Low energy elastic scattering of positrons by argon atoms

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Abstract. Positron scattering is complementary to electron scattering due to the difference in polarity of charge. This makes positrons an alternative tool to study atomic and molecular structure. In this paper, we report our calculations of differential and total cross sections for the elastic scattering of positrons with argon atoms in the energy range from 1 – 10 eV. A spherical optical potential approach is employed. The static potential is included exactly at the Hartree-Fock level, the short-range correlation and long-range polarization effects are target density functional and are free from any adjustable parameter. Our results are in fair agreement between experimental measurements and other theories.

1. Introduction

Study of electrons and positrons with atoms, ions and molecules can provide useful information for understanding of their structures, reaction mechanism and a lot of actual and prospective applications in the field of technology, environment and the biomedical sciences. The last decade is witness to a tremendous revival of interest in the general area of scattering processes involving positrons as projectiles with atoms and simple molecules in the gaseous phase as targets [1]. A variety of possible outcomes from the interaction of positrons obviously parallels that for electron projectiles. But in case of low energy positrons interactions, there is scarcity of experimental measurements, which is expected if the difficulties linked with weak yield of positron from radioactive sources are considered. However recently, there has been much attention in the experimental aspects of the scattering of positrons. This is because the dynamical processes involving energy losses and quenching of positron beam passing through either matter or molecular gases have gained importance in diverse fields ranging from the breakdown in the gaseous media to plasma chemistry. Consequently, an updated description of both elastic and inelastic scattering of positrons by atoms has always been in demand. More precisely, the accurate cross sections of elastic scattering events are highly desirable in Monte-Carlo simulations.

Initially, the collision cross sections observations with positron scattering were included in the ‘first generation experiments’ [2]. It was then observed that the scattering of positrons by only the rare-gas atoms exhibits the Ramsauer-Townsend (RT) minima. Thus argon may play an important role in showing this feature. Several groups [3-8] have calculated elastic scattering cross sections of electron/positron from the noble gases. In continuation of this, McEachran and Stauffer [9] have calculated differential cross sections for argon atoms using complex ab initio optical potential. This motivates us to do current work in low energy regime. This work is in continuation of our previous calculations [10]. In this paper, we demonstrate differential cross sections (DCS) and total cross sections (σ_t) for the elastic scattering of positrons by argon atoms in the energy range from 1 – 10 eV using spherical optical potential (SOP) model approach [11].
2. Methodology

In the usual potential scattering problem, the following Schrödinger-equation is solved for the scattered particle at energy $k^2$ i.e.

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} - V_R(r)\right]f_\ell(kr) = 0$$

(1)

where $V_R(r)$ is the real potential for the e$^+$ - Ar system written as

$$V_R(r) = V_{st}(r) + V_p(r)$$

(2)

The static potential is the average over the ground state atomic charge distribution of the electrostatic interaction of the positron and atom. The static potential is calculated accurately from

$$V_{st}(r) = \frac{Z}{r} - \int \frac{\rho_o(r') d^3 r'}{|r - r'|}$$

(3)

where $\rho_o(r)$ is the target unperturbed charge density.

The polarization effect arises from the distortion of the target electronic wave due to the incident charged particle. For the elastic scattering, the polarization-correlation contribution accounts for all virtual transitions to the excited states. We have used a parameter-free polarization potential ($V_p$), which is based on the correlation energy of the target atom [12]. It has two components, the short-range [$V_{SR}(r)$] and the long-range [$V_{LR}(r)$] parts, and is given by

$$V_p(r) = \begin{cases} 
V_{SR}(r), & r < r_c \\
V_{LR}(r), & r \geq r_c 
\end{cases}$$

(4)

Here, $r_c$ is the point where two forms cross each other for the first time. The crossing point for argon atoms occurs at 2.90 a.u. The short-range form for the positron scattering with atomic systems is given by

$$V_{SR}(r) = \begin{cases} 
0.0622 \ln r_s + 0.0187 r_s \ln r_s - 0.02 r_s - 0.096, & 0.7 \leq r_s \leq 10.0 \\
0.03796 \ln r_s - 0.1231, & 10.0 \leq r_s
\end{cases}$$

(5)

The long-range form of the polarization is taken as the following well known asymptotic form,

$$V_{LR}(r) = -\frac{\alpha_d}{2 r^4}, \quad r > r_c$$

(6)

where $\alpha_d$ is the dipole polarizability of the target atom. For the present calculations, its value is taken as 11.08 a.u. for the argon atom [13].

Both potential terms are function of electronic density of the target. The static potential ($V_{st}$) and the charge density ($\rho_o$) are obtained using non-relativistic Slater-type orbital of Roothan–Hartree Fock wave functions as given by McLean and McLean [14].

We have employed the variable - phase approach (VPA) as proposed by Calagero [15] to find the solution of the equation (1). The corresponding quantities i.e. DCS and $\sigma_t$ are then easily obtained from phase shifts at each energy by this method. All our phase shifts are converged with respect to the number of partial waves up to a value of 0.00001 radians.
3. Results and discussion

Figure 1 shows our elastic DCS for positron scattering with argon atoms at 5 eV. The results are compared with the theoretical calculations of McEachran and Stauffer [9] as well as elastic DCS of Nahar and Wadehra [16] along with experimental data of Kauppila et al [17]. It has been found that the present results are better than the calculations of Nahar and Wadehra [16]. These are also in agreement with the calculations of McEachran and Stauffer [9] as well as experimental measurements of Kauppila et al [17] reproducing a single broad minima.

![Figure 1](image)

**Figure 1.** Differential cross sections for $e^+ - Ar$ scattering at 5 eV. Calculations: ____ , present results; - - - - , McEachran and Stauffer [9]. ...., Nahar and Wadehra [16]. Experiment: ☐ ☐ , Kauppila et al [17].

In figures 2, we have compared our DCS results with the recent calculations of McEachran and Stauffer [9] along with experimental data of Kauppila et al [17] at 8.7 eV. It is noticed that there exist a variation in the magnitude of the DCS between both theoretical calculations and experimental measurements at small scattering angles. This is reflected as a shift in the minima towards the forward direction i.e. upto $\approx 40^\circ$. But the difference narrows down for scattering angle $> 40^\circ$ extending for large angles (backward direction). Although this is a disagreement between theoretical calculations and experimental data but on the other hand retrace prevailing trends.

Total cross sections ($\sigma_t$) are also evaluated from the DCS’s. In figure 3, the $\sigma_t$ cross sections are presented and compared with the latest experimental measurements of Coleman et al [18] in the energy range from 1 – 10 eV. It has been observed that our theoretical results are in good agreement with the experimental data below threshold energy. The disagreement may be due to the inelastic channels which play important role beyond threshold energy.
Figure 2. Differential cross sections for $e^+$ - Ar scattering at 8.7 eV. Calculations: ____, present results; - - -, McEachran and Stauffer [9]. Experiment: +, Kauppila et al [17].

Figure 3. Total cross sections for $e^+$ - Ar scattering. Calculation: ____, present results. Experiment: ⮞, Coleman et al [18].
4. Conclusions
We have presented the results of our calculations of the elastic differential and total cross sections for the scattering of positron with argon atom within a spherical optical potential approach. The calculated DCS reproduces the angular shape and size of the experimental results which is similar to other calculations. The total cross sections are also reported and compared with recent measurements.

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