



Effect of Exchange and Absorption Potential in the Distorted Wave Calculation of Electron Impact Excitation of Auto Ionizing State of Rubidium

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Authors' contributions

This work was carried out in collaboration between both authors. Author VOONA designed the study, performed the statistical analysis, wrote the protocol and wrote the first draft of the manuscript. Author CSS managed the analyses of the study. Author VOONA managed the literature searches. Both authors read and approved the final manuscript.

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ABSTRACT

This Research of electron impact excitation of autoionizing states of rubidium have calculated the integral cross section using Distorted Wave Method in the range of incident energy of 15.8 -1000 eV. Numerical calculations have been done using a modified dwba1 fortran computer program which was originally made for hydrogen atom. The results are compared with Borovik work which showed a systematic agreement with inclusion of absorption potential, it also clear that incomparision with Pangantiwar and Srivastava there is a good qualitative agreement though the quantitive is attributed to the Multi Zeta Hartree fork wave functions applied.

Keywords: *Autoionization; total cross section; negative ion resonances; absorption potential; distorted wave method.*

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1. INTRODUCTION

The study of atomic collision physics plays an important role in the development of different areas of physics mainly astrophysical science, laser physics, light industry, medicine and material science. For this reason, scientists have developed experimental and theoretical tools to help understand the field of atomic collisions in-depth in the form of evaluation of differential, integral cross sections and angular correlation parameters. Research on electron atomic collision has seen rapid increase in interests, using theoretical and experimental approaches. This is due to the fact that these processes produce a clear means of investigating the dynamics of the collision process. However, it is mostly because the information is relevant in many areas.

The study of atomic collision involves the scattering of a projectile by a target. A projectile may be any charged particle e.g. electron, positron, proton, an ion and any atom, ion or a molecule may be the target. Experimentally, a beam of free particles is scattered from the target and the scattered particles detected in the asymptotic region [1]. A theoretical study can be done using semi classical methods or quantal approaches. Semi classical methods include semi classical impact parameter method, classical trajectory and Monte Carlo method, classical impulse and binary encounter approximation, eikonal approximation, multi-channel eikonal treatment and Glauber approximation. Quantal approaches are classified into perturbative and non perturbative methods. Perturbative methods include Born series, Eikonal series, distorted wave series [1] and many body theory [2]. Non perturbative method includes R-matrix [3], convergent close coupling [4] and variational methods.

Distorted wave approximation methods were introduced because the Born approximation failed to give accurate account of differential cross-sections for low impact energies and large scattering angles. In distorted wave approximation, the incident electron is taken to be elastically scattered by the initial state atomic potential. In the direct process, the incident electron makes a transition to a state in which it is being elastically scattered by final-state atomic potential. If the excitation of the atom is through

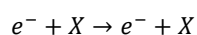
exchange process, the incident electron is captured into a bound state of the atom, while one of the initially bound electrons is ejected into an elastic-scattering state. The transition between the initial and final elastic state is calculated by perturbation method.

In experimental approach, developments have taken a great stride and this has also contributed greatly in the atomic collision and its applications. Instruments used have also been refined to give accurate result but the basic concept still remains the same. A typical set-up for electron-atom scattering experiments is illustrated in Fig. 1 [4].

The electron gun produces electrons and accelerates them at the required velocity towards the target atom for example rubidium. The incident electron is mono energetic with a momentum of k_1 . When a collision takes place, an electron with a momentum k_2 is deflected from its path and the target atom is either excited or ionized or remains in the same state. The deflected electron is detected by the detector. The direction of the scattered electron is determined by the polar θ and azimuthal angles ϕ .

The experiment (theory) measure (calculate) the differential cross-sections which are a measure of the probability that the electron will be scattered in a given direction, determined by the two angles θ and ϕ . However, integral cross section can be determined using differential cross-section values by integrating them over angle θ and ϕ . Differential cross-section measurements are carried out by crossing the target atom with mono energetic electron beam usually at 90° and determining the energy and angular distribution of the scattered electron. These distributions contain the information on the nature of the electron collision process, the energy level of target after collision and the corresponding cross-section.

In the electron-atom collision, such as the one studied, an elastic or inelastic collision can occur [1]. In the elastic collision, the target and the projectile energies are unaffected by the collision;



where X represent an atom.

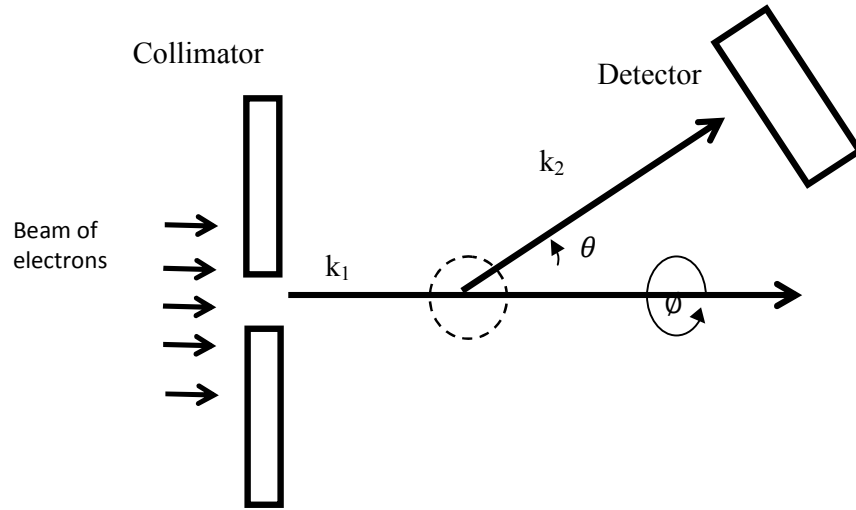
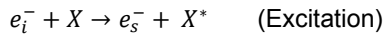
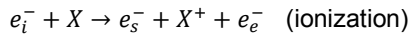


Fig. 1. Schematic diagram of a scattering experiment

In an inelastic collision, there is some energy transfer between the incident electron and the target. This results in either the target electron moving to higher energy level or one or more electron being removed from the atom;

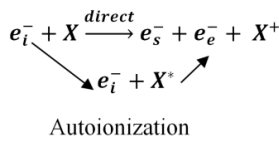


or



where e_i^- , e_s^- and e_e^- are respectively the incident, scattered and ejected electrons. X^* is the excited state of X .

The ionization can take place in two ways, either by direct process or through the excitation of the autoionizing state and then its subsequent decay to its ion by ejecting an electron. It can be shown as follows;



Here X^* is an autoionizing state. These autoionizing states lie above the first ionization threshold of the atom.

In inelastic scattering comparison of measured and calculated cross sections is important in the understanding of the nature of interactions of electrons with atoms. Cross sections for electron-

atom scattering are important in laser development and in plasma physics [4].

Elastic scattering cross sections are useful in X-ray photoelectron spectroscopy, XPS, and Auger-electron spectroscopy, AES, [5] the signal electrons are elastically scattered from within metal surfaces. These cross sections also provide vital input in the Monte Carlo simulation of conduction of electrons in solids [5].

1.1 Study Area

Integral cross sections.

2. METHODOLOGY

2.1 The Distorted Wave Method Applied to Electron-atom Collision

The total Hamiltonian for the system of the scattering of an electron from a neutral atom is expressed as;

$$H = H_\infty - \frac{1}{2} \nabla_0^2 + V \quad (1)$$

where H_∞ is the Hamiltonian for an isolated atom, the second term is the kinetic energy operator of an isolated projectile, V is the interaction between the projectile electron and the N -electron atom target and it is given by;

$$V = -\frac{N}{r_0} + \sum_{i=1}^N \frac{1}{r_{oi}} \quad (2)$$

Where $\frac{N}{r_0}$ and $\frac{1}{r_{01}}$ are the projectile electron target nucleus interaction term and projectile electron target electron interaction term respectively.

The initial state full scattering wave function Ψ_i is a solution of schrödinger's equation;

$$(H - E)\Psi_i^+ = 0 \quad (3)$$

where the + sign indicates the outgoing wave boundary conditions. In this case, the projectile electron experiences either elastic or inelastic collision with an N electron atom, the exact T-matrix in the two potential approach is given by [2];

$$T_{if} = (N + 1)\langle \chi_f^-(0) \psi_f(1, \dots, N) | V - U_f | A \Psi_i^+(0, \dots, N) \rangle + \langle \chi_f^-(0) \psi_f(1, \dots, N) | U_f | \psi_i(1, \dots, N) \beta_i(0) \rangle \quad (4)$$

In the equation 4, ψ_i and ψ_f are the properly antisymmetrized initial and final atomic wave functions for the isolated atom, which diagonalizes the atomic Hamiltonian H_α according to;

$$\langle \psi_n | H_\alpha | \psi_n \rangle = \varepsilon_n \delta_{nn} \quad (5)$$

β_i is an initial state plane wave (eigen function for an isolated projectile) and A is the antisymmetrizing operator for the N+1 electrons. If $\Psi_i^+(0, \dots, N)$ is chosen to be a product of a projectile wave function and an antisymmetrized atomic wave function of electrons 1, ..., N, then anti-symmetrization operator may be expressed as [6];

$$A = \frac{1}{N+1} (1 - \sum_{i=1}^N P_{i0}) \quad (6)$$

where the P_{i0} is the operator that exchanges electrons 0 and i. The potential U_f in equation 4 is an arbitrary distorting potential for the projectile, which is used to calculate χ_f^- by solving the equation;

$$\left(-\frac{1}{2} \nabla_0^2 - \frac{1}{2} k_f^2 + U_f \right) \chi_f^- = 0 \quad (7)$$

where the - superscript designates incoming wave boundary conditions and k_f is the final state wave vector of the projectile. Generally, the U_f is chosen to be any linear combination of initial and final state static potential of the target atom. In principle, however, U_f can be any potential as long as χ_f^- fulfils the appropriate

boundary conditions. All the working shown above and in the equations below is in atomic units. Forinelastic scattering, the second term in equation 4 vanishes for orthogonal atomic wave functions since U_f depends only on the single co-ordinate of the projectile. But for elastic scattering, the second term of the same equation is the dominant term, in fact it is generally the only contributing term since U_f is typically chosen such that the matrix elements of $V - U_f$ vanish.

The Lippmann Schwinger solution for Ψ_i^+ is given by;

$$\Psi_i^+ = [1 + G^+(V - U_i)] \psi_i \chi_i^+ \quad (8)$$

where G^+ is the full Green's function given by;

$$G^+ = (E - H + i\eta)^{-1} \quad (9)$$

But since Ψ_i^+ cannot be evaluated without making approximations, in the distorted wave approach Ψ_i^+ is expressed in terms of a product of an initial state distorted wave χ_i^+ and an initial atomic wave function ψ_i in its first order approximation of equation 8.

Then equation 4 takes the form (for excitation process considered);

$$T_{if} = (N + 1) \langle \chi_f^-(0) \psi_f(1, \dots, N) | V - U_f | A \chi_i^+(0) \Psi_i(1, \dots, N) \rangle \quad (10)$$

The initial state distorted wave is a solution of the schrödinger's equation;

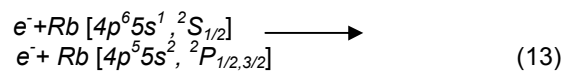
$$\left(-\frac{1}{2} \nabla_0^2 - \frac{1}{2} k_i^2 + U_i \right) \chi_i^+ = 0 \quad (11)$$

for an arbitrary distorting potential U_i which vanishes asymptotically. k_i is the incident wave vector and it is related to the incident energy by;

$$E_i = \frac{1}{2} k_i^2 \quad (12)$$

2.2 Evaluation of Direct and Exchange Matrix Elements

Equation 13 shows the excitation process;



where the 4p electron is excited to 5s. In the distorted wave approximation the transition

matrices for the one electron system excited from an initial state i to a final state f by electron impact is expressed using atomic units as;

$$T^{dir} = \langle \chi_f^-(r_0) \psi_f(r_1) | V(r_0 r_1) | \chi_i^+(r_0) \psi_i(r_1) \rangle \quad (14)$$

for direct excitation and;

$$T^{ex} = \langle \chi_f^-(r_0) \psi_f(r_1) | V(r_0 r_1) | \chi_i^+(r_1) \psi_i(r_1) \rangle \quad (15)$$

for exchange excitation, where $V(r_0 r_1)$ is the projectile-target atom interaction potential given by;

$$V(r_0, r_1) = z \left(\frac{1}{r_0} - \frac{1}{r_{01}} \right) \quad (16)$$

where Z is the charge of the incident particle and is taken as -1 for the electron: r_0 is the position vector of the incident electron and r_1 is the position vector of an atomic electron undergoing a transition and r_{01} is the position vector between the projectile and target electron.

In order to evaluate the direct and exchange scattering amplitudes given above, the radial distorted waves χ_f^- and χ_f^+ are expanded in terms of the partial waves as;

$$|\chi_f^+\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{k_f r} \sum_{l_i m_i} i^{l_i} \chi_{l_i}(k_i, r) Y_{l_i m_i}^*(k_i) \quad (17)$$

and

$$|\chi_f^-\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{k_f r} \sum_{l_f m_f} i^{l_f} \chi_{l_f}^* Y_{l_f m_f}^* Y_{l_f m_f}^*(k_f) \quad (18)$$

where Y_{lm} is a spherical harmonic.

In the expansion of χ_f^- the complex conjugate of radial part χ_{l_f} and is taken so that it satisfies the incoming wave boundary conditions. Substituting the above partial wave expansion of the distorted waves in the equation 7 and equation 11, it is found that the radial distorted waves are solutions of the following equation;

$$\left[\frac{d^2}{dr^2} - \frac{l_s(l_s+1)}{r^2} - U_s(r) + k_s^2 \right] \chi_{l_s}(r) = 0 \quad (19)$$

where $s=i$ for initial state and $s=f$ for the final state distorted wave. The equation 19 will be solved using Numerov's method. The differential cross section will be obtained using the relation;

$$\left(\frac{d\sigma}{d\Omega} \right)_{4p \rightarrow 5s} = \frac{1}{4\pi^2} \frac{k_f}{k_i} \sum_{m=-1}^{+1} \left[\frac{1}{4} |T_{4p \rightarrow 5s}^{dir} + T_{4p \rightarrow 5s}^{ex}|^2 + \frac{3}{4} |T_{4p \rightarrow 5s}^{dir} - T_{4p \rightarrow 5s}^{ex}|^2 \right] \quad (20)$$

And the total cross section shall be obtained as;

$$\sigma = \int_0^{2\pi} \int_0^\pi \frac{d\sigma}{d\Omega} \sin\theta d\theta d\phi \quad (21)$$

2.3 Distortion Potential

A complex local spherically symmetric optical model potential for distortion of projectile wave have been used [7];

$$V_{opt}(r) = V_{st} + V_{exch} + iV_{abs} \quad (22)$$

where V_{st} is the static potential, V_{exch} is a local energy dependent exchange potential and iV_{abs} is absorption potential arising because of the processes other than being considered i.e. because of absorption to other channels.

In this study the static potential of the target atom in its initial states as the distortion potential, V_{st} for the initial state of the projectile electron because, in initial state the projectile only 'sees' the initial state static potential of the target atom and a linear combination of the static potential of the target atom in its initial and final states as the distortion potential V_{st} for the final state of the projectile electron because when the energy of the projectile is transferred to the atom, it takes some time before the atom goes to its final state. Projectile in its final state 'sees' an intermediate potential between the initial and final state static potential of the target [8]. That is;

$$U_i = \langle \psi_i | V | \psi_i \rangle = V_{st} \text{ in the initial channel} \quad (23)$$

$$U_f = \frac{1}{2} \langle \psi_i | V | \psi_i \rangle + \frac{1}{2} \langle \psi_f | V | \psi_f \rangle = V_{st} \text{ in the final channel} \quad (24)$$

Exchange potential of [9] is given as;

$$V_{exc}(r) = \frac{1}{2} [E - V_{st}(r)] - \frac{1}{2} \{ [E - V_{st}(r)]^2 + 4\pi\rho(r) \}^{1/2} \quad (25)$$

Absorption potential due to [10] given as;

$$V_{abs} = -\frac{1}{2} T_{loc} \rho(r) \sigma_b \quad (26)$$

where $T_{loc} = [2(E - V_{se})]^{1/2}$ is the local kinetic energy of the incident electron, $\rho(r)$ is the

electron charge density of the target atom, V_{se} is the static plus exchange potential and σ_b is the average binary collision cross section.

2.4 Evaluation of Static Potentials

The general mathematical formulation of static potentials is expressed as;

$$U_s = \langle \psi_s | V | \psi_s \rangle \quad (27)$$

Where ψ_s is the target wave function $s=i$ or f for initial or final state respectively and V is the interaction between the target and the projectile. Hartree Fock wave functions of [5] have been used for the target states. In these wave functions ψ_s is summed over slater type orbitals of the basis set as;

$$|\psi_s\rangle = \sum_n C_n |\phi_n\rangle \quad (28)$$

and

$$\langle \psi_s | = \sum_n C_n^* \langle \phi_n | \quad (29)$$

The value of C_n represent the expansion coefficients and ϕ_n are the slater type orbitals of the basis set. Using equation 28 and 29 in equation 27 the distortion potentials can be written as;

$$U_s = \sum_n \sum_n C_n C_n^* \langle \phi_n | V | \phi_n \rangle \quad (30)$$

where V is the interaction potential in atomic units as given in equation 27. Since the target is being treated as one election atom, the interaction potential becomes;

$$V = -\frac{1}{r_0} + \frac{1}{r_{01}} \quad (31)$$

$\frac{1}{r_{01}}$ can be expanded in spherical harmonics as;

$$\frac{1}{r_{01}} = \sum_l \sum_{l'} \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{l,m}(r_0) Y_{l,m}^*(r_1) \quad (32)$$

Where $r_{<}$ and $r_{>}$ are the lesser or greater of r_0 and r_1 respectively and Y_{lm} 's are spherical harmonics.

In distorted wave calculations, the spherically symmetric distorting potential used consists of the nuclear term on the right hand side of equation 31 plus the monopole term ($l=0$) of the summation of equation 32 since the effects of non-spherical terms is very small [2]. Since;

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \quad (33)$$

The static potential is thus expressed as (in Rydberg units);

$$U_s = 2 \sum_n \sum_n C_n C_n^* \left\langle \phi_n \left| \frac{1}{r_{>}} - \frac{1}{r_0} \right| \phi_n \right\rangle \quad (34)$$

The slater type orbitals are expressed as a product of radial wave functions and spherical harmonics $Y_{l,m}$ [5] and are given as;

$$\phi_n = N_n r^{\mu_n - 1} \exp(-\xi_n r) Y_{l,m}(\hat{r}) \quad (35)$$

where μ_n is the principal quantum number of the n^{th} orbital of the basis set ξ is a constant and the normalization factor N_n of the orbital is given as;

$$N_n = \frac{(2\xi)^{\mu_n + \frac{1}{2}}}{\sqrt{(2\mu_n)!}} \quad (36)$$

When the values of the wave function are substituted in equation 34 and replace the Bra and Ket notation with the standard integrals a fully expanded static potential given below is obtained;

$$U_s = 2 \sum_{nlm} \sum_{n'l'm'} C_n C_n^* N_n N_n^* \int_{r_0}^{\infty} r_1^{\mu_n + \mu_n'} \left(\frac{1}{r_1} - \frac{1}{r_0} \right) \exp(-[\xi + \xi'] r_1) dr_1 \int Y_{l,m}(r_0) Y_{l',m'}(r_1) d\Omega \quad (37)$$

In equation 37 above partial integration of the radial component is made use of such that from the radial distance 0, r^0 is considered to be greater than r^1 , while from r^0 to infinity, r^1 is considered to be greater than r^0 . Since the spherical harmonics are orthonormal, the last integral on the right hand side of equation 37 vanishes unless $l=l'$ and $m=m'$

As a result the distortion potential reduces to;

$$U_s = \sum_{nn'lm} C_n C_n^* N_n N_n^* \int_{r_0}^{\infty} r_1^{\mu_n + \mu_n'} \left(\frac{1}{r_1} - \frac{1}{r_0} \right) \exp(-kr_1) dr_1 \quad (38)$$

$$\text{where } k = [\xi_n + \xi_{n'}] \quad (39)$$

In this case the integral of equation 38 above is evaluated analytically in order to get the exact static potentials which have been used as the distortion potentials. The analytical solutions of equation 38 depends on the sum of the principal quantum numbers, μ_n and $\mu_{n'}$ and the sum varies from 2 to 10 for the problem that was solved.

3. ANALYSIS AND RESULTS

The present results (with static potential, static plus exchange potential, static plus exchange plus absorption potential) have been compared amongst themselves and with the available experimental and calculated results. Multi zeta (MZ) wave functions have been used in this work. The results have been compared with those of [4,11,12] and [13] for electron impact excitation of rubidium. The result for [11] was obtained through experiment, [13] was obtained theoretically by employing a fully relativistic Dirac B-spline R-matrix (close-coupling) model and for [14] and [12] results is a calculation using the distorted wave method.

In this study integral cross sections (ICS) for inelastic scattering of electrons by a rubidium atom were calculated at the range of 15.8–1000eV. Table 1 gives the present inelastic integral cross sections, obtained using static potential, static plus exchange potential and static plus exchange plus absorption potential. The present integral cross sections results for electron impact excitation of the $4p^55s^2$ state of Rubidium are compared with the works [14,11] and [13]. The present integral cross section results indicate that when only static potential is taken as the distortion potential, it gives larger cross sections compared to those obtained when static plus exchange and static plus exchange plus absorption potentials [7] are used as distortion potential. This study also reveals that

with absorption potential the cross sections are lowered compared to when only exchange potential is included in the distortion potential.

At lower energies between 15.8-18.6eV and at energies above 50eV the present three sets of cross sections are nearly the same. Energies between 19.0 – 50eV the cross sections are so different with static potential results having the highest cross sections followed by static plus exchange and static plus exchange plus absorption potential results having the lowest values. This can be attributed to the opening of several or an infinite number of channels in addition to the elastic channel.

It is also clear that there is an abrupt increase in the integral cross sections at electron energy just above threshold energy [12] of the lowest autoionizing state of rubidium and it peaks at about 18.6eV. This is due to formation of a composite state of negative ion Rb^- which then decays into the rubidium atom in the autoionizing state and a free scattered electron with low energy which explain a sharp increase in the cross section near threshold energy. It can also be as a result of exchange effects between projectile electron and atomic electron at low impact energies.

From 19 to 50eV the effect of exchange and absorption potential is very much apparent, with the absorption potential lowering the cross section much more than exchange potential and brings the cross section closer to the experimental results of [11].

Table 1. Integral cross sections for electron impact excitation of $4p^55s^2$ state of rubidium atom

Energy (eV)	Static potential	Static and exchange potential	Static, exchange and absorption potential
15.8	5.962E-03	8.61E-03	8.61E-03
15.9	2.146E-03	2.94E-02	2.94E-02
16	4.233E-03	5.61E-02	5.61E-02
17	3.191E-01	3.46E-01	3.46E-01
18	4.491E-01	4.53E-01	4.53E-01
18.2	4.565E-01	4.58E-01	4.58E-01
18.4	4.601E-01	4.59E-01	4.59E-01
18.8	4.578E-01	4.54E-01	4.54E-01
19	4.533E-01	4.49E-01	4.49E-01
20	4.141E-01	4.08E-01	4.08E-01
30	2.475E-01	2.49E-01	1.53E-01
50	2.980E-01	2.98E-01	2.90E-01
60	2.920E-01	2.92E-01	2.86E-01
80	2.733E-01	2.73E-01	2.69E-01
100	2.567E-01	2.57E-01	2.54E-01
200	1.936E-01	1.94E-01	1.93E-01
600	1.002E-01	9.83E-02	9.82E-02
1000	5.971E-02	5.93E-02	5.93E-02

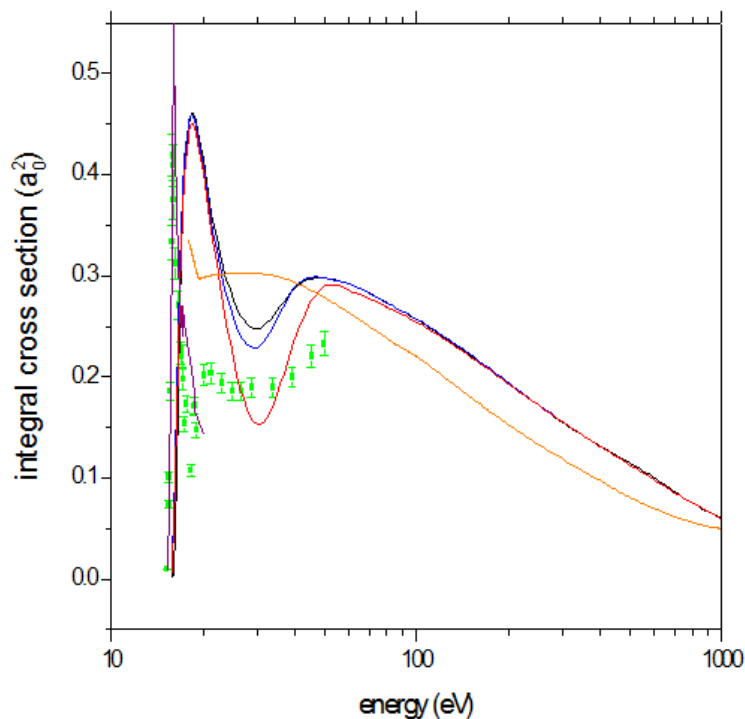


Fig. 2. Integral cross section for excitation of the lowest autoionising level in rubidium

■ Borovik experimental (2013) results, ■ present static distortion potential results, ■ present static and exchange distortion potential results, ■ present static, exchange and absorption distortion potential results, ■ Borovik theoretical (2012) results; ■ Srivastava and Pangantiwar (1987) results

At higher projectile energies the effects of exchange and absorption potentials are not visible and that's why the present three sets of cross section results are nearly equal. This is due to minimal interaction between the projectile electron and the target atom.

The present results for energies greater than 50eV are slightly higher than those of [14] this can be attributed to the choice of distortion potential. The present calculation we have applied as proposed by [8], initial state static potential as the initial channel distortion potential while a linear combination of initial and final state static potentials as the final channel distortion potential while in [14] calculation initial state static potential is the initial channel distortion potential while the final state static potential is the final channel distortion potential. In addition, it could be attributed to the present results as we applied MZ Hartree fork wave functions by [5] while they used MZ Hartree fork wave functions by [15]. When compared with [11,12] and [13] results they are in good qualitative agreement with both experimental and theoretical results.

4. SUMMARY

From this study, the following conclusions have been arrived at:

The present results are in good qualitative agreement compared to [14], at all the projectile energies the present cross sections are relatively higher. This may be attributed to the choice of distortion potential which is more apparent at low impact energies than at high energies. The energy of the projectile determines the level of interaction in the target atom. When the projectile energy is lowered, it leads to higher interaction.

Absorption distortion potential lowers the cross section at low energies and this is due to the opening of more channels at this point and considerable amount of time spent by the incident electron in the vicinity of the atom.

Near threshold strong negative ion resonances (due to the existence of an extra electron in the vicinity of the target atom electron cloud which

makes the target behave like a negative ion) there is sharp rise in the cross section though the exchange has less effect [6].

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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