Positron scattering from argon: total cross sections and the scattering length

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Abstract

We report results from new positron–argon total cross-section (TCS) measurements. Agreement with the corresponding recent data of Jones et al (2011 Phys. Rev. A 83 032701) is found to be very good, except at the lowest energies of common measurement. Excellent qualitative agreement is also found between our measurements and an improved convergent close-coupling (CCC) calculation which was undertaken as a part of this study. This level of accord between our experimental and theoretical TCSs has enabled us to determine an experimental scattering length ($a$) of $a = -4.9 \pm 0.7$ au for the positron–argon system. That value is in excellent agreement with the relativistic polarized orbital optical potential approach result of Jones et al ($a = -4.7$ au) and our CCC result of $a = -4.3$ au.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

A very thorough review of the available experimental and theoretical investigations into positron scattering from argon was recently provided by Jones et al [1], and so we do not repeat all of those details again here. Rather, we note that there is a sizeable body of previous work, both experimental [1–7] and theoretical [1, 8–14], that remains, in general, in only marginal to fair agreement with one another [1]. This is a serious problem, as the noble gases represent systems, for a variety of experimental and theoretical reasons [1], for which you might hope to be able to provide detailed ‘benchmark’ cross sections [15]. Indeed at least part of the rationale behind this study is the desire to shed more light, at the total cross-section (TCS) level, on positron–argon scattering as a possible ‘benchmarked’ system.

The scattering length ($a$) is a fundamental concept in quantum physics, with applications in both atomic and molecular and nuclear scattering phenomena [16]. Of particular relevance to this study is its utility in aiding our understanding of the physics for positron–atom interactions at low energies. For instance, targets with relatively large dipole polarizabilities ($\alpha$), argon has $\alpha = 11.07$ au [17], lead to a strong attractive scattering potential for the positron, which manifests itself in quite large negative values in their scattering lengths [15]. Unfortunately for positron–argon scattering (see table 1), agreement between the various theories [1, 9, 10, 18–20], between the various experiments [21–23] and between theory and experiment for the scattering length is, like the TCS, also only fair. Clarification of these discrepancies also represents a partial motivation for this investigation.

In section 2, we provide some details of our measurement techniques and analysis procedures, while in section 3, a description of the present convergent close-coupling (CCC) computations is given. Note that the present CCC results
supersede those previously reported by Jones et al [1], as here we have incorporated a more realistic description of the polarization. Thereafter, in section 4, we present and discuss our results. Finally, some conclusions from this investigation will be drawn.

2. Experimental details

The Trento University spectrometer was developed by Zecca and colleagues and has been described previously many times (see for example [24, 25]). We therefore do not repeat those details again, except to note that a tungsten moderator of thickness 1 μm [26] was employed in conjunction with a radioactive 22Na isotope (current activity ~ 1.5 mCi) and some electrostatic optics in order to produce the positron beam. These optics were originally designed to produce a stable and well-focused (into the scattering cell) positron beam with energies between ~ 0.1 and 50 eV [25]. Note that the energy range of the present positron–argon measurements was in fact 0.3–50.2 eV. The operational performance of the Trento spectrometer, over many years now, suggests that those design criteria have been met.

The basis of all linear transmission experiments is the Beer–Lambert law as defined by

\[ I_1 = I_0 \exp \left( -\frac{(P_1 - P_0) L \sigma}{kT} \right) \]  \hspace{1cm} (1)

where \( I_1 \) is the positron beam count rate at pressure \( P_1 \), the target gas pressure being measured with argon (Ar) routed to the scattering cell, \( k \) is Boltzmann’s constant and \( T \) is the temperature of the Ar vapour (K), as measured by a calibrated platinum (PT100) resistance thermometer that is in thermal contact with the scattering chamber. In equation (1), we also note that \( \sigma \) is the TCS of interest at a given incident positron energy, \( I_0 \) is the positron count rate at \( P_0 \), the pressure with the Ar gas diverted into the vacuum chamber, i.e. away from the scattering cell and \( L \) is the length of the scattering region.

For a physical application of equation (1), several crucial precautions should be taken and care must be exercised during the measurements. These considerations include minimizing the double-scattering events and ensuring the TCSs are independent of pressure. In addition, only a high-purity argon source (⩾ 99.998%) was used (Air Liquide). The geometrical length of the scattering region is 22.1 ± 0.1 mm, with apertures of 1.5 mm diameter at both the entrance and exit of the scattering cell. In our application of equation (1), the value of \( L \) used is always corrected to account for the path increase caused by the gyration of the positrons in the focusing axial magnetic field present in the scattering region. For incident positron energies from 0.3 to 30.2 eV, \( B \sim 11 \text{ G} \) and the value of \( L \) increased by ~5.5%, while for positron energies between 35.2–50.2 eV, \( B \sim 4 \text{ G} \) leading to an increase in \( L \) of ~2%. It is crucial for the energy scale to be calibrated accurately. The zero for the energy scale, in the absence of the target gas, was determined using a retardation potential analysis of the positron beam [27]. Note that an electronic copy of [27] is available on request from the corresponding author of this paper. We believe that the error in our energy scale is ±0.05 eV. The same measurements allow us to evaluate an energy width of the positron beam of ~0.25 eV (FWHM), with an uncertainty on this determination of at most ±0.05 eV. It is also very important to accurately measure the scattering cell pressure, which we achieve with an MKS 627B capacitance manometer operating at 45 °C. As the manometer temperature was different to that for the argon gas in the scattering cell (\( T = 22 \pm 1 \text{ °C} \)), thermal transpiration corrections to the pressure readings are made using the model of Takaishi and Sensui [28]. Typically, this led to a maximum correction on the TCS of +3%.

All linear transmission scattering-cell–based experiments invariably have some angular discrimination limitations. They arise from the inability to distinguish between positrons that are elastically scattered at small angles from those in the primary (unscattered) beam and result in the directly measured TCSs being somewhat smaller than the ‘true’ value. The extent of this problem depends on the angular discrimination of the apparatus in question and the nature of the elastic differential cross section (DCS) in this forward angle region [29]. From a consideration of the size of the entrance and exit apertures of our scattering cell, and their separation, the angular acceptance (\( \Delta \theta \)) of the Trento spectrometer is ~4° [25], which compares favourably with that from the Yamaguchi spectrometer (\( \Delta \theta \sim 7^\circ \)) and the Detroit apparatus [30] (\( \Delta \theta \sim 16^\circ \)). The gyration of the positrons can also potentially increase the angular discrimination correction compared to the no-field case [31]. Using some of the analytic formulae detailed in Kauppila et al [30], but for the typical experimental conditions of our measurements, estimates of the present energy-dependent angular discrimination varied from ~17° at 1 eV to 5.4° at 10 eV positron energy [25]. These can then be used in conjunction with the approach of Hamada and Sueoka [31] to determine the corrections to the TCSs to account for this effect. An alternative approach to using the formulae from Kauppila et al [30] and [31], would be to conduct a Monte Carlo simulation of the behaviour of the positrons in our scattering cell. We have preliminary results from such a study, using the krypton CCC cross sections from

<table>
<thead>
<tr>
<th>Origin</th>
<th>Scattering length (au)</th>
</tr>
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<tbody>
<tr>
<td><strong>Experimental</strong></td>
<td></td>
</tr>
<tr>
<td>Present result</td>
<td>−4.9 ± 0.7</td>
</tr>
<tr>
<td>Lee and Jones [21]</td>
<td>−4.4 ± 0.5</td>
</tr>
<tr>
<td>Tsai et al [22]</td>
<td>−2.8 ± 0.7</td>
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<tr>
<td><strong>Empirical</strong></td>
<td></td>
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<tr>
<td>Hara and Fraser [23]</td>
<td>−4.0 to −3.0</td>
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<tr>
<td><strong>Theoretical</strong></td>
<td></td>
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<tr>
<td>Present CCC</td>
<td>−4.3</td>
</tr>
<tr>
<td>McEachran et al [9]</td>
<td>−5.3</td>
</tr>
<tr>
<td>Datta et al [18]</td>
<td>−3.5</td>
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<tr>
<td>Schrader [19]</td>
<td>−4.1</td>
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<tr>
<td>Nakanishi and Schrader [10]</td>
<td>−4.5</td>
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<tr>
<td>Jones et al [1]</td>
<td>−4.7</td>
</tr>
<tr>
<td>Assafrão et al [20]</td>
<td>−3.4</td>
</tr>
</tbody>
</table>
Zecca et al [15] and a modified version of a Monte Carlo code that was originally employed for studying $E \times B$ discharges in swarm physics [32]. In any event, the results from the Monte Carlo simulation were in quite good agreement (typically to better than 5%) with those predicted using the formulae of Kauppila et al and the procedure of Hamada and Sueoka thereby giving us more confidence in their validity. Further note that the present energy-dependent angular discrimination estimates compare well with those determined by the ANU group (see table II in Jones et al [1]) for their apparatus. The ANU group subsequently employed these estimates and their relativistic polarized orbital optical potential (RPO) approach elastic DCSs [1] for argon, to quantify the forward angle scattering effect on their measured TCSs. That correction varied from 13.4% at 0.5 eV to 2.4% at 8.5 eV. Of course, we can adopt the same approach (following [31] and references therein) using the table of correction factors, for the present spectrometer, listed in table 2 of Zecca et al [25] and the present elastic CCC DCS (see figure 1). On doing this we determine an increase in our measured argon TCS of $\sim 12\%$ at 0.3 eV, $\sim 4\%$ at 10 eV and $\sim 2\%$ at 30 eV. The problem is that there is currently no independent verification of the validity of the present CCC results, or for that matter of the RPO elastic DCS results used by Jones et al [1]. As a consequence, the very real question as to which theory is to be preferred at the DCS level needs to be addressed and at this time the answer is that we simply do not know. Therefore, we decided not to make such a correction to our measured TCSs (see table 2) until this matter has been resolved, quite simply we think it would be premature to do so at the moment.

Finally, we note that all the present data collection and analysis codes were driven by software developed at the University of Trento, for application on a personal computer.
The positron energy range of the present TCS measurements was 0.3–50.2 eV, with the overall errors on our TCSs estimated as being within the 5–12% range. Note that the overall errors are formed from the quadrature sum of quantities such as the statistical uncertainties on our data (0.1–8.8%), the uncertainty in our thermal transpiration corrections, the uncertainty in the value of $L$, the uncertainty in the value of $T$ and the uncertainty in the absolute pressure readings (∼0.3%), as per the manufacturer’s specification.

3. Theoretical details

The CCC theory for positron scattering on inert gases other than helium assumes a frozen-core model of the form $\ldots np^5$ for the target. In the case of Ar, we may write its structure as $[\text{Mg}]2p^5nl$. The $[\text{Mg}]2p^5$ orbitals are obtained in a self-consistent field Hartree–Fock approach. The $nl$ orbitals are obtained using an orthogonal Laguerre basis of size $N_l$ with exponential fall-off $\lambda_l$ [33]. CCC results using such a structure were reported recently [1] for the positron–argon collision system. Unfortunately, such a model yields a static dipole polarizability of 13.7 au which is somewhat larger than the experimental value of 11.1 au [17]. This is particularly problematic at low energies and resulted in the overestimation of the cross sections. Here, as for the heavier inert gas Kr [15], to reduce the polarizability we apply the phenomenological di-electronic core polarization potential

$$V_p(r_1, r_2) = -\frac{\alpha}{r_1^2 r_2^2} \times \sqrt{1 - \exp(-r_1/\rho)}(1 - \exp(-r_2/\rho)),$$

(2)

where $\alpha$ and $\rho$ are parameters chosen to yield the required target static dipole polarizability. Having two parameters to determine one number results in many possibilities. We make the choice that $\alpha$ is the same as the required experimental value, and then choose just $\rho$. Presently, we took $\alpha = 11.1$ and $\rho = 4.7$. Additionally, given our interest in very low energy scattering we have utilized radial grids that extend to 1000 au.

Having decided on the model for the target, we need to define the target states used in the expansion of the positron–argon collision system. We take $\ell \leq \ell_{\text{max}} = 8$ and $N_l = 20 - \ell$. The target Hamiltonian is diagonalized for all possible target symmetries resulting in a total of 334 states, all of which are included in the close-coupling expansion [34].

Results from the present computations for elastic DCS, at 0.2, 2 and 20 eV incident positron energies, can be found in figure 1 while the present CCC TCS is presented in figure 2.

4. Results and discussion

In figure 2, we plot the present experimental TCSs and the TCSs from our CCC calculations, along with the results from the previous measurements of Jones et al [1]. An extensive body of earlier experimental and theoretical work [2–14] is not plotted, rather we refer the reader to figure 4 in Jones et al in order to view that data. Note that we will also comment on that comparison shortly. The present measured TCSs, uncorrected for the forward angle scattering effect, are also listed in table 2. It is clear from figure 2 that the present data and CCC calculations are in good qualitative agreement over most of their common energy range, our CCC theory generally being some ∼20% lower in absolute magnitude compared to the measured data for energies less than the positronium formation threshold energy ($\text{Ps}$ = 8.96 eV). This is an interesting observation given the treatment of the polarization (see section 3) for argon that we employed here, and perhaps suggests that the preferred experimental value for $\alpha$ [17] is in fact a little low. We highlight the very strong increase in the magnitude of both our measured data and CCC TCSs (see figure 2), as the incident positron energy decreases below 1 eV. A similar observation was also made by us in our recent study of positron–krypton scattering [15]. We believe that this behaviour reflects the relatively strong dipole polarizabilities of the noble gas atoms and in particular argon in this case. The present data are also seen to be in largely very good agreement with the measured results of the ANU from Jones et al [1]. Again, in this case for positron energies greater than about 1.5 eV, this accord would only improve if the present TCS was corrected for the angular discrimination effect. Note, however, that as we estimate the overall errors on our measured TCS to be in the 5–12% range, the actual level of agreement between ANU and the current TCS is really very good. Indeed, this level of agreement is particularly pleasing given that the TCSs from each group were determined on very different spectrometers employing completely different measurement techniques. An exception to this is at energies below 0.55 eV where the magnitude of the ANU TCS appears a little low, possibly reflecting a technical problem with the operation of their trap below that energy. We note that a similar
problem was also identified by us when comparing our TCSs for positron–krypton scattering [15]. Nonetheless, given the overall comparison indicated in figure 2, for the present and ANU data, a case might now be made for considering the positron–argon scattering TCSs to have been experimentally ‘benchmarked’. If this is in fact the case, then it is an important result, as it provides a set of accurate TCS, over a quite wide energy range, against which theory might be intimately tested. With respect to the level of agreement between the present measurements and the other earlier data and computations [2–14, 20], we find only a fair-to-marginal level of accord between them over the common energy ranges studied. Indeed, in terms of the earlier experimental data, the agreement appears to be best above the Ps-formation threshold. The discrepancy at the lower energies might well simply be a reflection of the earlier data needing more significant angle-discrimination corrections being made to them (they are all uncorrected for this effect at this time) [29], relative to the present and ANU data, rather than an error in their measurement and/or analysis procedures.

It is well known from quantum mechanics [16] that, at low energy, the integral elastic cross section (σel) in atomic units (au) is related to the scattering length via

\[ \sigma_{el} \approx 4\pi a^2. \]  

(3)

For incident positrons with energies lower than the positronium formation threshold, σel is equivalent to the TCS. Thus, TCS can replace σel in equation (3). The rationale for conducting our CCC computations to very low energies is now clear in figure 2. Here it is quite apparent that by \(10^{-5}\) eV the magnitude of the CCC TCS has plateaued to a value of \(65.1 \times 10^{-20}\) m\(^2\), so that with equation (3) being valid, a CCC scattering length (\(a_{\text{CCC}}\)) for positron–argon scattering of \(a_{\text{CCC}} = -4.3\) au can be derived. Note that the negative root from equation (3) is chosen due to the strongly attractive nature of this scattering system at lower energies [9]. This value of the scattering length compares favourably with those found previously by Nakanishi and Schrader [10], Schrader [19] and Jones et al [1], as summarized in table 1. Given the very good level of qualitative accord between the CCC and present measured TCS over most of their common energy range, we have used the shape or form of the low-energy CCC result to extrapolate our measured data to \(10^{-5}\) eV. This extrapolation is shown as the dashed line in figure 2, and we believe it to be a fair representation of the low-energy TCS for our data. Note that this approach was recently used to similarly extrapolate our positron–krypton TCS data to very low energy [15]. An alternative approach would be to try and employ a modified effective range theory (MERT) expansion to try and analyse the present TCS. Indeed this was initially attempted. However, it quickly became apparent that the derived values of the coefficients were very sensitive to the number of terms actually retained in the MERT expansion. This therefore cast significant doubt as to the uniqueness of the MERT coefficients we derived, so that this approach was abandoned. Using our preferred extrapolation we determine an ‘experimental’ TCS at \(10^{-5}\) eV of magnitude \(83.8 \times 10^{-20}\) m\(^2\) leading via equation (3) to a value of the scattering length \(a_{\text{expt}} = -4.9 \pm 0.7\) au. Note that our error estimate on the current scattering length incorporates for the effect of our forward angle-discrimination correction to the measured TCS. The present scattering length value can also be found in table 1, where we see it is in good agreement with an earlier measurement-based result from Lee and Jones [21] of \(a = -4.4 \pm 0.5\) au. We believe that the present approach for deriving an experimental scattering length from TCS data measured to low energies is the most straightforward and transparent of the procedures applied for this task (so far) [21–23] in the literature. As such we assert that our value for \(a_{\text{expt}}\) is probably the most reliable of those experimental values available (see table 1). We can also compare \(a_{\text{expt}}\) to the various theoretical results (again see table 1), where we find good agreement with the values from McEachran et al [9], Jones et al [1], Nakanishi and Schrader [10] and our CCC result. As the magnitude of the scattering lengths in table 1 is larger than argon’s mean radius, it follows that the scattering cross section will be greater than its geometric size. This enhancement can be viewed [36] as arising from the existence of a virtual level for the positron projectile, at an energy (in au) given by [15]

\[ \varepsilon = \frac{1}{2a^2}. \]  

(4)

These virtual levels are also known to lead to enhanced positron annihilation cross sections [14]. Hence using our experimental scattering length in equation (4), we determine that the energy of the positron–argon virtual state is at \(\varepsilon = 0.57 \pm 0.08\) eV.

5. Conclusions

We have reported on measurements and CCC calculations for positron–argon scattering. The measurements were made at some of the lowest energies to date, and with the aid of our CCC theory, which is in good qualitative accord with our TCS data, we have determined a robust value for the experimental scattering length. We believe that this value is probably the most reliably currently available, and it was found to be in good agreement with our corresponding CCC result and those from some of the other calculations including the RPO approach [1]. From this estimate of the scattering length we were also able to determine the energy of the virtual state formed when positrons interact with argon atoms. Finally, at the TCS level, the very good agreement between the ANU data and the present data enabled us to make a case for why this system might now be considered to have been experimentally ‘benchmarked’. Such ‘benchmarked’ systems are very useful in the development of new approaches to theoretical studies.

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References