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Polarization Potential Influence on Positron-Magnesium Elastic Scattering in Distorted Wave Calculations

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Abstract

The effects of polarisation potential in scattering of positrons by magnesium is investigated by performing elastic scattering calculations using the distorted wave method. The two potential formalism is employed in which the residual interaction may include or exclude polarisation potential. Differential cross sections as well as integral elastic cross sections have been calculated at incident energies between 10 eV and 200 eV for both cases. Results show that low energy cross sections are more sensitive to the polarisation potential. It is shown that the polarisation potential has a significant influence on differential cross sections at small angles.

Key words: differential cross section; integral cross section; magnesium atom; distorted wave method.

Introduction

The applied science community has seen rapid growth in the demand for accurate cross sections of electron and positron interactions with different systems some being atomic and others being molecular (Surko and Gianturco, 2001). In statistical physics, Monte Carlo simulations in different areas such as micro-dosimetry, radiation dosimetry, radiation therapy, radiation protection, nuclear medicine, atmospheric and plasma physics and other various spectroscopic techniques require detailed information of elastic scattering of both electron and positron by atoms. A similar need arises in modelling the energy deposition associated with the interaction of any form of ionising radiation with matter. Through a combination of theoretical calculations and experimental measurements, various researchers have developed models and techniques aimed at gaining a deeper understanding of the scattering process of positrons from various atoms such as, helium, neon, magnesium, argon, krypton and xenon (Charlton and Humberston, 2000).

The theoretical models which have been developed to describe e^+-Mg scattering are based on various approximations and assumptions. The polarised orbital method is based on the idea that the atom can be represented by a set of polarized orbitals (Szmytkowski, 1993; Bromley *et al.,* 1998; Campeanu *et al.,* 1998). Beginning with the research conducted by Hewitt and colleagues (1996), using a method known as two-centre close-coupling (CCC), more focus has been on the development of theory which incorporates positronium formation. In their research, Techniques from many-body theory were utilized to compute phase shifts and total cross sections for the interaction between positrons and magnesium atoms, with a specific focus on considering the channels that involve the formation of positronium (Gribakin and King, 1996).

Analyzing phase shifts and elastic cross sections, Mitroy and Bromley (2007) investigated the low-energy scattering of positrons by magnesium atoms. They made a significant theoretical prediction, suggesting that at positron energies of approximately 0.1 eV, there is a noteworthy p-wave shape resonance. This prediction was in contrast to earlier findings reported by Gribakin and King (1996), which did not support the existence of such a resonance in this energy range. Additionally, the authors did not detect any resonance behaviour in the case of d-wave scattering.

Two different types of close-coupling calculations were employed in e^+ -Mg scattering, leading to complementary insights into the scattering process (Savage *et al.,* 2011; Utamuratov *et al.,* 2012). These calculations corroborated the presence of a low-energy shape resonance, which had been previously theorized by other researchers (Mitroy *et al.,* 2008). The one-centre as well as two-centre close coupling calculations predicted a p-wave shape resonance at an energy level of approximately 0.17 eV in the energy regime where positronium cannot form. This observation closely aligned with a similar resonance predicted at 0.1 eV in previous research (Mitroy *et al.,* 2008).

In the high-energy regime, where the incoming positron's velocity is significantly exceeds that of the electrons within the target material, the first Born approximation is known to provide reasonably precise estimates of elastic scattering cross sections. Importantly, this approximation predicts that the elastic scattering cross sections will be identical for both positrons and electrons under these conditions (Charlton and Humberston, 2000). The DWBA, being superior to the first Born approximation, provides an opportunity to extend the study of e^+-Mg scattering beyond the current state. In particular, understanding the contribution of polarisation potentials to the cross sections provides the motivation for this study.

Theory

The incident positron introduces an electric field that distorts the negative cloud of electrons of magnesium atom. This fields varies with time and the resulting charge distribution establishes a field which interacts again with the positron thereby changing the electronic energy of the atom. The interaction potential between the positron and magnesium is the sum of the static potential V_{st} and the polarisation potential V_{pol}, namely, $V_{\int ¿} = V_{st} + V_{pol}. ¿$

For the elastic scattering process for which the full Hamiltonian and the approximate initial-state Hamiltonian for the system are denoted by H and H_0 respectively, the exact T-matrix is given as (Joachain, 1975):

$$T = ¿ \Psi_f \left| H - H_0 \right| \Phi_i >, \tag{1}$$

where

$$H \left| \Psi_f \geq E \right| \Psi_f >, H_0 \left| \Phi_i \geq E \right| \Phi_i >. \tag{2}$$

Within the standard DWBA approach, the initial-state Hamiltonian is chosen to be the sum of the atomic Hamiltonian H_A, the kinetic energy operator for the free positron T_0 and potential influencing the free positron in the incident (exit) channel $U_i(U_f)$

$$H_0 = H_A + T_0 + U_i = H_{A'} + T_0 + U_f. \tag{3}$$

Note that for elastic scattering, H_A and H_A' should be equal, hence U_i and U_f should be equal as well. An eigenfunction derived from the initial-state distorting potential is the initial-state distorted-wave χ_i

$$\left(T_0 + U_i \right) \chi_i = \varepsilon_i \chi_i, \tag{4}$$

In the above equation ε_i is the energy of the incident projectile. The wave functions for each of the final particles are multiplied to approximate the exact wave function of the final state, that is,

$$\Psi_f \simeq \psi_f \chi_f, \tag{5}$$

where ψ_f is the final-state wave function for magnesium atom. From the final-state distorting potential U_f, the final-state distorted waves χf are obtained.

$$\left(T_0 + U_f \right) \chi_f = \varepsilon_f \chi_f. \tag{6}$$

As a result, in the two-potential formalism, the direct-scattering T-matrix is given by (Joachain, 1975)

$$T_{fi} = \langle \chi_f^- | U | \Phi \rangle + ¿ \quad (8)$$

Distorted-wave series

To evaluate a multiparticle expression, such as the one described in Equation 8, certain assumptions about the characteristics of atomic wave functions must be made. In this study, the following assumptions are made:

i. The expression of $^{\Psi_i^+}$ is given by the product of the initial atomic wavefunction ψ_i and the initial-state distorted-wave χ_i^+.
ii. The central field model is utilised to derive the single-particle wave functions, from which the atomic wave functions are created as suitable combinations.
iii. It is assumed that the single-particle wave functions associated with bound states are mutually orthogonal to each other.

With these assumptions, the Lippmann-Schwinger expansion of $\Psi_i^{+¿¿}$ in terms of the distorted waves is

¿ (9)

The quantity $(E - H - i\varepsilon)^{-1}$ is the Green's function. Denoting this Green's function by G^+ and introducing another Green's function $g^+ = (E - H_A - T_0 - U - i\varepsilon)^{-1}$ associated with an arbitrary potential U, the full Green's function admits a series expansion of the form

$$G^{+¿} = g^{+¿} + g^{+¿(V-U)g^{+¿}} ¿ \ldots \quad (10)$$

By using Equation 9 in Equation 8 the first-order term is

$$T_1 = ¿ \quad (11)$$

Distorting potentials

The initial-state distorting potential is the interaction potential $V_{\int ¿¿}$. The static potential is composed of two main components: the nuclear contribution and an approximation for the interaction between the projectile positron and the electrons in magnesium.

$$V_s(r) = \left\langle \psi \left| \frac{Z}{r} - \sum_{i=1}^{Z} \frac{1}{r_i - r} \right| \psi \right\rangle \quad (12)$$

where Z is the nuclear charge of magnesium atom. The basis functions for the expansions of ψ are the Slater-type orbitals (STO) given by

$$\Phi_{\lambda p}(r)=\sum_{i=1}^{M} c(\lambda,p,i)\frac{\left[2\zeta(p,i)\right]^{n(p,i)+1/2}}{\{\left[2n(p,i)\right]!\}^{1/2}} r^{n-1}\exp\left[-\zeta r\right]Y_{lm}(\hat{r}). \qquad (13)$$

The values of the constants used in the present study were obtained from Bunge *et al.,* (1993). The multipole expansion of the positron-electron interaction was suppressed to the first term. Consequently, the static potential Equation 12 can be written as

$$V_s=\sum_{\lambda=1}^{3}\sum_{p=0}^{\lambda-1} N_{\lambda p}\sum_{i}\sum_{j} a\exp(-zr)\left[\frac{s}{r}+\sum_{t=0}^{v-2} m r^{t}\right] \qquad (14)$$

where $v=ni+nj$, $z=\zeta(p,i)+\zeta(p,j)$, $a=c(\lambda,p,i)c(\lambda,p,j)v!$, $s=z^{-v-1}$ and $m=\left[1/(t+1)!-1/(vt!)\right]/z^{v-t}$.

The polarisation potential V_p, varies with the spatial position of the positron. It does not have spherical symmetry and mainly it exerts an attractive force. It is given by (Bromley *et al.,* 1998)

$$V_p(r)=-\frac{\alpha_d r^2}{2\left(r^2+\rho^2\right)^3} \qquad (15)$$

The constant α_d is the dipole polarizability and ρ is an energy dependent parameter. The values used in this project for α_d and ρ were $72a^3_0$ and 1.5906 respectively. These values were obtained by Bromley *et al.,* (1998) by matching the binding energies of Mg^{e+}.

Cross sections

The first order direct scattering amplitude in the DWBA is given by (Madison and Bartschat, 1996)

$$f^{\mathrm{dir}}=¿ \qquad (16)$$

Since $U_i=U_f$, $\psi_i=\psi_f$ and $U_i=V_{ii}$ with $V_{kj}=\langle\psi_k|V|\psi_j\rangle$ the partial wave expansion of the T-matrix becomes

$$T=\sum_{l,m} D_l Y_{l,m}\left(\hat{k}_f\right)Y^{*}_{l,m}\left(\hat{k}_i\right)\equiv\sum_{l} D_l\frac{2l+1}{4\pi}P_l(\cos\theta) \qquad (17)$$

where

$$D_l = \frac{2}{\pi}\frac{1}{k_i^2}\int \chi_{l_i}(k_i, r)\, V_{ii}(r)\, j_{l_i}'(k_i r) \quad (18)$$

and θ is the scattering angle. The differential cross sections were obtained using

$$\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 = (2\pi)^4 |T|^2 \quad (19)$$

and the integral cross sections were calculated as

$$\sigma_I = \int \frac{d\sigma}{d\Omega}\, d\Omega = 2\pi \int_0^{2\pi} \left(\frac{d\sigma}{d\Omega}\right) \sin\theta\, d\theta. \quad (20)$$

Results

Differential Cross Sections

The differential cross sections (DCS) which are obtained from a distorting potential in which only the static potential is included are denoted as DCS_s and DCS_{sp} denotes those calculations where both static and polarisation potentials are included. For incident energies 50 eV and 100 eV, these results are compared with the calculation of Khare *et al*. (1983) and Hossain *et al*. (2016). No experimental data could be found for these energies for comparison.

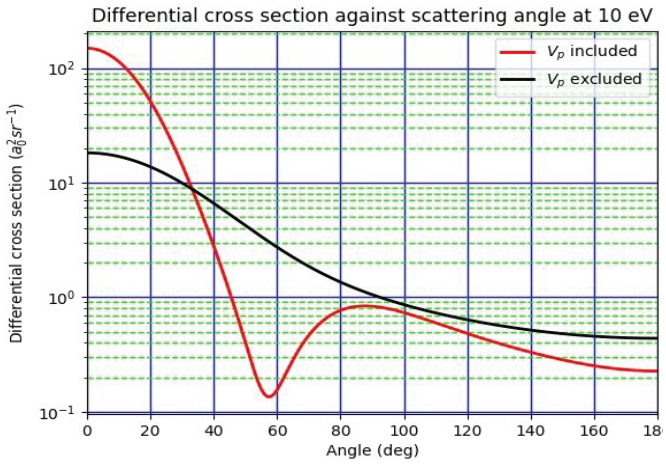

Figure 1: DCS results for e^+-Mg scattering at 10 eV.

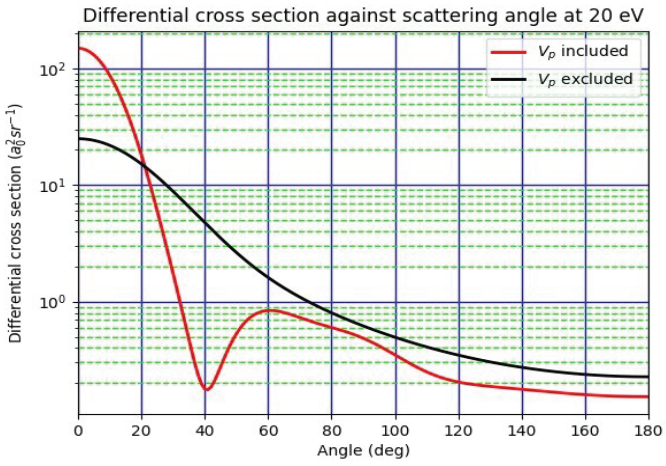

Figure 2: DCS results for e^+-Mg scattering at 20 eV.

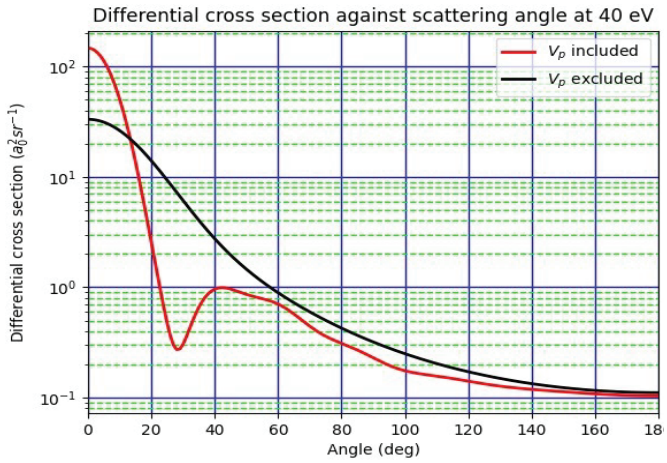

Figure 3: DCS results for e^+-Mg scattering at 40 eV.

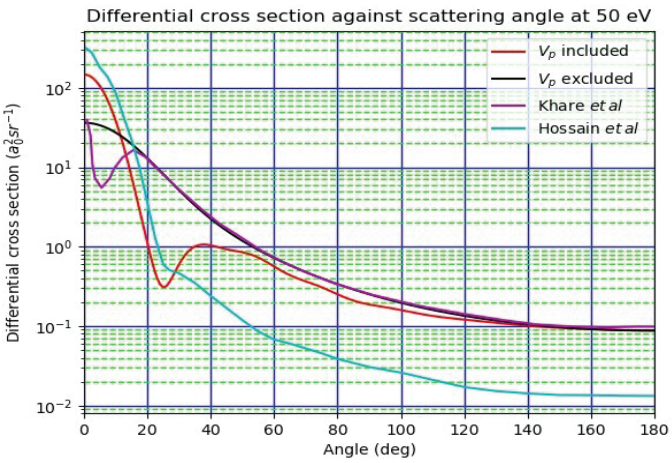

Figure 4: Elastic DCS results for e^+-Mg scattering at 50 eV. A comparison is made with the results of Khare *et al*. (1983) and Hossain *et al*. (2016).

At impact energy of 10 eV, figure 1, when the polarisation potential is included the present result show a local minimum at 58°. At angles less than 30° the effect of including the polarisation potential is to produce DCS which exceed those obtained when V_{pol} is excluded from the distorting potential. As the impact energy increases the range for which the calculated DCS_{sp} is greater than DCS_s decreases. This can be seen in the graphs for higher energies.

For 20 eV impact energy, (figure 2), DCS_s have the same profile as those of 10 eV. The DCS_{sp} however show the minimum at 40° and the difference between the two curves for angles greater than 60° is less pronounced. Although the maximum value of DCS_s at the energy 20 eV is greater than that of 10 eV, the maximum value of DCS_{sp} at 20 eV is slightly smaller than that of 10 eV. This narrowing of the maximum values of DCS can be observed as the energy of incident positron increases.

The calculated DCS at 40 eV, figure 3, are similar to the one at 20 eV albeit with slightly larger values between 0° and 16°. The DCS_{sp} and DCS_s agree better for angles above 60°. Figure 4 shows the comparison between the present result and the calculated results of Khare *et al*. (1983) using the optical potential method and those of Hossain *et al*. (2016) using the polarised orbital method at projectile incident energy of 50 eV. Absorption effects were not included in both the present study and that of Khare *et al*. (1983) and the results tend to agree at large angles and disagree at small angles. This can be attributed to the difference in the methods used as well as the different polarisation potentials employed. It indicates that the effect of polarisation in elastic scattering is not appreciable for large angles. The potential used by Hossain *et al*. (2016) included absorption and

their results underestimated the present and those of Khare *et al*. (1983) at angles above 20 eV. This can be attributed to the use of complex potential by Hossain *et al*. (2016) which can be interpreted that some incident flux was removed from the elastic channel.

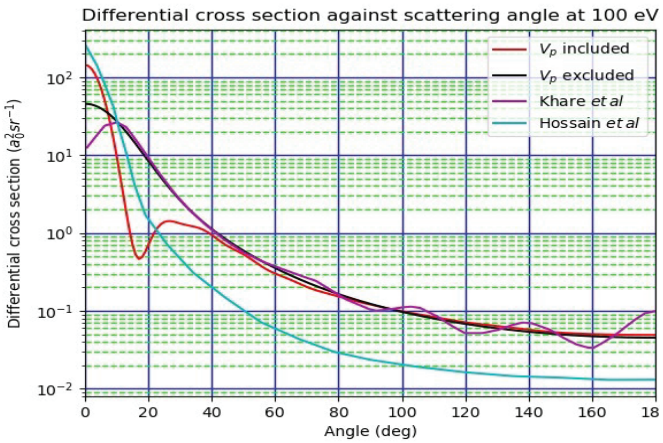

Figure 5: Elastic DCS results for e^+-Mg scattering at 100 eV as compared with the results of Khare *et al*. (1983) and Hossain *et al*. (2016).

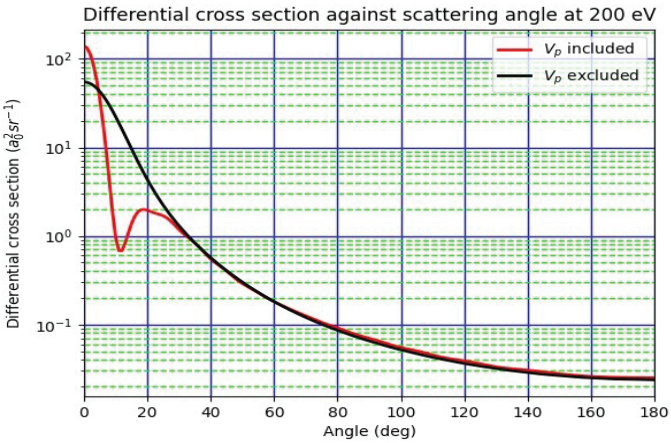

Figure 6: Elastic DCS results for e^+-Mg scattering at 200 eV.

Figure 5 shows good agreement, for all scattering angles above 10°, between DCS_s and the results of Khare *et al*. (1983). The results of Hossain *et al*. (2016) and DCS_{sp} agree only at small scattering angles. However, the present results (DCS_{sp}) agree well with those of Khare *et al*. (1983) for scattering angles above 50°. Similar to the 50 eV results, the results of Hossain *et al*. (2016) are smaller than the present due to the removal of some incident flux from the elastic channel as a result of the complex potential used in their calculation.

Figure 6 shows the elastic DCS at impact energy 200 eV. The range of angles where the DCS_s differs from DCS_{sp} is from 10° to about 30°.

Integral Cross Sections

The elastic cross sections (ICS) for positron-atom scattering for magnesium atom has been computed at 10-200 eV. Two set of results are calculated depending on the distortion potential in order to investigate the effect of polarisation. Table 1 shows the present ICS results obtained using DWM method, together with other theoretical. The ICS_s results were obtained by excluding the polarisation potential from the distorting potential while ICS_{sp} results were obtained by including the polarisation potential in the distorting potential.

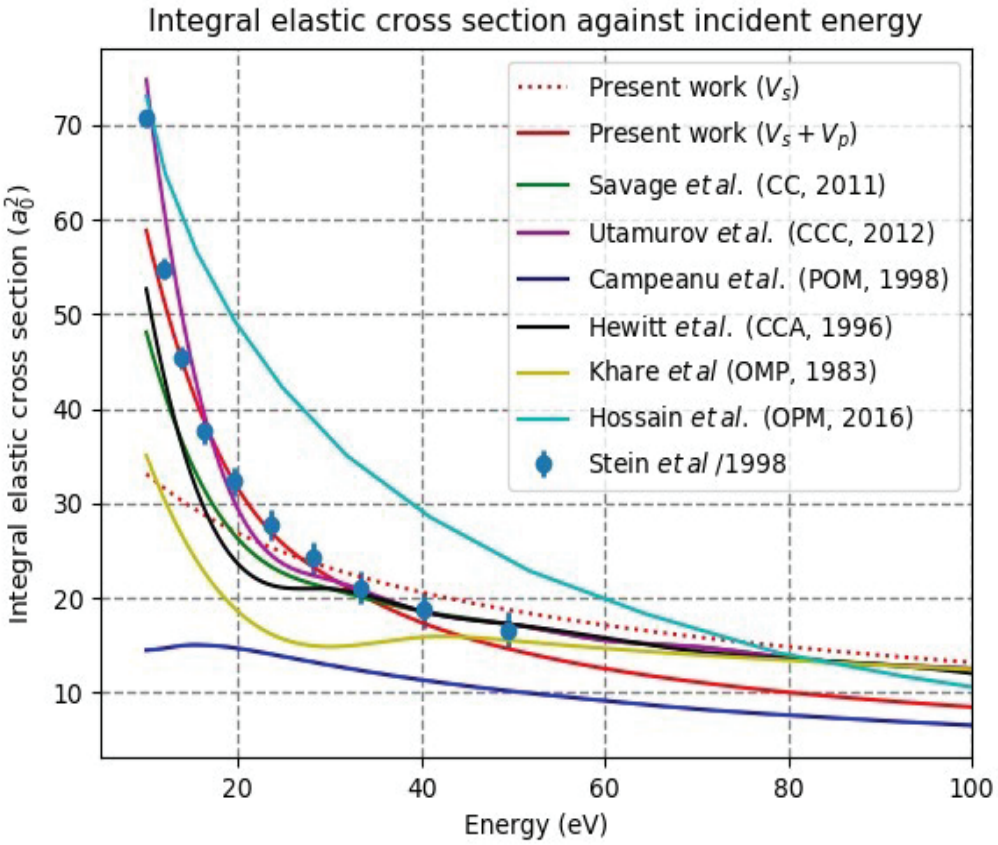

Figure 7: A comparison with other integral cross section calculations. Except for Khare *et al.* (1983), the other calculations have included inelastic cross-sections as well in their results.

Figure 7 shows how the present results compare other results on total cross sections of positron-magnesium scattering. The ICS_s results agree well with most results in the energy regime above 40 eV. The ICS_{sp} results are in satisfactory agreement with the experimental results of (Stein *et al.,* 1998) as well as the theoretical results of (Utamuratov *et al.,* 2012) between 10 eV and 40 eV impact energies.

Discussion

The differential cross-sections exhibit a distinct pattern when considering the polarisation potential. Starting from a peak in the forward direction, a steep decline follows as the scattering angle increases until a local minimum is reached. Subsequently, they increase to a local maximum before gradually decreasing in the backward direction to a much lower value. Similar angular distributions from elastic scattering processes have been observed in other studies (e.g., Franz *et al.,* 2008). As the energy increases, the angles corresponding to the local minimum and maximum in the differential cross-sections decrease. For instance, at 10 eV, these angles are observed at 58° and 90°, but at 200 eV, they occur at much smaller angles, specifically 13° and 20° respectively. For electrons,

however, the DCS exhibits a different behaviour. It shows a relatively higher value in the forward direction, gradually decreasing to a minimum between 90 and 100 degrees, and then sharply rising in the backward direction (Kariuki *et al.,* 2014).

In the context of positron-magnesium interactions, the behaviour of the projectile as it approaches the target becomes significant. As the distance between the two decreases, the repulsive Coulombic forces emanating from the target's nucleus start to impede the projectile's motion, acting as a decelerating factor. Simultaneously, the attraction exerted by the bound electrons within the target atom intensifies, exerting a strong influence on the projectile's trajectory. This modification in motion is intricately linked to a correlation mechanism reminiscent of the effects observed in multiple scattering phenomena (Puska and Nieminen, 1983). Furthermore, the magnitude and nature of this effect are dependent on the energy of the projectile.

This short-range effect ultimately leads to the emergence of polarization effects, wherein the presence of the projectile causes the redistribution of electrical charge within the target atom. The dominant term in these polarization effects is determined by the dipole-polarizability of the target atom, signifying its crucial role in shaping the overall interaction. The difference between DCS_{sp} and the result of Khare *et al*. (1983) can therefore be attributed to the different dipole-polarizabilities used in the respective calculations. The exact values of the polarizabilities for Mg, despite being the subject of numerous calculations, are currently unknown. The values of dipole and quadrupole polarizabilities used by Khare *et al*. (1983) were based on calculated values from Eades *et al*. (1982) while the ones used in this study were adjusted to match the binding energies of Mge^{+} by Bromley *et al*. (1998). These calculations are anticipated to encompass several factors beyond those arising solely from the dipole polarization of the target. These additional factors include the short-range correlation potential which emerges from virtual positronium formation and the effects of higher-order polarization potentials.

Table 1: Present elastic integral cross section results (in a^2_0) for positron impact elastic scattering of magnesium at various energies, together with calculated results of Campeanu *et al*. (1998) and Khare *et al*. (1983).

Energy (eV)	ICS_s	ICSsp	Campeanu *et al*. (1998)	Khare *et al*. (1983)
1.000E+01	3.310E+01	5.885E+01	7.339E+00	3.505E+01
2.000E+01	2.687E+01	3.156E+01	4.149E+00	1.857E+01
3.000E+01	2.317E+01	2.217E+01	3.025E+00	-
4.000E+01	2.059E+01	1.740E+01	2.434E+00	1.585E+01

5.000E+01	1.865E+01	1.450E+01	2.064E+00	1.547E+01
6.000E+01	1.712E+01	1.253E+01	1.806E+00	-
7.000E+01	1.587E+01	1.110E+01	1.616E+00	-
8.000E+01	1.483E+01	1.002E+01	1.468E+00	-
9.000E+01	1.395E+01	9.167E+00	-	-
1.000E+02	1.318E+01	8.475E+00	1.252E+00	1.243E+01
1.500E+02	1.051E+01	6.330E+00	9.406E-01	-
2.000E+02	8.872E+00	5.191E+00	7.703E-01	8.750E+00

Conclusion

It has been demonstrated that the polarisation potential has a significant effect on the scattering of positrons from magnesium. We employed a fully adiabatic positron-Mg polarisation potential with a specific cut-off to investigate elastic scattering. Our method yielded total cross sections which, when compared to total cross sections obtained from experiment, agreed quite well even at energies where inelastic channels are important.

Therefore, the findings of the present DWBA calculations can be considered as an initial step in the direction of understanding the role of polarisation in positron-magnesium interactions.

Although the integrated cross sections reported here as obtained from DWBA underestimate the experimental data in the energy range 0-10 eV, at the energy range 10-200 eV the calculation did fit the data well.

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