Excitation Cross-section Evaluation for the Lowest Auto-ionizing State of Potassium

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The accuracy and reliability of any theoretical scattering model relies on the wave functions used and the energy of the projectile. Perturbation methods are known to be accurate at intermediate and high energies of the incident projectile but this accuracy also depend on the distortion potentials employed and the consideration given to higher order terms and the exchange effects. In a distorted wave model the initial state distorted wave is generated by the static potential of the target atom in the initial state and the final state distorted wave is generated by a potential taken as the sum of one-half of the initial state static potential and one-half of the final state static potential of the target atom. We used this model to evaluate the integral and differential cross-sections as well as alignment and lambda parameters for electron-impact excitation of the lowest auto-ionizing states of *K* in the energy range of 18-1000 eV. The wave functions employed are the multi-zeta Hartree-Fock single electron wave functions. The numerical calculations are performed using DWBA1 program, which we modified to evaluate the exchange amplitudes exactly without any approximation. We have compared our results with other known theoretical and experimental results. From our alignment parameter results, we observed a near threshold resonant structure.

1. Introduction

Electron impact excitation of the lowest auto-ionizing state of potassium has been a subject of investigation for over two decades [1,2,3,4]. Nygaard [5] observed that excitation of the auto-ionizing states leads to a rapid rise in ionization cross sections for neutral atoms. Borovik [1] also reported strong resonances near the excitation threshold in their measured excitation functions of the lowest auto-ionizing fine structure states of potassium. Matterstock [4] measured alignment parameter for the lowest auto-ionizing state of potassium from the threshold to 1000 eV.

In this paper, we have attempted to model these measurements using a non-relativistic distorted wave method with a variation in the distortion potential from near threshold to 1000 eV incident energies of the projectile. The distorted wave method is more reliable at intermediate and high energies. It has been successful in predicting electron impact excitations cross sections for various processes and typically gives results qualitatively similar to the R-matrix approach [6]. In the distorted wave approximation, the choice of the distorting potential is in principle arbitrary and can be selected in a suitable manner [7,8]. Our distorted wave method, suggested by Singh [9], uses a linear combination of final and initial state static potentials as distortion potential and with different coefficients in either channel. We have also included the polarization potential in either channel to account for the polarization of the target within the vicinity of the projectile electron. Using these distortion potentials, we have calculated integral cross sections, differential cross sections, and alignment parameters using the multi zeta Hartree-Fock wave functions of Clementi and Roetti [10]. In our calculations, the exchange amplitude has been evaluated exactly without making any approximation within the distorted wave Born approximation (DWBA) frame work. For numerical calculations, we modified the code originally developed by Madison and Bartschat [11] for electron-hydrogen scattering from an s state to higher orbital states.

The major difference between this study and other distorted wave approaches is in the choice of the arbitrary distortion potential. Here, we employed the initial state static potential as the initial distortion potential, and a simple average of the initial state static potential and the final state static potential as the final distortion potential. This choice was necessitated by the reasoning that when the projectile is in the initial state, for all the time it is in the field of the initial state of the target, the distortion potential should therefore be taken as the static potential of the target atom in its initial

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state. When the energy from the projectile electron is transferred to the target atom, the atom takes time (relaxation time) to go to its final state. That is, there is a time lag between the time of transfer of energy and the instant when the atom reaches its final state. Thus the projectile electron in its final state 'sees' a potential which is intermediate between the initial- and final-state static potentials. Hence the final state distortion potential has been taken as the sum of one-half of the initial state static potential and one-half of the final state static potential of the target atom [9]. We also included the dipole polarization potential in the distortion potential in order to investigate polarization effects.

2. Theory

The excitation process that we considered for our calculations are expressed as

$$e^- + K(3p^6 4s)^2 S_{1/2} \rightarrow e^- + K^*(3p^5 4s^2)^2 P \quad (1)$$

In this excitation process, we assume that the transitions only involve one atomic electron that is $3p \rightarrow 4s$ in potassium. Thus, we have treated it as behaving like one electron system. We chose the distorted wave model to solve this scattering problem owing to its suitability in this energy range. The general T matrices for the electron impact excitation of one electron atom [11] are expressed as

$$T^{dir} = \langle \chi_f^-(\mathbf{r_0})\psi_f(\mathbf{r_1}) \mid V(\mathbf{r_0},\mathbf{r_1}) \mid \chi_i^+(\mathbf{r_0})\psi_i(\mathbf{r_1})\rangle \quad (2)$$

$$T^{ex} = \langle \chi_f^-(\mathbf{r_0})\psi_f(\mathbf{r_1}) \mid V(\mathbf{r_0},\mathbf{r_1}) - U_f(\mathbf{r_0}) \mid \chi_i^+(\mathbf{r_1})\psi_i(\mathbf{r_0})\rangle \quad (3)$$

Where, T^{dir} and T^{ex} are the direct and exchange transition matrices, respectively, and $\psi_{i(f)}$ represents the initial (final) state target atom wave function. In this study, we used the multi zeta Hartree-Fock Slater type orbitals [10] to represent the single electron atomic wave functions in either initial or final state. The function $\chi^{-(+)}$ represents the distorted waves with incoming (outgoing) wave boundary conditions and $U_{i(f)}$ is the distortion potential experienced by the target atom in its initial (final) state.

The distorted waves are obtained by solving the following second order differential equations

$$(\nabla_0^2 + k_f^2 - U_f)\chi_f^- = 0 \quad (4)$$

$$(\nabla_0^2 + k_i^2 - U_i)\chi_i^+ = 0 \quad (5)$$

Where, $k_{i(f)}^2$ is the initial (final) kinetic energy of the projectile electron given in Rydberg units. As explained in the introduction, the distortion potentials that we used in the above equations are given by the expressions

$$U_i = V_{ii} + V_{pol} \quad (6)$$

$$U_f = \frac{1}{2}(V_{ii} + V_{ff}) + V_{pol} \quad (7)$$

Where, we used V_{ii} as the static potential of the target in its initial state, V_{ff} as the static potential of the target in its final state and V_{pol} as the polarization potential that describes the behavior of the target atom when the projectile is within the interaction region. These potentials are expressed as

$$V_{ii(ff)} = \langle \psi_{i(f)} \mid V(\mathbf{r_0},\mathbf{r_1}) \mid \psi_{i(f)} \rangle \quad (8)$$

and

$$V_{pol} = -\frac{\alpha_d}{r_0^4} \quad (9)$$

Where, α_d a non-negative constant is called the dipole polarizability of the atom. For ground state potassium atom, α_d is 43.4 x 10^{-30} in units of $4\pi\varepsilon_0$ cubic meters [12].

The interaction potential between the projectile electron and the target atom, $V(\mathbf{r_0},\mathbf{r_1})$ is expressed as

$$V(\mathbf{r_0},\mathbf{r_1}) = -\frac{2}{\mathbf{r_0}} + \frac{2}{\mathbf{r_{01}}} \quad (10)$$

Where, $\mathbf{r_0}$ and $\mathbf{r_{01}}$ refer to the projectile electron-target nuclear and projectile electron-target electron displacement vectors, respectively.

To evaluate the direct and exchange scattering amplitudes given by the Eqns. 1 and 2, the distorted waves χ_i^+ and χ_f^- are first expanded, respectively, in terms of the partial waves as

$$|\chi_i^+\rangle = \sqrt{\frac{2}{\pi}}\frac{1}{k_i r}\sum_{l_i m_i} i^{l_i}\chi_{l_i}(k_i,r)Y_{l_i m_i}(r)Y_{l_i m_i}(k_i) \quad (11)$$

$$|\chi_f^-\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{k_f r} \sum_{l_f m_f} i^{l_f} \chi_{l_f}^*(k_f, r) Y_{l_f m_f}(r) Y_{l_f m_f}^*(k_f) \tag{12}$$

Where, the function Y_{lm} is a spherical harmonics. In the expansion of, χ_f^-, the complex conjugate of radial part χ_{l_f} is taken so that it satisfies the incoming wave boundary conditions. Substituting the above partial wave expansions of the distorted waves in the Eqns. 3 and 4, it can be shown that the radial distorted waves are solutions of the following equation

$$\left(\frac{d^2}{dr^2} - \frac{l_s(l_s+1)}{r^2} - U_s(r) + k_s^2 \right) \chi_{ls}(r) = 0 \tag{13}$$

Here $s = i(f)$ for the initial (final) state distorted waves. In the asymptotic region they satisfy the boundary condition.

$$\lim_{r\to\infty} \chi_{l_s}(k_s, r) = j_{ls} + \alpha_l(-\upsilon_{l_s} + i j_{l_s}) \tag{14}$$

Where, j_l and υ_l are regular and irregular Ricatti-Bessel functions, and α_l is a complex number expressed as

$$\alpha_l = \exp(i\delta_l)\sin\delta_l \tag{15}$$

Where, δ_l is the elastic scattering phase shift.

The radial distorted wave equations for initial- and final -states are solved by using Numerov method. The transition matrices have been fully expanded by making use of vector addition coefficients (Clebsch-Gordan coefficients) and the incident electron is considered to be along the z-axis to simplify the problem [11]. The differential cross-sections have been obtained using the relation

$$\left(\frac{d\sigma}{d\Omega}\right)_{2p\to 3s} = 4\pi^4 \frac{k_f}{k_i} \sum_{m=-1}^{+1} \left(\frac{1}{4} \left| T_{2p\to 3s}^{dir} + T_{2p\to 3s}^{ex} \right|^2 + \frac{3}{4} \left| T_{2p\to 3s}^{dir} - T_{2p\to 3s}^{ex} \right|^2 \right) \tag{16}$$

The total cross-section is obtained as:

$$\sigma = \int_0^{2\pi} \int_0^{\pi} \frac{d\sigma}{d\Omega} \sin\theta d\theta d\phi \tag{17}$$

And the alignment parameter, A_{20}, which is the measure of angular anisotropy of the ^2P state, is given by the expression below for unresolved fine structure splitting;

$$A_{20} = \frac{\sigma_1 - \sigma_0}{\sigma} \tag{18}$$

Where, σ_0 and σ_1 give total cross sections for the magnetic sublevels, 0 and 1, respectively. $\sigma_0(\theta,\phi)$ and $\sigma_1(\theta,\phi)$ are the differential cross sections for $np_m \to (n+1)s$ transition with $m = 0$ and 1, respectively. These differential cross sections are related to their scattering amplitude $f_m(\theta,\phi)$ by

$$\sigma_m(\theta,\phi) = \frac{k_f}{k_i} \left| f_m(\theta,\phi) \right|^2 \tag{19}$$

While, the scattering amplitude is directly connected to the transition matrix T_{if} using the relation

$$f_m(\theta,\phi) = -2\pi^2 T_{if}(m) \tag{20}$$

Generally, the transition matrix including excitations from both singlet and triplet states are evaluated as

$$T_{if} = \left[\frac{1}{4} \left| T^{dir} + T^{ex} \right|^2 + \frac{3}{4} \left| T^{dir} - T^{ex} \right|^2 \right]^{\frac{1}{2}} \tag{21}$$

In this study, we evaluated the above transition matrix exactly and then used it to calculate the differential cross sections, integral cross sections, and alignment parameters for the excitation under consideration.

3. Results

We report here the evaluation of non relativistic excitation cross sections, differential cross sections and alignment parameter results for electron impact excitation of the lowest auto-ionizing state of potassium evaluated using a distorted wave method from 19 eV to 1000 eV. We used multizeta

Hartree-Fock wave functions of Clementi and Roetti [10] for both ground and excited states of the target. This wave function is not very realistic for the excited state but it resolves the non-orthogonality issue associated with a more realistic wave function [6].

Fig.1 shows our excitation cross section results for direct excitation (DWMD) and excitation with exchange (DWME) and compared to cross sections with exchange (DWE) for Pangantiwar and Srivastava [13], relativistic cross sections (RDW) of Kaur and Srivastava [14] and the experimental (Expt) results of Feuerstein et al. [15]. We normalized the experimental results with our DWMD at 1000 eV, since at this energy the results converge with the Plane wave approximation results, which are known to be accurate at higher energies. All the results except RDW [14] are in both quantitative and qualitative agreement for incident electron energies above 80 eV. Above the ionization threshold (18.72 eV) to 80 eV, our DWME results agree in shape with the experimental results [15] although our cross sections are higher in this region. It is interesting to note that the maxima for both DWME and experimental results coincide at about 22 eV, the broader resonant structure observed for both $K^*(3p^5 4s^2 P_{\frac{3}{2},\frac{1}{2}})$ results. It may be important to note that when we included the polarization potential in both channels of the distortion potential there was no significant difference in the evaluated potentials.

Feuerstein et al. [15] also reported a DWBA results whose peak coincides with the sharp resonance at 19.5 eV. Their distorted wave method differs with ours in the choice of distortion potential. Their distortion potential includes the exchange potential for Furness and McCarthy [16], and a static potential which is evaluated differently from ours. Results similar to Feuerstein et al. [15] were also observed by Borovik et al. [1] in their experimental and theoretical results for the fine structure components.

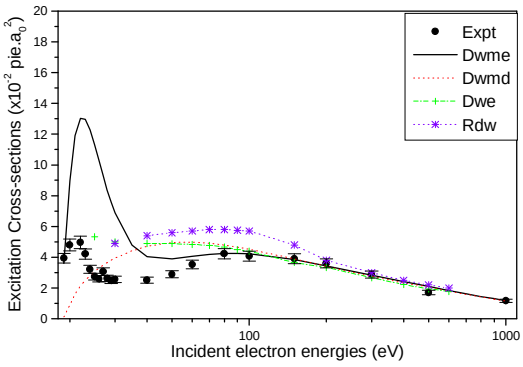


Fig.1: Integral cross sections for electron impact excitation of $(3p^6 4s)^2 S_{\frac{1}{2}} - (3p^5 4s^2)^2 P$ state of potassium. The solid (black) line represents DWME result, the dotted (red) line represents DWMD result, the dashed (green) line with (+) symbol represents DWE result [13], the dotted (violet) line with (*) symbol-RDW result [14], and the solid (black) circles with error bars represents the experimental result [15].

In Fig.2, we present our DWME alignment parameter results as compared to experimental results of Matterstock et al. [4] and the relativistic distorted wave (RDW) results [14]. The DWME result is in shape resonance with the experimental results given, although our results are higher in absolute values. In the DWME results, there is a resonant structure with a peak at about 26 eV. This can be attributed to exchange effect that dominates transitions at lower energies.

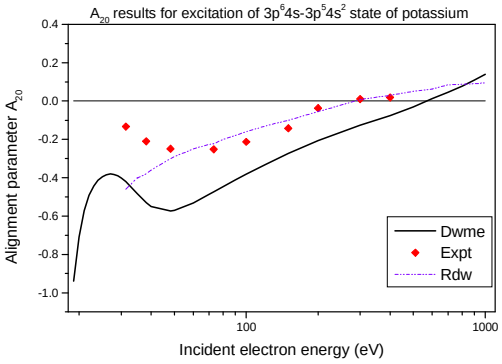
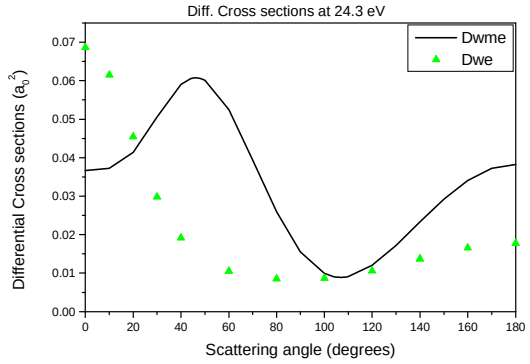
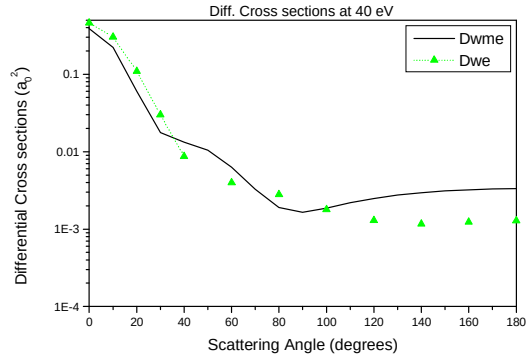
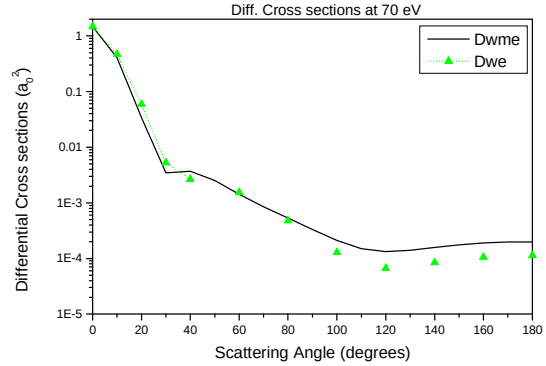


Fig.2: Alignment Parameter A_{20} for the excitation of $(3p^6 4s)^2 S_{\frac{1}{2}} - (3p^5 4s^2)^2 P$ state of sodium. The solid (black) line represents DWME result, the symbol diamond (red) represents experimental results of Matterstock et al. [4], and the dash-dot-dot (violet) line represents RDW results [14].

Fig.3 shows the present DWME differential cross section result for 24.3 eV, 40 eV, 70 eV and 100 eV and compared with the DWE results of Pangantiwar and Srivastava [13]. The near threshold enhancement can be seen in the differential cross section results at 24.3 eV. As the projectile energies increase, the exchange contribution dies out leaving only the direct cross sections. It can be seen from the figure that as the energy of incident electron increases, both results tend to converge despite the difference in their method of evaluation.







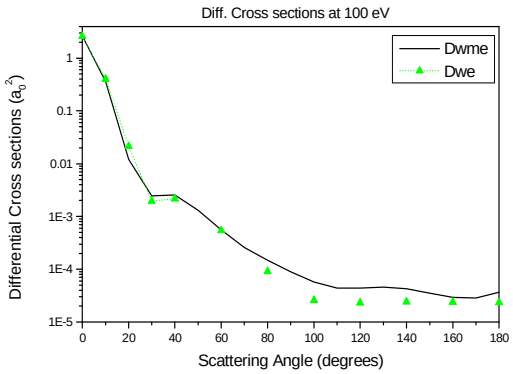


Fig.3: Differential cross section results for electron impact excitation of $(3p^6 4s)^2 S_{1/2} - (3p^5 4s^2)^2 P$ state of potassium at 24.3, 40, 70, and 100 eV. Solid (black) line-represents DWME results and the dotted (green line with solid squares) represent DWE result [13].

4. Conclusion

We have reported total cross sections, differential cross sections and alignment parameter results for electron impact excitation of the lowest auto-ionizing state of potassium evaluated using a distorted wave method with a variation in the distortion potential at near threshold energies up to 1000 eV. Our results show a high enhancement of cross sections at energies less than 30 eV, a feature that we attribute to the exchange effect. Just as observed in Pangantiwar and Srivastava [13], there is no significant change in results when the polarization potential is included in the distortion potential in both channels.

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Received: 8 October, 2011
Accepted: 18 January, 2012