Elastic Scattering of e⁺-K-atom

Research Article

Mukesh Kumar Sinha[1] and Tarun Kumar Dey[2,*]

[1] *Department of Physics, L. N. J. P. Institute of Technology* (*Aryabhata Knowledge University*),
  Chapra 841 302, Bihar, India
[2] *Post Graduate Department of Physics, L. S. College* (*B.R.A. University*), *Muzaffarpur 842 001,*
  Bihar, India
*Corresponding author:** tkdeyphy@gmail.com

Abstract.   The differential cross-section for elastic scattering of positron by potassium atom have been calculated in intermediate energy range by using modified form of Born approximation. Born approximation has been modified and improved by taking into account the effect of nuclear interaction terms in the form of distorted wave. The impact of polarisation effect has been analysed. The results are compared with theoretical predictions of Khare and Vijayshri [3] .

Keywords. Elastic scattering; Cross section; Polarization potential

PACS. O.365.Nk

1. Introduction

Large number of channels including continuum are open in positron-atom scattering at intermediate energies. In practice it is difficult to include effects of all channels including continuum in calculation. Although all the dynamics of the system can not be incorporated in a single distorted wave method. A suitable distorted wave method that accounts for the effect of higher excited states and continuum is required to predict cross-sections.

In present method, we include a part of Coulomb potential in continuum wave function in initial channel. The nucleus of target atom has been taken as screened due to presence of target electrons. So, incoming positron will see an effective charge. The valence electron of potassium is loosely bound, hence, its polarizability is very high.

Therefore, the reliable prediction of scattering parameters is not possible without including dipole polarization. By including the polarization potential in our calculation, few excited state is partially included. Moreover, the effect of continuum in present model is taken via distorted continuum wave function.

2. Theoretical Basis

The Hamiltonian H for positron-alkali atom can be expressed as follows:

$$H = \left[-\frac{1}{2}\nabla^2_{r_1} - \frac{1}{2}\nabla^2_{r_2} - \frac{1}{r_1} \right] + \left[\frac{1}{r_2} - \frac{1}{r_{12}} \right]. \tag{1}$$

In centre-of-mass reference frame $\vec{r}_1$ and $\vec{r}_2$ are the position vectors of the atomic electron and the incident positron with respect to the screened nucleus of the target atom. $\nabla^2_{r_1}$ and $\nabla^2_{r_2}$ are the kinetic energy operators. Atomic units are used throughout the paper.

The Hamiltonian H is partitioned and expressed as follows:

$$H = H_1 + W \tag{2}$$

with

$$H_1 = H_0 + U, \tag{3}$$

where

$$U = \frac{\delta}{r_2}, \tag{4}$$

$$W = \frac{(1-\delta)}{r_2} - \frac{1}{r_{12}}, \tag{5}$$

where δ = screening parameter; H_0 = Free Hamiltonian

The function ϕ_r, χ_r and ψ_r satisfy the following Schrodinger equations with Hamiltonian H_0, H_1 and H, respectively.

$$\left. \begin{array}{l} H_0\phi_r = E_r\phi_r \\ H_1\chi_r = E_r\chi_r \\ H\psi_r = E_r\psi_r \end{array} \right\}, \tag{6}$$

where E_r is the total energy of the system.

Let the system move from initial bound state $|i\rangle$ with momentum $\overline{K}_i$ to the final state $|f\rangle$ with momentum $\overline{K}_f$. Then T-matrix elements can be expressed as follows:

$$T_{i \to f} = \langle \phi_f | V | \psi_i^{(+)} \rangle, \tag{7}$$

where

$$V = \frac{1}{r_2} - \frac{1}{r_{12}}. \tag{8}$$

Here, $\psi_i^{(+)}$ can be expanded with respect to H_1 as

$$\psi_i^{(+)} = \sum_{n=0}^{\infty} (G^{(+)}W)^n \chi_i^{(+)}, \tag{9}$$

where $G^{(+)}$ is the Green function for H_1.

It would not be crude approximation to retain the first order term in the above expression.

$$T_{i \to f} = \langle \phi_f | V | \chi_i^{(+)} \rangle. \tag{10}$$

In atomic unit, differential cross section is expressed as follows:

$$\frac{d\sigma}{d\Omega} = \frac{\mu^2}{4\pi^2} \frac{K_f}{K_i} |T|^2 . \tag{11}$$

In present case, wave functions have been taken in the following forms:

$$\phi_r = \exp(i\overline{K} \cdot \overline{r}_2) \phi_{nlm}(\overline{r}_1), \tag{12}$$

$$\chi_i^{(+)} = \Gamma(1 + ia) \exp\left(i\overline{K} \cdot \overline{r}_2 - \frac{\pi a}{2}\right) {}_1F_1(-ia; 1; iK_i r_2 - i\overline{K}_i \cdot \overline{r}_2) \phi_{nlm}(\overline{r}_1), \tag{13}$$

where

$$a = \frac{\delta}{K}. \tag{14}$$

Here, $\overline{K}$ is the momentum for the direct channel, in which distortion is introduced. The screening parameter δ is evaluated by the method of Junker [1, 5, 8].

This method takes the part of Coulomb potential in incident continuum wave function. Physically, the effect of continuum is taken into account partially.

The radial part of wave function is expressed as follows (*Hartree Fock wave function*):

$$\varphi_{40}(r) = \sum_{i=1}^{2} a_i r \exp(-b_i r) + \sum_{i=3}^{4} a_i r^2 \exp(-b_i r) + \sum_{i=5}^{6} a_i r^3 \exp(-b_i r) \tag{15}$$

$$\text{(in ground state)}$$

Now, T-matrix can be expressed in the following form :

$$T_{i \to f} = MF' \left[I_0 + \sum_{i=1}^{2} \sum_{j=1}^{2} N_{ij} \frac{\partial^2 I}{\partial \lambda_{ij}^2} + \sum_{i=1}^{2} \sum_{j=2}^{4} N_{ij} \frac{\partial^3 I}{\partial \lambda_{ij}^3} + \sum_{i=1}^{2} \sum_{j=5}^{6} N_{ij} \frac{\partial^4 I}{\partial \lambda_{ij}^4} \right.$$
$$\left. + \sum_{i=3}^{4} \sum_{j=3}^{4} N_{ij} \frac{\partial^4 I}{\partial \lambda_{ij}^4} + \sum_{i=3}^{4} \sum_{j=5}^{6} N_{ij} \frac{\partial^5 I}{\partial \lambda_{ij}^5} + \sum_{i=5}^{6} \sum_{j=5}^{6} N_{ij} \frac{\partial^6 I}{\partial \lambda_{ij}^6} \right]. \tag{16}$$

In (16)

$$\overline{q} = \overline{K}_i - \overline{K}_f , \tag{17}$$

$$\left. \begin{array}{l} MF' = \Gamma(1 + ia) \exp\left(-\frac{\pi a}{2}\right) \\ \lambda_{ij} = b_i + b_j \\ N_{ij} = \left(-\frac{1}{4\pi}\right) a_i a_j \end{array} \right\}, \tag{18}$$

$$I = \iint \exp(i\overline{q} \cdot \overline{r}_2) {}_1F_1(-ia; 1; iK_i r_2 - i\overline{K}_i \cdot \overline{r}_2) \exp[-(b_i + b_j) r_1] \left(\frac{1}{r_{12}}\right) d\overline{r}_1 d\overline{r}_2, \tag{19}$$

$$I_0 = \int \exp(i\overline{q} \cdot \overline{r}_2) {}_1F_1(-ia; 1; iK_i r_2 - i\overline{K}_i \cdot \overline{r}_2) \frac{1}{r_2} d\overline{r}_2 . \tag{20}$$

Polarization potential [2, 4, 6].

$$V_p = \left(-\frac{\alpha}{2r^4}\right). \tag{21}$$

It is in asymptotic form.

The differential cross sections are calculated with polarization potential (DCSPP) and without polarization potential (DCSWP) so that effect of polarization may be properly analysed.
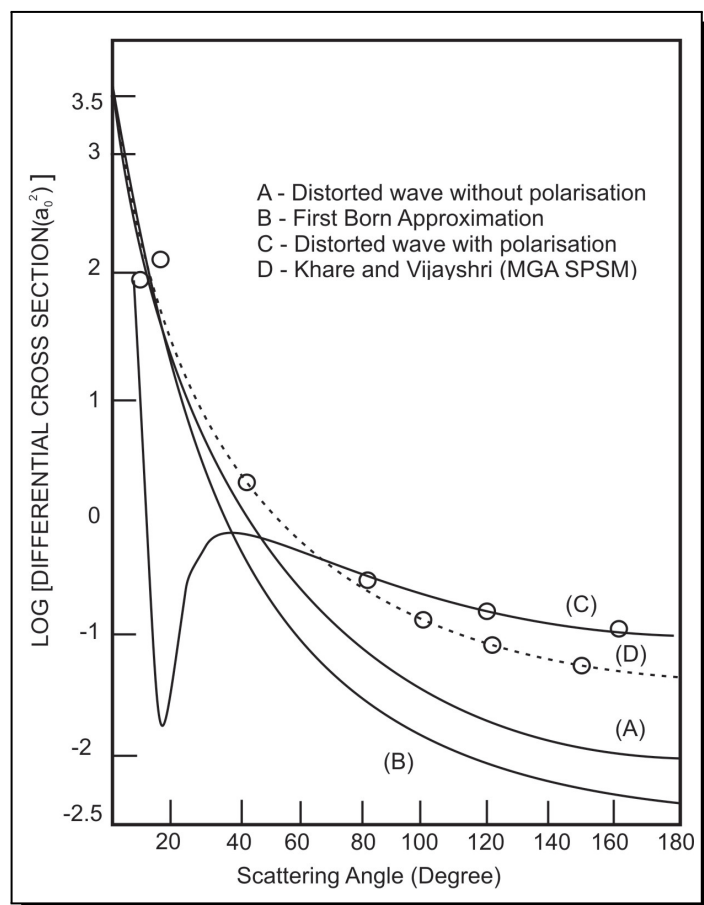

Figure 1. e^+K atom scattering at 400 eV

3. Results and Discussion

In intermediate energy-range, infinite number of channels are open and effect of loss of inleeastic flux is not negligible. As literatures reveal the positronium formation cross-section for positron-alkali atom is very high at low energy. With enhancement of energy capture cross-section decreases very rapidly. As a consequence the effect of capture channel on direct channel is not expected to be appreciable. Since, alkali atom has loosely bound valance electron, so, the effect of polarization is very significant.

The values of differential cross-sections calculated by employing distorted wave method without polarization, the first Born approximation and distorted wave method with polarization are represented by curve A, B and C, respectively.

At 400 eV energy of incident positron curves A and B are closer throughout the entire angular range of scattering. This is expected. The curve D which represents MGA-SPSM results of Khare and Vijayshri [3, 7] is closer to curve A up to 60° angle of scattering. But

at angle of scattering above 70°, curve D is closer to curve C. This shows present approach is suitable.

The polarization shows its greater influence within angular range 5° to 50°. The relative reduction in value of DCSPP with respect to DCSWP is maximum at angle of scattering 15°. Thus it is observed that the position of minima has shifted to 15° with increase in energy. The shift in forward direction has been observed by all investigators. These features have been shown in figure. It is observed that polarization potential is the most effective near forward direction of differential cross-section. As a great deal of cancellation between polarization potential, which is attractive and the static potential, which is repulsive in nature. DCSPP near the forward direction are found to be less than DCSWP. This cancellation gives rise to the minimum in the curve.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

References

[1] B. R. Junker, *Phys. Rev. A* **11**, 1552 (1975), DOI: 10.1103/PhysRevA.11.1552.

[2] A. Nordsieck, *Phys. Rev.* **93**, 785 (1954), DOI: 10.1103/PhysRev.93.785.

[3] S. P. Khare and Vijayshri, *Atomic Phys. with Positron*, in Proc. of Nato Adv. Research Workshop of London, New York, Plenum, p. 417 (1987).

[4] T. T. Gien, *J. Phys. B : At Mol. Opt. Phys.* **22** (1989), L129 – L134, DOI: 10.1088/0953-4075/22/6/005.

[5] S. J. Ward, M. Horbatsch, R. P. McEachran and A. D. Stauffer, *At. Mol. Opt. Phys.* **21** (1989), L611 – L616.

[6] T. T. Gien, *J. Phys. B: At. Mol. Phys.* **20** (1987) L427 – L432, DOI: 10.1088/0022-3700/20/13/005.

[7] S. A. Elkilany, *J. Theoretical Chemistry*, **2014**, Article ID 820672 (2014), DOI: 10.1155/2014/820672.

[8] L. A. Poveda, D. Assafrao and J. R. Mohalleus, *Eure. Phys. Jour. D* **70** (2016), 152, DOI: 10.1140/epjd/e2016-70120-y.