	2.35	2.19
350	1.55	0.39	0.20	2.14	2.01
400	1.40	0.37	0.20	1.97	1.85
500	1.18	0.33	0.19	1.70	1.60
600	1.02	0.31	0.16	1.49	1.43

700	0.90	0.28	0.17	1.35	1.28
800	0.80	0.26	0.16	1.22	1.16
900	073	0.24	0.15	1.12	1.07
1000	0.66	0.23	0.14	1.03	0.98

Table 2. Electron impact single ionization cross-sections of Xe in units of 10^{-16} cm^2

Energy (eV)	**Contributions of 5p**	**Contributions of 5s**	**Contributions of 4d**	**Contributions of 4p**	**Total**	**Expt. [21]**
14	2.56	-	-	-	2.56	0.73
16	4.70	-	-	-	4.70	1.37
18	6.08	-	-	-	6.08	2.01
20	7.00	-	-	-	7.00	2.43
22	7.63	-	-	-	7.63	2.90
24	8.05	-	-	-	8.05	3.33
26	8.34	0.01	-	-	8.35	3.62
28	8.52	0.08	-	-	8.60	3.80
30	8.64	0.13	-	-	8.77	4.01
35	8.72	0.22	-	-	8.94	4.48
40	8.63	0.27	-	-	8.90	4.59
45	8.46	0.30	-	-	8.76	4.60
50	8.24	0.32	-	-	8.56	4.58
60	7.76	0.35	-	-	8.11	4.62
70	7.29	0.36	-	-	7.65	4.67
80	6.85	0.35	0.05	-	7.25	4.64
90	6.44	0.35	0.14	-	6.93	4.53
100	6.08	0.34	0.19	-	6.61	4.44
120	5.45	0.33	0.26	-	6.04	4.19
130	5.18	0.32	0.28	-	5.78	4.05
140	4.94	0.31	0.30	-	5.55	3.97
150	4.72	0.30	0.31	-	5.33	3.89
160	4.52	0.29	0.32	-	5.13	3.78
170	4.33	0.28	0.32	-	4.93	3.67
180	4.16	0.28	0.33	-	4.77	3.58
190	4.00	0.27	0.33	0.01	4.61	3.51
200	3.86	0.26	0.33	0.01	4.46	3.44
225	3.53	0.25	0.33	0.02	4.13	3.25
250	3.26	0.23	0.33	0.02	3.84	3.06

300	2.83	0.21	0.32	0.03	3.39	2.77
350	2.50	0.19	0.31	0.03	3.03	2.48
400	2.24	0.17	0.29	0.03	2.73	2.31
500	1.86	0.15	0.27	0.03	2.31	2.00
600	1.59	0.13	0.25	0.03	2.00	1.75
700	1.39	0.11	0.23	0.03	1.76	1.58
800	1.24	0.10	0.21	0.03	1.58	1.42
900	1.12	0.09	0.20	0.03	1.44	1.32
1000	1.02	0.09	0.19	0.02	1.32	1.21

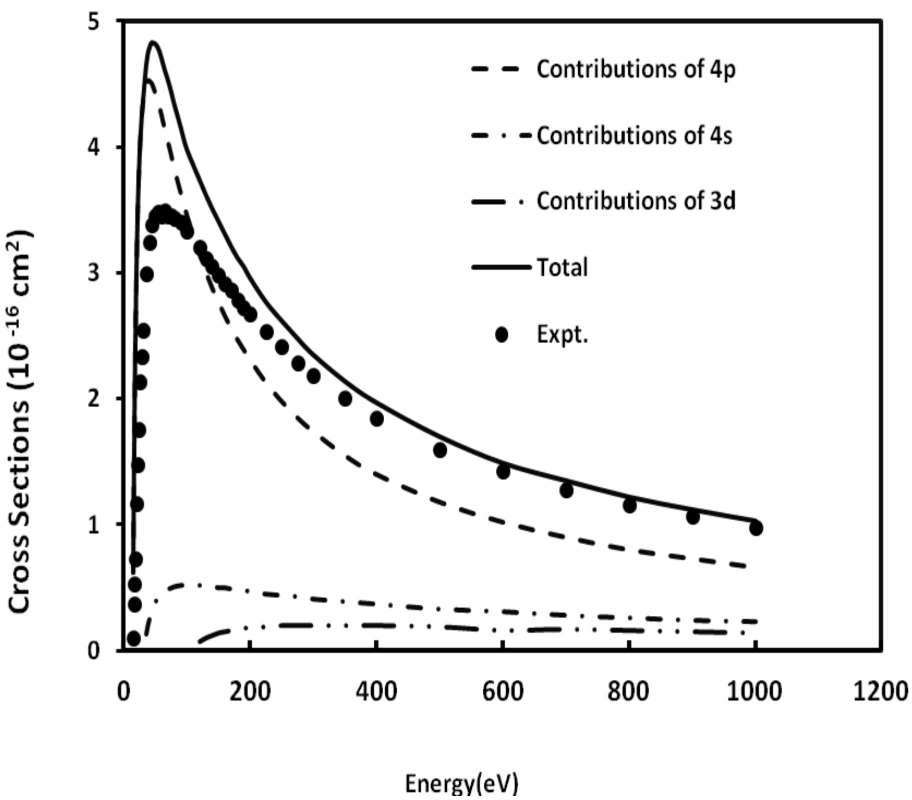

Figure-1-Single ionization of Kr by electron impact ($10^{-16}cm^2$)

Electron Impact Single Ionization of Kr

In the case of Kr we have calculated the ionization cross sections from the threshold 15 eV to 1000 eV impact energies. Such calculations over a wide energy range have never been reported earlier. In case of Kr we have calculated single ionization cross sections for 4p, 4s and 3d shells. The remaining inner shell contributions are almost negligible. Therefore we have not taken the contributions of these shells into account. Near the threshold the magnitude of the calculated cross sections are larger in comparison to the experimental result which is a usual feature of the model because the present model is valid for high energy range. Our calculated results come closer to the experimental data with increase of energy value. The calculated peak has magnitude 4.83 x 10^{-16} cm^2 while the peak measured by Rejoub et al. [21] has a magnitude 3.49 x 10^{-16} cm^2. The peak is obtained in the present calculations at impact energy 45 eV while the experimental peak is observed at 65 eV impact energy. The ratio of the calculated peak to the theoretical peak is 1.38 but the calculated peak is shifted towards low energy side. The ratio of calculated cross section to the experimental cross section becomes greater than 2 at impact energies 22 eV and 24 eV respectively. Beyond 24 eV impact energy the ratio of theoretical cross sections to the experimental cross sections decreases gradually and it is minimum at impact energy 600 eV. Beyond 24 eV calculated cross sections are within a factor of 2. The ratio of theoretical cross sections to experimental cross section at impact energy between 35 eV to 40 eV becomes less than 1.55. At impact energy 170 eV and 180 eV the ratio remains same having magnitude 1.12 eV. The magnitudes of theoretical value at 170 eV, 180 eV and 190 eV are 3.21 x 10^{-16} cm^2, 3.12 x 10^{-16} cm^2 and 3.05 x 10^{-16} cm^2 respectively and the magnitudes of experimental cross section are 2.86 x 10^{-16} cm^2, 2.78 x 10^{-16} cm^2 and 2.72 x 10^{-16} cm^2. From impact energy 700 eV to 1000 eV the ratio of theoretical cross sections to experimental crosssection are nearly almost same about 1.05. From a close inspection of the results it is concluded that the calculated results are in excellent agreement with the experiment in the energy region 100 to 1000 eV.

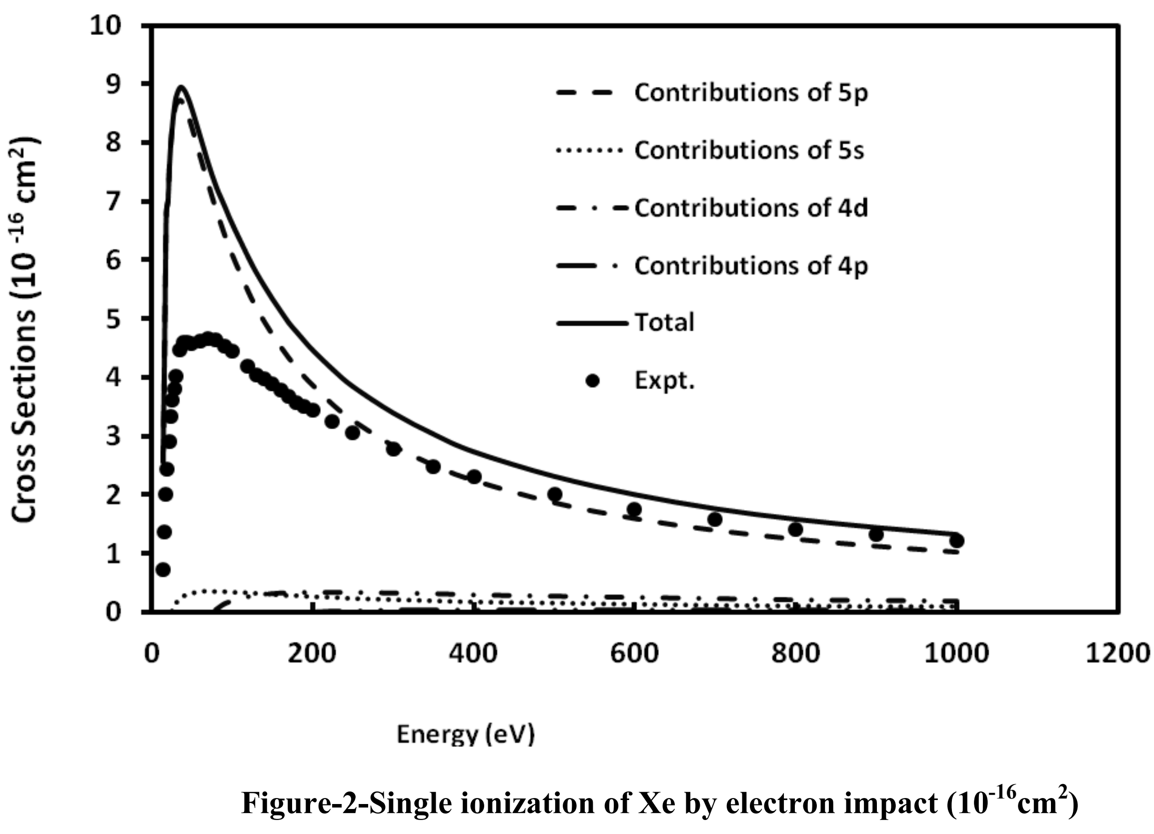

Figure-2-Single ionization of Xe by electron impact ($10^{-16}$$cm^2$)

Electron Impact Single Ionization Cross Section of Xe

In the case of Xe, we have calculated electron impact ionization cross sections from the threshold 14 eV to 1000 eV. In the case of Xe we have taken the contributions of 5p, 5s, 4d and 4p shells for the calculation of single ionization cross sections. The calculated maximum peak value of Xe is 8.94 x 10^{-16} cm^2 at impact energy 35 eV while the experimental peak value is 4.67 x 10^{-16} cm^2 at impact energy 70 eV. Thus our calculated peak value is shifted towards the low energy region. The ratio of theoretical peak to the experimental peak is about 1.91. Beyond 40 eV impact energy the ratio of the calculated results to the experimental values of cross sections is always within a factor of 2. Below 40 eV the value of the ratio of theoretical to the experimental cross sections gradually increases up to 3.51 at impact energy 14 eV i.e. ratio increases as impact energy decreases. The ratio of the calculated cross sections to the experimental cross sections gradually decreases by increasing impact energies. At impact energies 900 eV and 1000 eV the value of the ratio of calculated to experimental cross sections becomes minimum 1.09. The magnitudes of the calculated cross sections and experimental values are 1.44 x 10^{-16} cm^2, 1.32 x 10^{-16} cm^2 and 1.32 x 10^{-16} cm^2 , 1.21 x 10^{-16} cm^2 at impact energies 900 eV and 1000 eV respectively. Between 40 eV to 90 eV the ratio becomes greater than 1.5. Beyond 90 eV impact energy the ratio becomes less than 1.5. In this case the calculated maximum cross section becomes flat having magnitude 8.94 x 10^{-16} cm^2, 8.90 x 10^{-16} cm^2 at impact energy 35 eV and 40 eV respectively. Our calculated flat peak is shifted towards the low energy region but the experimental flat peak shifted toward high energy region at 60 eV, 70eV and 80 eV having magnitude 4.62 x 10^{-16} cm^2, 4.67 x 10^{-16} cm^2 and 4.64 x 10^{-16} cm^2 respectively. Our calculated results are greater than the experimental values throughout the energy range considered. The calculated results show good agreement with the experiment in the entire energy range.

CONCLUSION

On the basis of discussion of the results it is apparent that our theoretical cross sections of electro impact single ionization cross section of Kr and Xe atoms are in good agreement with the experimental observations. From the close inspection of the calculated cross sections substantiate the view point that the BE model gives reasonably good agreement with the experimental results in intermediate and high energy regions. Keeping the view of above mentioned facts we have used the symmetrical collision model of Vrien's including exchange and interference in the present work and used Hertree-Forck velocity distribution for the target atoms. We have also taken into consideration of inner shells. In the past BEA has been found successful in the calculation of electron impact single ionization cross sections ions.

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International Journal of Advance Research in Science and Engineering
Volume No.06, Issue No. 11, November 2017
www.ijarse.com
IJARSE
ISSN: 2319-8354

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

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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])

$$Q_i(s,t) = \frac{4}{s^2u^2}\left[1+\frac{2t^2}{3}-\frac{1}{4(s^2-t^2)}\right]; \qquad 1 \quad \leq \quad 4s(s-t)$$
$$= \frac{2}{s^2u^2t}\left[\frac{1}{4(s+t)}+t+\frac{2}{3}\left\{2s^3+t^3-(1+t^2)^{3/2}\right\}\right]; \qquad 4s(s-t)\leq 1 \leq 4s(s+t)$$
$$= 0; \qquad 1 > 4s(s+t)$$

(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)

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])

$$\sigma_{\Delta E} d(\Delta E) = \begin{cases} Ad(\Delta E); & \Delta E \le 4su(s-t) \\ Bd(\Delta E); & 4su(s-t) \le \Delta E \le 4su(s+t) \\ 0; & \Delta E > 4su(s+t) \end{cases}$$

(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.

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

(7)

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

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

when $(s-1/4s)$ is negative

(8)

In the above expressions

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

(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

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

(11)

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

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

(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 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.

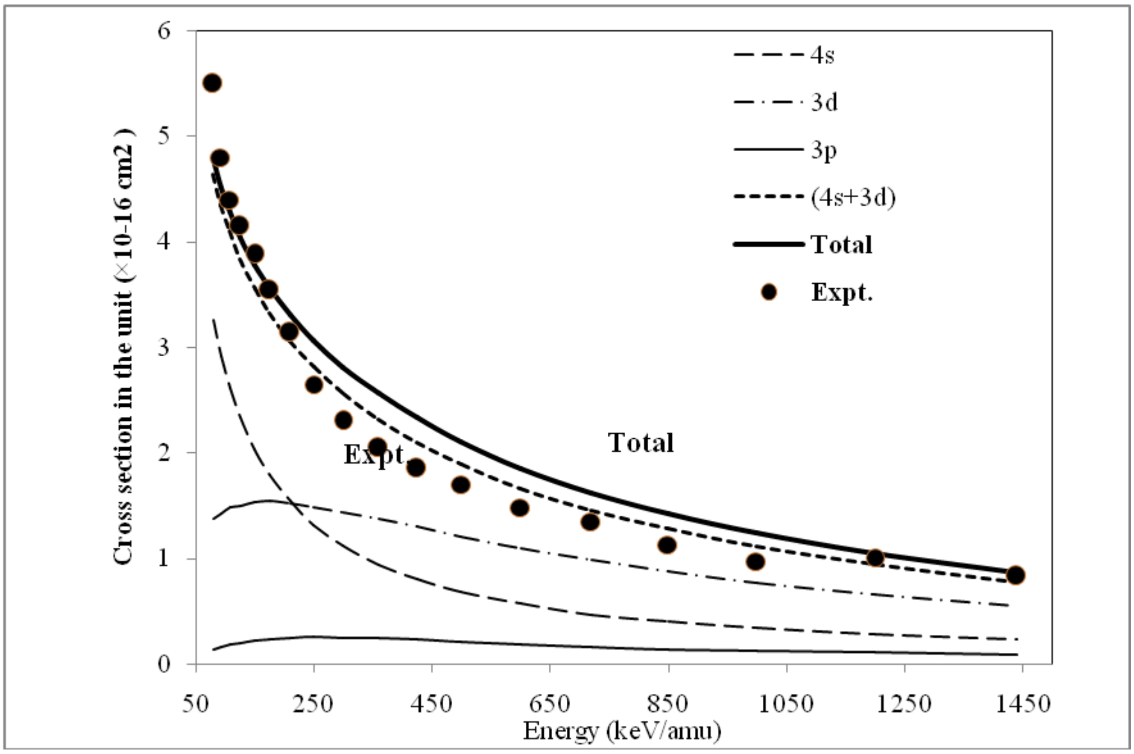

Figure1: Proton impact single ionization cross sections of Cu in the unit of ×10-^{16} cm^2.

[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 $\times 10^{-16}$ cm^2 and 0.82 $\times 10^{-16}$ 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.

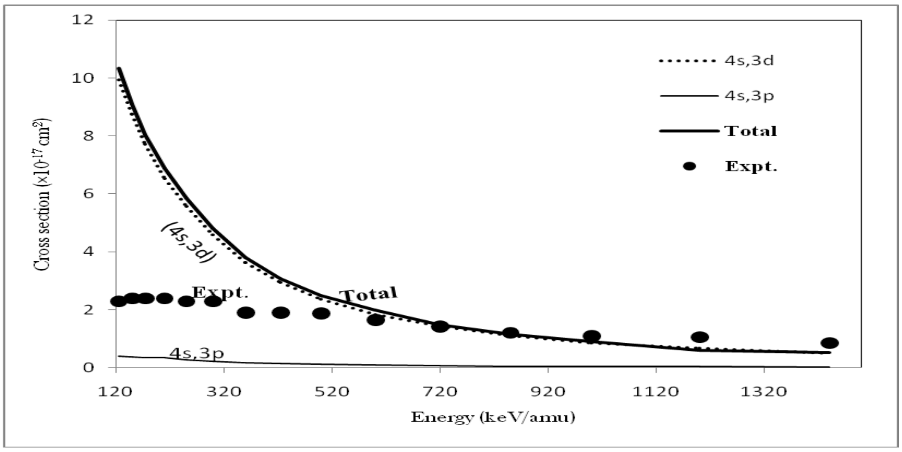

Figure2: Proton impact double ionization cross sections of Cu in the unit of $\times10^{-17}$ cm^2.

[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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