Relativistic distorted wave approach to electron impact excitation of argon gas using a complex potential

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Abstract
In this study, we apply relativistic effects to excitation of the lowest lying resonance states of argon gas with inclusion of absorption, polarization and exchange effects to the electrostatic distortion potential to form an overall complex distortion potential. The atomic wave functions are constructed in the multi-configuration Dirac Fork approach by modifying the general-purpose relativistic atomic structure code GRASP for numerical procedures, while differential cross sections (DCS) and integral cross sections (ICS) have been obtained using our new code RDWBA1. Our results are compared with available experimental and theoretical results in literature. Present results from this study predict that use of a complex distortion potential in the relativistic approach to excitation of argon generally lowers integral and differential cross sections as impact energies of the incident electron increases, specifically beyond 50 eV, and that the energy dependent polarization potential adopted in this work plays a major role in improving shapes of cross-sections at near threshold impact energies up to around 30 eV, where available distorted-wave methods fail to give satisfactory results when compared to experiments.

1. Introduction

The distorted-wave Born (DWB) method is known to be a very successful and not computationally demanding method for electron impact excitation of atoms and ions, especially at intermediate and high energies (Itikawa 1986). It is a kind of first-order perturbation theory in terms of distorted waves, hence a proper distortion potential has to be chosen (Zuo et al 1991). Relativistic effects in excitation of the target arise from two main sources, namely relativistic effects in target wave functions and the relativistic interaction of the free and bound electrons in the target (Chen 1996). The excitation of the ground np⁶ state of heavy rare gases to the first excited-electron np⁶⁷(n+1)s configuration results in the excitation of four levels with total angular momentum of the collision system J = 0, 1, 1 and 2. Those with J = 0 and 2 represent the metastable states while the remaining two with J = 1 represent the resonance states for which configuration interaction is taken into account. Previously, most theoretical and experimental studies on the excitation of argon gas have emphasized primarily the excitation of the lowest lying excited states [3s⁵3p⁵4s]¹⁺, ³P_j, from the ground state [3s⁵3p⁴]¹S₀, with theoretical calculations considering only the non-local exchange and the energy independent polarization effects. For excitation of the resonance states of argon, relativistic distorted-wave (RDW) studies have not yet included absorption effects (The imaginary part of the interaction potential), which accounts for the loss of flux into other possible open inelastic channels.

Bartschat and Madison (1987) carried out a non-relativistic study on electron impact excitation of rare gases. In this work they used the first-order distorted-wave Born approximation (DWBA) method where results were calculated using the excited-state static potential plus the dynamic local electron-exchange potential. No polarization or absorption potential was applied in this study. For Ar, DCS results yield an overall satisfactory agreement at all scattering angles for both singlet and triplet excited states with the available experimental data at incident-electron energies above 50 eV, but not below 30 eV. Zuo et al (1992) carried out a RDW calculation of...
electron impact excitation of heavy noble gases Ar, Kr and Xe from ground state to the lowest lying excited states for incident electron energies of 20, 30 and 50 eV. They applied a fully relativistic distorted-wave method with a non-local exchange potential and energy independent polarization potentials. Comparing their data with that of Filipovic (1984), first order many body theory (FOMBT) of da Paixao et al (1984) and DWBA of Bartschat and Madison (1987) results, satisfactory agreement is seen only for the optically allowed transitions at 50 eV. The singlet transition results do not give satisfactory agreement below 30 eV impact energies. Madison et al (1998) calculated ICS and DCS for electron-impact excitation of argon to 12 different target states using a semi-relativistic first-order distorted-wave Born theory. Their cross sections results are very large at energies below 30 eV compared with experimental data from Chutjian and Cartwright (1981) and Tsurubuchi et al (1996) for the excitation of the lowest resonance states of argon, but yield reasonably good agreement at higher energies up to 150 eV. Khakoo et al (2004) carried out an electron-impact differential cross section (DCS) and DCS-ratio measurements for electron impact excitation of lowest excitation levels of argon. They made both relativistic and semi-relativistic calculations which include; 41-state R-matrix, unitarized first order many body theory (UFOMBT), RDW and semi relativistic DWA methods for energies ranging from 14 to 100 eV. Non relativistic calculations in this study fail to agree with experimental measurements at impact energies below 30 eV, but agree well as energies tend toward 100 eV. Zatsarinny et al (2014) used the R matrix method with close-coupling with target state wave functions ranging from 5 up to 500 to make calculations for electron impact excitation of the lowest lying excited states of argon over an extended energy range from threshold up to 300 eV. Cross sections obtained with less target states wave functions are very large compared to experimental results although inclusion of many more target states in their calculation wave functions improves ICS and DCS results.

In all the studies on excitation of low lying states of argon by different workers described here, the distorted-wave methods apply real potentials. The inclusion of relativistic effects for distorted-wave methods greatly improves the agreement of results for both cross-sections and angular correlation parameters but still fail to yield an overall satisfactory agreement at all scattering angles and projectile energies below 30 eV, even after the inclusion of electron exchange and energy independent polarization effects to the projectile-target interaction potential. Therefore in this work, we have used the relativistic distorted-wave method (RDW) to excitation of the lowest resonance states of argon and together with the static potential, we modified the distortion potential to include more effects such as the absorption of incident projectile flux into other open channels and used an energy dependent polarization potential in addition to a local exchange potential, in order to check its effect on cross sections at low and intermediate electron impact energies. Cross sections results presented are calculated using four treatments of the RDWBA model namely; SEPA-RDWBA (static + exchange + polarization + absorption potentials), SEP-RDWBA (static + exchange + polarization potentials), SE-RDWBA (static + exchange potentials and S-RDWBA (static potential).

2. The relativistic distorted wave method

2.1. Theoretical framework

We consider an atom target excited by an incident projectile electron from an initial state ‘a’ to a final state ‘b’ for transition \([3s^23p^6]S_0 \rightarrow [3s^23p^54s]^{1,3}P_1\). The Dirac form of the Hamiltonian for an atom with N electrons, in atomic units \((m = e = \hbar = 1, c = 1/137)\) is (Grant 1970)

\[
H = \sum_{i=1}^{N} H_i + \sum_{i<j}^{N} \frac{1}{r_{ij}}
\]  

(1)

where \(r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|\) and \(\mathbf{r}_i\) is the position vector of the electron \(i\), while

\[
H_i = c\alpha \cdot p + \beta c^2 + V(r)
\]  

(2)

The quantity \(V(r) = -Z/r\) is the potential energy of electron \(i\), \(Z\) is the atomic number, \(c\) is the relativistic velocity of light, and \(p = -i\hbar \nabla\) is the momentum operator while \(\alpha\) and \(\beta\) represent the usual Dirac matrices. For electron impact excitation of an atom with N electrons from state ‘a’ to state ‘b’, the distorted-wave T-matrix element is given by (Zuo et al 1991)

\[
T^\text{RDW}_{a \rightarrow b} = \langle \chi_b^- | V - U | A \chi_a^+ \rangle
\]  

(3)

U is the distortion potential which is taken as a function of only the radial coordinate of the projectile electron. \(A\) is the anti-symmetrizing operator to account for electron exchange. The total wave function for channel \(a\) and \(b\) is given respectively as

\[
\chi_a^+ = \Psi_a^{|0 \rangle \langle 1, 2, ..., N|} F^\text{RDW}_{a|b} (N+1)
\]  

(4a)
\[ \chi_{\pm} = \Phi_{\pm}^r(1, 2, \ldots, N)F_{\kappa_{\mu_{\text{rel}}}}(N + 1) \]  

(4b)

\[ \Phi_{\pm}^r \text{ and } \Phi_{\pm}^a \text{ are bound state wave functions constructed from central field Dirac-Fock orbitals. That is} \]

\[ \phi_{\kappa_{\mu_{\text{rel}}}}(r, \sigma) = \frac{1}{r} \left( \frac{P_{\kappa_{\mu_{\text{rel}}}}(r)\chi_{\kappa_{\mu_{\text{rel}}}}(r, \sigma)}{Q_{\kappa_{\mu_{\text{rel}}}}(r)\chi_{-\kappa_{\mu_{\text{rel}}}}(r, \sigma)} \right) \]  

(5)

where \( P \) and \( Q \) are the ‘large’ and ‘small’ components of the radial wave function while \( \chi_{\pm\kappa_{\mu_{\text{rel}}}} \) are the spin angular momentum functions given in terms of spherical harmonics \( Y_{\mu_{\text{rel}}}(r) \) and normalized two-component spinors \( \psi_{\pm}(\sigma) \) by

\[ \chi_{\kappa_{\mu_{\text{rel}}}}(r, \sigma) = \sum_{\mathbf{lm}_{\kappa_{\mu_{\text{rel}}}}} (\mathbf{lj}_{\mu_{\text{rel}}}) Y_{\mu_{\text{rel}}}(r) \psi_{\sigma}(\sigma) \]  

(6a)

\[ \chi_{-\kappa_{\mu_{\text{rel}}}}(r, \sigma) = \sum_{\mathbf{lm}_{\kappa_{\mu_{\text{rel}}}}} (\mathbf{lj}_{\mu_{\text{rel}}}) Y_{\mu_{\text{rel}}}(r) \psi_{\sigma}(\sigma) \]  

(6b)

In this study, the configurations of concern are those with total angular momentum \( f = 1 \), which can be expressed in single-configuration representation, in the intermediate-coupling scheme in a similar way as that of Khakoo et al (2004). Taking into account the configuration interaction, the atomic wave functions of the first two \( f = 1 \) excited states of argon are

\[ 4s[1/2]^2 = c_1 \Phi(a_1^pJ_M^a) - c_2 \Phi(a_2^pJ_M^a) \]  

(7a)

\[ 4s[3/2]^2 = c_2 \Phi(a_1^pJ_M^a) - c_1 \Phi(a_2^pJ_M^a) \]  

(7b)

Here, \( c_1 = 0.8978 \) and \( c_2 = 0.4405 \) are the configuration mixing coefficients calculated using the GRASP program (Dyall et al 1989). The wave functions above are written in the common Racah notation. The total angular momentum of the channel is related to the orbital angular momentum by the relation \( l = 2j - l \), while \( \psi \) represents the normalized two component spinors. An angular state is characterized by the quantum number \( k \) or alternatively by quantum numbers \( (l, j) \).

\[ j = |k| - 1/2 \]  

(8)

Parity of the orbital is given in terms of the orbital quantum number as \((-1)^l\). Following the formulation by Zuo et al 1991, the equation for \( T \)-matrix, the distorted waves describing the incident and scattered electrons in the channel ‘ch’ in the general relativistic version of the partial wave expansion is

\[ F_{\kappa_{\mu_{\text{rel}}}}(\kappa_{\mu_{\text{rel}}}) = \frac{1}{(2\pi)^{1/2}} \sum_{\kappa_{\mu_{\text{rel}}}} e^{h\xi_{\kappa_{\mu_{\text{rel}}}} d_{\kappa_{\mu_{\text{rel}}}}(\hat{\kappa}_{\mu_{\text{rel}}})} \left( \frac{f_{\mu_{\text{rel}}}(r) \chi_{\kappa_{\mu_{\text{rel}}}}(r, \sigma)}{g_{\mu_{\text{rel}}}(r) \chi_{-\kappa_{\mu_{\text{rel}}}}(r, \sigma)} \right) \]  

(9)

where

\[ d_{\kappa_{\mu_{\text{rel}}}} = 4\pi \left[ \frac{E_{\kappa_{\mu_{\text{rel}}} + c^2}}{2E_{\kappa_{\mu_{\text{rel}}}}} \right]^{1/2} \sum_{\mathbf{lm}_{\kappa_{\mu_{\text{rel}}}}} (\mathbf{lm}_{\kappa_{\mu_{\text{rel}}}}J_M^a) Y_{\mu_{\text{rel}}}^a(r) \hat{\kappa}_{\mu_{\text{rel}}} \]  

(10)

The plus and minus signs indicate the usual outgoing and incoming asymptotic boundary conditions. The \( l \) and \( j \) refer to the orbital and total angular momentum of the projectile electron while \( \mu_{\text{rel}} \) denotes the spin orientation of the channel. Furthermore, \( \xi_{\kappa_{\mu_{\text{rel}}}} \) is the phase shift of the partial wave, \( (\mathbf{lm}_{\kappa_{\mu_{\text{rel}}}}J_M^a) \) is a Clebsch–Gordan coefficient while \( E_{\kappa_{\mu_{\text{rel}}}} \) is the energy of the projectile electron. Generally, the quantum number \( k \) is given by

\[ k = \pm(j + 1/2) \]  

(11)

The radial distorted waves \( f_{\mu_{\text{rel}}}(r) \) and \( g_{\mu_{\text{rel}}}(r) \) are solutions of the following pair of coupled integro-differential equations below (see Zuo et al 1991 and Zeman et al 1994)

\[ \begin{align*}
\left( \frac{d}{dr} + \frac{k}{r} \right) f_{\mu_{\text{rel}}}(r) - \frac{1}{hc} (2mc^2 - U + E_{\kappa_{\mu_{\text{rel}}}}) \\
\times g_{\mu_{\text{rel}}}(r) - \frac{1}{hc} W_Q(k; r) = 0
\end{align*} \]  

(12)

\[ \begin{align*}
\left( \frac{d}{dr} - \frac{k}{r} \right) g_{\mu_{\text{rel}}}(r) + \frac{1}{hc} (-U + E_{\kappa_{\mu_{\text{rel}}}} - f_{\mu_{\text{rel}}}(r)) \\
+ \frac{1}{hc} W_P(k; r) = 0
\end{align*} \]  

(13)

Here, \( W_Q(k, r) \) and \( W_P(k, r) \) are non-local exchange potentials, \( E_{\kappa_{\mu_{\text{rel}}}} \) is the relativistic kinetic energy of the scattered electron while \( k_{\kappa_{\mu_{\text{rel}}}} \) is the corresponding linear momentum. Furthermore, \( U \) is the distortion potential used in calculation of the radial distorted-wave functions which satisfy the asymptotic conditions.
2.2. Distorting potentials $U_A$ and $U_B$

In this study, we employ the complex potential of the ground state argon atom as the initial channel distortion potential and the complex potential of the excited state argon atom as the final channel distortion potential. The complex potential $U$ is such that; the real part is the static, exchange and polarization potentials while the imaginary part is the absorption potential. That is

$$U = (V_A + V_{ex} + V_{pol}) + iV_{abs}$$

The static potential is given by;

$$V_0(r) = -\frac{Z}{r} + \int \frac{\rho(r')}{r'^2} r'^2 dr'$$

$Z$ is the atomic number of the target atom and $r_0$ is the greater of $r$ and $r'$. The charge density is defined as

$$\rho(r) = \frac{1}{4\pi r^2} \sum_{n,k'} N_{n,k'} [P^{a}_{n,k'}(r') + Q^{a}_{n,k'}(r')]$$

$N_{n,k'}$ is the occupation number of the atomic orbital. The absorption potential adopted in this work is that of Staszewska et al (1984) and Sharma (2014) which is given in terms of the local velocity of the scattering electron $[2(E - V^{SE})]^{1/2}$ and the mean binary collision cross section $\sigma$, that is

$$V_{abs}(r, E) = -\frac{1}{2} [2(E - V^{SE})]^{1/2} \rho(r) \sigma$$

The polarization potential is given as (Jhanwar and Khare 1976)

$$V_{pol}(r, E) = -\frac{\alpha_d r^2}{(r^2 + d^2)^3} - \frac{\alpha_q r^4}{(r^2 + d^2)^5}$$

where $\alpha_d = 11.07$ and $\alpha_q = 52.25$ is the dipole and quadrupole polarizabilities for argon and $d = 0.75 k_{CH}/\Delta$ is an energy dependent parameter with $\Delta$ as the mean excitation energy and $k_{CH}$ is the channel’s linear momentum.

We adopt the exchange potential of the form given by Furness and McCarthy (1973)

$$V_{ex}(r, E) = -\frac{1}{2} [(E - V_{st}(r))^2 + \rho(r)]^{1/2} - [E - V_{st}(r)]$$

2.3. Evaluation of transition matrix elements

Following the formulation by Zuo et al (1991), the $T$ -matrix elements in equation (3) are evaluated by substituting (4) and (9) into (3) then after performing a lengthy but straight-forward angular momentum algebra numerically, we obtain

$$T_{a\rightarrow b}^{RDW} = \sum_{k_a k_b \mu_a \mu_b} e^{i(n_a + n_b)} T_{a\rightarrow b} \left[ \frac{2I_a + 1}{4\pi} \right]^{1/2}$$

$$\times \{ T_{a\rightarrow b}^{D} + (-1)^S T_{a\rightarrow b}^{E} \} \left[ \frac{\hat{I}_a}{\mu_a M_a m_a} \right]$$

$$\times (l_a 0 1/2 \mu_a l_b \mu_b) (l_b m_b 1/2 \mu_b l_a m_a) Y_{l_b m_b}^k(\Delta_k)$$

The direct and exchange T matrix elements of (22) can be shown to be

$$T_{a\rightarrow b}^{D} = \frac{3}{2\pi} \sum_{l_{k_a}} \left[ \frac{E_a + c^2}{2E_a} \right]^{1/2} \left[ \frac{E_b + c^2}{2E_b} \right]^{1/2} (2j + 1)^{1/2}$$

$$\times (2j_b + 1)^{1/2} \left( \frac{l_a}{2} \right)^{1/2} (l_b m_b 1/2 \mu_b l_a m_a) Y_{l_b m_b}^k(\Delta_k)$$

(23)
and
\[
T_{\ell a \rightarrow \ell b}^E = \frac{2}{\pi} \sum_{\ell_k} \left\{ \frac{E_a + \ell^2}{2E_a} \right\}^{1/2} \left\{ \frac{E_b + \ell^2}{2E_b} \right\}^{1/2} (2\ell + 1)^{1/2} \\
\times (2\ell_a + 1)^{1/2}(2\ell_b + 1)^{1/2} \\
\times (\sqrt{3}) \begin{pmatrix} j & j_a & j_b \\
1/20 & 1/20 & 1/20 \\
-1/2 & -1/2 & -1/2
\end{pmatrix} \begin{pmatrix} j_a & j_b \\
j/j & j/j \end{pmatrix}
\]
\[(-1)^{\ell_a + n_a + \lambda} \Gamma_{\ell}(nk, c_{a,k}; n_k, c_{b,k})
\]
which contain the radial integrals for the direct and exchange T matrix elements respectively as
\[
\Gamma_{\ell}(nk, c_{a,k}; n_k, c_{b,k}) = \int_0^\infty \int_0^\infty (P_{a,k}(r)P_{b,k}(r) + Q_{n,k}(r)Q_{a,k}(r)) \gamma_{\ell}(r, s) \\
\times (f_{c_{a,k}}(s)f_{c_{b,k}}(s) + g_{c_{a,k}}(s)g_{c_{b,k}}(s)) dr ds
\]
and
\[
\Gamma_{\ell}(nk, c_{a,k}; n_k, c_{b,k}) = \int_0^\infty \int_0^\infty (P_{a,k}(r)f_{c_{a,k}}(s) + Q_{n,k}(r)g_{c_{a,k}}(s)) \gamma_{\ell}(r, s) \\
\times (P_{b,k}(s)f_{c_{b,k}}(s) + Q_{n,k}(s)g_{c_{b,k}}(s)) dr ds
\]
Here, \(\ell_a\) and \(j_a\) represent quantum numbers for the incident electron partial wave while \(\ell_b\) and \(j_b\) represent the outgoing electron partial wave. Furthermore, \(n\), \(\ell\), and \(j\) are quantum numbers for the active \(\bar{p}\) or \(p\) electron, while \(n\), \(\ell\), and \(j\) represent the excited \(s\) electron. Parity conditions requires that \(\ell_a + \ell_b + B\) and \(l + l + j\) be an even integer. Furthermore, the symbol \(\lambda\) satisfies the triangular condition \(|j - j| \leq \lambda \leq j + j\).

From the calculated T-matrix elements the various collisional parameters can be determined. Here we define the relativistic scattering amplitude and cross sections expressions as that of Kaur et al (1998b) which is,
\[
f(J_bM_b, \mu_b, J_aM_a, \mu_a) = (2\pi)^{1/2} \left(\frac{k_b}{k_a}\right)^{1/2} \\
\times T(J_bM_b, \mu_b, J_aM_a, \mu_a)
\]

2.4. Cross sections
For a given value of \(J_a\) and \(J_b\) the DCS for scattering is defined as
\[
\frac{d\sigma}{d\Omega} = \frac{1}{2(2\ell + 1)} \sum_{M_a,M_b,M_{\mu_a},M_{\mu_b}} |f(J_bM_b, \mu_b, J_aM_a, \mu_a)|^2
\]
The angular integration over the scattering angles of equations above respectively, gives us total cross sections for individual final magnetic sub-states and their summed value. That is
\[
\sigma_{\text{tot}} = \int \frac{d\sigma}{d\Omega} d\Omega
\]

2.5. Top-up procedure
In order to obtain improved cross sections, it is important to include high \(l\) partial wave contributions in the RDW calculations. The challenge however involves the lack of convergence of the partial-wave expansion as \(l\) approaches infinity. The analytic Born Subtraction Technique detailed by Fontes and Zhang 2007 and Bostock et al (2013) has been used however to give more accurate calculations of the excitation cross sections in a fully relativistic treatment and ensure convergence of results for high partial waves. That is
\[
T_{D,a \rightarrow b} = T_{D,a \rightarrow b}^{\text{born}} + \sum_{l=0}^{l_{\text{max}}} (T_{D,a \rightarrow b}^{D} - T_{D,a \rightarrow b}^{\text{born}})
\]
First, exchange is neglected beyond a set limit for \(l\), say \(l_{\text{max}}\), and then it is assumed that beyond this point, plane waves dominate, hence we get the relativistic Born approximation T-matrix formula
\[
T_{D,a \rightarrow b}^{\text{born}} = (\Phi^a_{D}(N)F^{PW}_{D,a\mu_a}(N + 1)|V - U|\Phi^a_{D}(N)F^{PW}_{D,a\mu_a}(N + 1))
\]
Here $P_{ch_{i,\mu a}}^{PW}$ is a relativistic plane wave in channel $'ch'$. $T_{b \rightarrow b}^{D,born}$ is obtained by replacing the relativistic version of the partial wave expansion used in deriving $T_{b \rightarrow b}^{D}$ with a partial wave expansion of the relativistic plane wave (see, Rose (1961) pages 70 and 162) and ignoring the phase shifts.

2.6. Data analysis

Obtained algorithms are solved using a new program RDWBA1 to obtain continuum radial wave-functions ($f$ and $g$), Transition matrix elements ($T$), Scattering amplitudes, differential cross-sections (DCS) and Integral cross sections (ICS), while the General Relativistic Atomic Structure Program, GRASP program (Dyall et al 1989) is modified in order to calculate the atomic radial wave-functions ($P$ and $Q$). The program RDWBA1 is written in FORTRAN77 language, designed to run on windows operating system with a typical running time of approximately 60 seconds on PENTIUM 4 computers with minimum processor speed of 2.1 gigahertz and 2048 random access memory. Atomic radial wave functions from the GRASP program together with their grid are used as input for the RDWBA1 program which further uses the Wentzel-Kramers-Brillouin (WKB) approximation in solving the Dirac equations (12) and (13) to obtain continuum wave functions. The continuum wave functions are then used in calculating the transition matrix elements (22–26), scattering amplitudes, and differential and integral cross sections equations as presented in this paper.

3. Results and discussion

3.1. Differential cross sections

Present differential cross sections results for electron impact excitation of the lowest resonance ($J = 1$) of Ar are compared with experimental results of Chutjian and Cartwright (1981), Filipovic et al (2000a and 2000b) and Khakoo et al (2004) and theoretical results of Bartschat and Madison (1987) using DWBA and the R-matrix, the unitarized first-order many body theory, the semi-relativistic distorted-wave Born, and the relativistic distorted-wave results due to Khakoo et al (2004) for impact energies from excitation threshold up to 100 eV.

At 17.5 eV (figure 1), present SEPA (static + exchange + polarization + absorption potentials) RDWBA and SEP (static + exchange + polarization potentials) RDWBA results are similar at all scattering angles and both are in good agreement both in shape and magnitude with experimental results of Khakoo et al (2004) especially for excitation of $4s\, (3/2^+)$ state, while the present SE (static + exchange potentials) RDWBA and S
(static potential) RDWBA results disagree with experimental results at all angles. The semi relativistic DWB and R matrix results of Khakoo et al (2004) do not yield very satisfactory agreement with the experimental results at this low energy, unlike our present SEPA-RDWBA and SEP-RDWBA results. This may be attributed to the difference in type of distortion potential they adopted (absorption and polarization potentials not adopted) in their calculations and relativistic effects not being fully applied in their semi relativistic DWB calculations.

At 20 eV (figure 2), experimental results of Cartwright and Chutjian (1981) are generally lower at all angles, though the shapes are similar, with other experimental results. Present SEPA-RDWBA model again predict DCS results of about the same shape and magnitude as the experimental results for this impact energy. This trend is the same for present SEP-RDWBA results. The overlap in present SEP-RDWBA and SEPA-RDWBA results suggests that the effect of the absorption potential is not yet very critical at low electron impact excitation energies for argon. Present SE-RDWBA and S-RDWBA results which predict cross sections that lack agreement in both shape and magnitude also verify the importance of the polarization potential at low impact energies.

At 30 eV (figure 3), present SEP-RDWBA and SEPA-RDWBA results predict DCSs in good agreement in both shape and magnitude with experimental results of Cartwright and Chutjian (1981) for 4s[1/2]s only in shape with those of Khakoo et al (2004), unlike the R-matrix method of Khakoo et al (2004) and the DWBA method of Bartschat and Madison (1987) which present larger cross sections. Present SE-RDWBA and S-RDWBA results still predict large cross sections for both 4s[1/2]s and 4s[3/2]s excitations, while the RDW method of Zuo et al (1992) has better agreement with only the experimental results of Khakoo et al (2004), our SEP-RDWBA and SEPA-RDWBA results tend to match in shape with both experimental results of Cartwright and Chutjian (1981) and of Khakoo et al (2004) at larger scattering angles and at lower scattering angles respectively.

For impact energies greater than 30 eV (figures 4–5), the trend of DCSs across the calculations and experimental measurements remains similar in shape, both for excitation of 4s[3/2]s and 4s[1/2]s levels, although the present SEPA and SEP results are still in good agreement with the experimental results compared to SE RDWBA and S RDWBA. At 50 eV of figure 4, the RDW result of Zuo et al (1992) (which adopted static, exchange and polarization potentials) differ with present SEP RDWBA result mainly due to the difference in the
Figure 3. DCS results for electron impact excitation of the lowest resonance ($J = 1$) states of argon. — S-RDWBA present result; — SE-RDWBA present result; — SEP-RDWBA present result; — SEPA-RDWBA present result; — Zuo et al. (1992) RDW result; — Cartwright and Chutjian (1981) experimental result; — Bartschat and Madison (1987) DWBA result; Khakoo et al. (2004): + experimental result; ▲ RDW result; ★ R Matrix result.

Figure 4. DCS results for electron impact excitation of the lowest resonance ($J = 1$) states of argon. — S-RDWBA present result; — SE-RDWBA present result; — SEP-RDWBA present result; — SEPA-RDWBA present result; — Zuo et al. (1992) RDW result; — Filipovic et al. (2000a and 2000b) experimental result; Khakoo et al. (2004): + experimental result; ★ DWBA result; ★★★★★★ R Matrix result.
type of exchange, polarization and lack of absorption in their calculations. Present calculations use an energy
dependent polarization and a local exchange potential compared to the energy independent polarization and
non-local exchange potential adopted by Zuo et al. (1992).

Generally, at low impact energies, the differential cross section values are not so varied with angles as at high
impact energies. This is because at impact energies near excitation threshold, there is more interaction between
the projectile electron and the target electrons compared to larger impact energies and the electrons are scattered
evenly in different directions. The effect of the distortion potential thus is always very active at low energies
nearing excitation threshold. At high impact energies, the projectile electron tends to move in a near straight line
inside the target atom electron cloud, and encounters less interaction with the target atom electrons, hence it is
scattered at small angles.

3.2 Integral cross sections
In figures 6 and 7 present integral cross sections results for electron impact excitation of the lowest resonance states of
Ar are compared with the experimental results of Chutjian and Cartwright (1981), Filipovic et al (2000b) and Khakoo

![Figure 5. DCS results for electron impact excitation of the lowest resonance (l = 1) states of argon. —— S-RDWBA present result; —— SE-RDWBA present result; — SEP-RDWBA present result; — SEPA-RDWBA present result; ■ Khakoo et al (2004) experimental result.](image)

![Figure 6. ICS results for electron impact excitation of the lowest resonance states of Argon. —— S RDWBA present result; —— SE RDWBA present result; — SEP RDWBA present result; — SEPA RDWBA present result; ◊ Cartwright and Chutjian (1981) experimental result; Zatsarinny et al (2014): •, 5-state R Matrix result; •, 500-state R matrix result; ◆, Filipovic et al (2000b) experimental result; •, Madison et al (1998) Semi RDW result; Khakoo et al (2004): ■, experimental result; ▲, RDW result.](image)
et al (2004) and theoretical results of Bartschat and Madison (1987) using DWBA, semi RDW result of Madison et al (1998), R-matrix result due to Zatsarinny et al (2014), the unitarized first-order many body theory, the distorted-wave Born and the relativistic distorted-wave results of Khakoo et al (2004) for impact energies up to 100 eV.

Apart from the Filipovic et al (2000b) results which remain slightly higher than other experimental results, the present SEPA-RDWBA results predict ICS that are in a satisfactory agreement with the measurements for excitation of the 4s[1/2] 2 0 level, while for 4s[1/2] 2 0 level, measurements of Khakoo et al (2004) have close agreement with our present SEPA-RDWBA results at high energies (50 eV and above), whereas those of Cartwright and Chutjian (1981) tend to agree well with our calculations even at lower energies up to 20 eV. The sharp increase in cross sections near the threshold excitation energy for electron impact can be attributed to large interaction between target electrons and projectile electrons which leads to an increase in the number of particles scattered. The large interaction between electrons is mainly due to attraction of the projectile electron by the positive nucleus, exchange effects between electrons during impact and the polarization effect of the incident electron on the target electrons. The polarization potential plays a major role in improvement of cross section results at low energies for the excitation of the lowest resonance states of argon.

As impact energy increases, say beyond 50 eV, the effect of absorption becomes more important in obtaining cross sections, as seen from the ICS graphs (figure 6 and 7) and tables 1 and 2 for both singlet and triplet excitations. Present SEPA-RDWBA results (more pronounced for excitation of the 4s[1/2] 2 0 state) are most reliable at higher energies. Apart from the RDW calculations of Khakoo et al (2004), other non-relativistic and semi-RDW calculations predict slightly higher cross sections. Relativistic effects may thus be attributed to better cross sections apart from the effect of the absorption of incident electrons to other open scattering channels, which leads lower differential cross sections. Furthermore, at high impact energies, there are more available open scattering channels apart from the inelastic channel under consideration. This makes the absorption potential more dominant.
4. Conclusions

Calculations with static potential (present S-RDWBA) alone cannot be used to describe an atomic collision process accurately as the cross sections obtained are very large especially at low electron impact energies and at all scattering angles compared to actual measurements. Exchange between target and projectile electrons and polarization of the target electrons by the incident electron lowers the cross sections, though its effect reduces as impact energy increases. Furthermore, the impact energy dependent polarization potential adopted in this work plays a major role in improving shapes of cross sections at energies below 30 eV, where other distorted wave methods cited in this work usually fail to give accurate shapes. It is also important to note that the absorption potential has minimal effect on cross sections results for inelastic scattering of electrons by argon at low energies and that it only becomes important in improvement of cross section results where impact energies are higher than 50 eV, as shown by the graphs of integral cross sections. This means that as the impact energy increases, complex potentials (present SEPA-RDWBA) generally begin to lower argon cross sections. The present RDW differential cross sections for electron impact excitations and the experimental results of Khakoo et al. (2004) are in good agreement at all impact energies. This can be attributed mainly to the choice of distortion potential adopted in this work.

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Data availability statement

All data that support the findings of this study are included within the article.

Author contribution statement

Alex M. Marucha, Peter K. Kariuki, John Okumu, and Chandra S. Singh contributed equally towards the design and implementation of the research, to the analysis of the results and to the writing of the manuscript.

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