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Forward angle scattering effects in the measurement of total cross sections for positron scattering

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Abstract

Measurements of total scattering by positron impact have typically excluded a significant portion of the forward scattering angles of the differential cross section. This paper demonstrates the effect that this can have on measurements of the total cross section. We show that much of the apparent disagreement between experimental measurements of positron scattering from atoms and molecules may be explained by this excluded angular range. It is shown that this same effect may also lead to an anomalous energy dependence of some cross sections.

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

1. Introduction

Significant disagreement exists in the literature between various experiments for the absolute magnitude of positron total scattering cross-section measurements, with the noble gases being a particular case in point. These systems have been measured extensively over recent decades and variations of up to 20% in neon, 25% in Ar and Kr and up to a factor of 2 in Xe are seen across the energy range below 100 eV (see [1], for instance). There are several possible explanations for this situation but one, which is perhaps the most prominent, is the role that strong angular scattering, particularly at forward angles, may play in the determination of the total cross section.

A common feature of attenuation-type experiments for the total scattering cross section is that all suffer, to some extent, from the inability to discriminate against small angle elastic scattering. This is a consequence of the simple fact that the attenuation cells that are used have entrance and exit apertures of finite size to enable the passage of the primary positron beam. This means that some particles that are scattered through small angles may be transmitted to the detector, resulting in a potential error in the determination of the cross section. The normal approach to the determination of the total cross section is to use the Beer–Lambert law:

$$\sigma_T = \frac{1}{NL} \ln\left(\frac{I_0}{I_T}\right) \qquad (1)$$

where I_T and I_0 are the transmitted (or unscattered) and incident positron intensities, respectively, N is the gas number density and L is the length of the scattering cell. It can thus be readily seen that an inability to discriminate against forward elastic scattering will potentially result in an overestimation of the measured transmitted intensity, I_T, and hence an underestimation of the total cross-section value.

Attempts have been made to correct for this in various experiments. If one has knowledge of the nature of the differential cross section, and the range of angles over which forward scattered positrons are being detected in any given experiment, then the total cross section can be corrected for this effect. In many cases, these corrections can result in a substantial difference in the true measured value of the total cross section. This is particularly the case for targets which have either a large dipole polarizability or a large permanent dipole moment, or both. Both result in long-range interactions that can have a profound effect on the magnitude of forward scattering. In the rare gases the dipole polarizability increases from 1.38 au in He to 27.3 au for Xe, and this is strongly manifested in the shape of the low energy differential cross sections, with the heavier gases exhibiting strong forward scattering. In the case of strong dipole scattering, water is a spectacular case in point and this has recently been shown to have a significant impact in the case of positron total scattering measurements [2, 3].

As positrons are relatively rare in nature, and thus difficult to produce in an energy-resolved, high-intensity beam, a common feature across many such experiments is the use of guiding magnetic fields to help maintain the positron flux. With a relatively weak guiding magnetic field (1–10 Gauss), the cyclotron radius of the positrons may be as big as the beam spot size, making it even more difficult to distinguish between forward elastically scattered positrons and the unscattered incident beam. The range of angles, $\theta < \theta_c$ (where θ_c is the critical angle) for which forward scattered particles cannot be discriminated from the primary beam varies from experiment to experiment, but typical values range between 5° and 20°. For forward angle inelastic scattering, some experiments overcome this problem by the use of a retarding potential device following the scattering cell to retard the progress of inelastically scattered particles to the detector. However, for elastic scattering this technique is not useful.

An alternative experimental approach which, in principle, is not as susceptible to these effects, particularly at energies above about 2 eV, uses the positron beams generated in buffer-gas trap and beam systems [4, 5]. This technique employs much stronger magnetic fields (∼500 Gauss), such that all positrons, including those that are scattered, are transmitted to the detector. In this case the cyclotron radius of the positrons is also very much smaller and the angular resolution, and hence θ_c, is directly related to the energy resolution of the beam (see [5] for details). At very low energies, the values of θ_c that are obtained are similar to those mentioned above, but these improve significantly at higher incident energy.

This paper examines the role the degree of forward angular discrimination can play in the experimental determination of the absolute total positron scattering cross section, and demonstrates that, in many cases, if these effects are not accounted for, they can lead to the measured cross sections that may be substantially underestimated. The focus has been restricted to elastic scattering in the rare gases, but the concepts are generally applicable to all measurements of positron (and electron) total scattering. We have used both theoretical and experimental cross sections to investigate these effects, the latter being measured using a trap-based positron beam in which the forward angular discrimination can be arbitrarily varied. Such effects have, of course, been discussed in the past (see for example [6]), and we do not claim this to be a new revelation. However, in the majority of cases in the literature, the cross sections that are presented have not been corrected for these effects.

2. The effect of finite angular discrimination on the total cross section

The total elastic cross section can be determined by integrating the elastic differential scattering cross section (DCS) over the entire angular range:

$$\sigma_T = 2\pi \int_0^{\pi} \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \sin\theta \, \mathrm{d}\theta. \qquad (2)$$

In the case of any measurement of the total cross section using a transmission technique, however, we have discussed how there will be a certain fraction of the angular scattering that is not distinguished from the unscattered incident beam. In the case of positron scattering, most measurements of the total cross section have been made using a transmission-type experiment, with the positrons confined in a relatively weak magnetic field. The forward angular discrimination (θ_c) for these measurements varies, but typical values cited in the literature range from 40° [7], 13°–20° [8, 9], to around 6.5° [10]. In some cases corrections have been applied to the measured cross section but in the overwhelming majority of cases they have not.

If we know the value of θ_c for any experiment and have some knowledge of the elastic DCSs as a function of energy and angle, the effect of forward scattering on the total cross section can be estimated. For example, using a given theoretical DCS calculation, we can estimate the fraction of the total cross section which may be missed as a result of this effect. Argon is one of the most studied targets in the positron scattering literature, and there are many theoretical calculations of differential and total elastic scattering. An example of how theory can be used to this effect is shown in figure 1(a). DCSs calculated using our own relativistic polarized orbital (RPO) approximation have been used to derive the total scattering cross section from equation (2), with various values of θ_c (5°, 10°, 15°, 20°, 30°) being used as the lower limit on the integration. It can be seen that the magnitude of the 'effective' total cross section is progressively reduced as the level of forward scattering discrimination is reduced (or θ_c is increased). For instance when θ_c is 20° as in figure 1(a) the cross section is reduced by about 30%. The increasing neglect of forward scattering also appears to change the energy dependence of the total cross section, producing a shallow minimum at around 2 eV, when between 20° and 30° of the measured DCS is overlooked. This also seems to be the case irrespective of the theory that one uses for the test. Varying the nature of the polarization potential used in the present calculation does change the energy dependence and magnitude of the cross section at low energies, but does not significantly affect the percentage reduction we observe when excluding portions of the forward scattering. A similar process using cross sections calculated with a recently developed convergent close coupling approach [11] yields the same overall picture, even though there are some differences between the calculated cross sections as to the absolute magnitude of the cross section in the low energy region.

The experimental apparatus that we use for positron scattering measurements has been described in detail elsewhere [12], as have the techniques that are used for

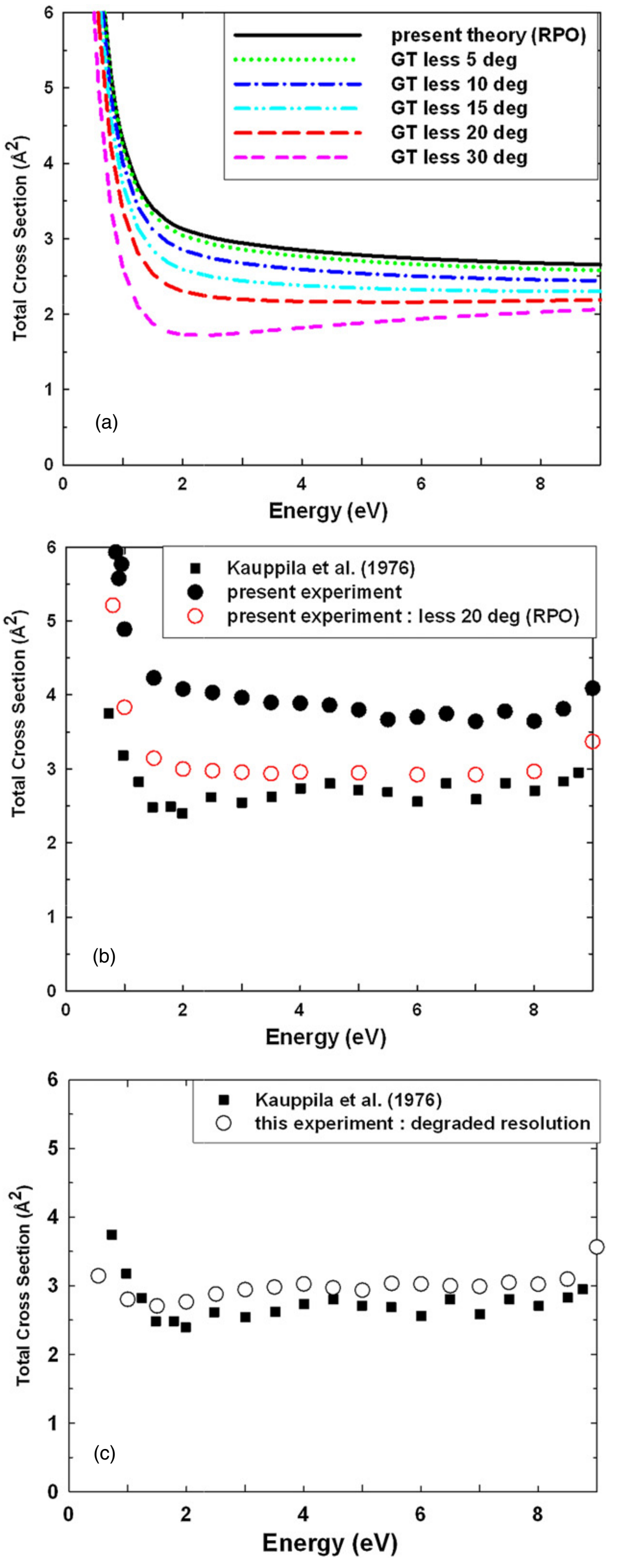

Figure 1. (a) Relativistic polarized orbital calculation for the total positron scattering cross section for argon (—) and with 5°, 10°, 15°, 20° and 30° excluded from the integration of the DCS—curves descending with increasing missing angle; (b) (•) present data for the argon total cross section, (○) present data with the forward 20° of scattering omitted using the RPO cross sections, (■) data of Kauppila *et al* [13]; (c) (○) present data measured with an experimentally degraded angular discrimination (see the text) compared with the (■) data of Kauppila *et al* [13].

measuring cross sections in a high magnetic field [5]. For this type of experiment all positrons are transmitted through the scattering cell under the influence of the strong field and the scattering information is extracted from a measurement of the flux transmitted through a retarding potential analyser, as a function of the retarding potential applied. In this way the loss of parallel energy incurred due to elastic scattering can be interpreted readily in terms of the DCS (see [5] for details). Using this retarding potential analyser technique, the forward angle discrimination (θ_c) is determined by the energy resolution of the beam, and we also have the ability to arbitrarily choose the extent of the forward angle discrimination by selecting an appropriate part of the RPA transmission spectrum.

Figure 1(b) shows the present experimental measurements of the total scattering cross section together with data from the literature of Kauppila *et al* [13]. We use the data of [13] merely as an example, and because the authors have clearly articulated the value of θ_c in their measurements. Our measurements, which have been taken with an angular discrimination that varies from 21° at 0.5 eV to 6.5° at 5 eV, and then corrected accordingly using the RPO theoretical DCS values, are shown as solid black circles and are seen to lie well above the data of Kauppila *et al* (squares) across this energy range. The data of Kauppila *et al* were taken with an angular discrimination that varied from 15° to 20°, but they have not been corrected for any forward scattering effect. The open circles show our experimental data after removing the contribution from the forward 20° of scattering at each energy, as given by the RPO calculation. This is done to mimic the situation for the upper end of the angular discrimination in the data of [13], and we see that the resulting agreement between the present, effectively uncorrected result, and that of [13] is markedly improved.

In addition to this adjustment and comparison using theoretical cross sections, we can also measure cross sections, using the retarding potential techniques described above, which have an arbitrarily set forward-angle discrimination (θ_c). This is done in figure 1(c) where the retarding analyser potential is set such that the measured cross sections correspond to a missing angular region of 30° at 0.5 eV reducing to 8° at 8 eV. Once again the agreement between the present cross section, with degraded angular discrimination, and that of [13] is considerably improved.

From figures 1(b) and (c) it can be seen that the magnitude of the result is very sensitive to the level of forward angle discrimination, in accord with the discussion above, and the results shown in figure 1(a) based on the theoretical calculation. When the forward angle discrimination of the two experimental data sets are roughly matched, the agreement between the two is extremely good. Of particular interest is the appearance of a dip at around 2 eV in the cross sections with the poorer forward angle discrimination. It was previously speculated that this may be due to the Ramsauer–Townsend effect [13], but it also seems possible from this demonstration that such a feature may arise simply from the effect on the cross section of a finite level of discrimination against forward angle scattering.

A similar study is presented in figure 2 for xenon. Again, cross sections from our relativistic polarized orbital calculation are used to ascertain the effect on the total cross section of different levels of forward angle discrimination. It can be clearly seen in figure 2(a) that there is a significant reduction in the cross section depending on the extent of the forward angle portion that is excluded. Once again at 2 eV, the consequence of not accounting for 20° forward scattering is a reduction in the cross section of about 30%.

Through recent measurements of the xenon total cross section in our laboratory we have found that the magnitude of the cross section, at low energies, is substantially higher than any previous measurements, and we attribute this largely to the superior angular discrimination of our experiment at energies above about 2 eV. Figure 2(b) shows a comparison between the present (corrected) data and those from Dababneh *et al* [14], which have not been corrected for any forward scattering effects. Note that the rise in the cross sections above 5.33 eV is due to positronium formation, which is not included in the calculated cross sections in figure 2(a). In figure 2(b) we have used two different techniques in an attempt to mimic the angular discrimination of the measurement of [14]. First, we have reduced our corrected cross section at energies below 5 eV using the RPO cross sections and an angular discrimination of 20°, as was the case in the data of [14]. This is shown as the open circles in figure 2(b) and the agreement between these data, and those of [14] is excellent. Second, at three energies (4.4, 6.4, 8.4 eV) we have experimentally degraded the angular discrimination to 20° and repeated cross section measurements. These data, the open triangles in figure 2(b), are also in excellent agreement with the cross section of [14].

Once again, in xenon, we find that although our measured cross-section magnitude is in disagreement with those of [14], once the angular resolution is adjusted to match that of the previous result, using theoretical cross sections or our experimental technique, the experimental data are in good agreement.

Finally, to further illustrate the extent and influence of the forward-peaked nature of the differential scattering cross section, we show the RPO elastic DCS for Xe at 2 eV, weighted by $\sin\theta$ as in the integrand of equation (2), in figure 2(c). This shows quite clearly the dominant effect that forward scattering plays in the determination of the total cross section, even at these relatively low energies.

3. Conclusion

We believe that this paper has demonstrated that relatively small changes in the level of discrimination against forward scattering can lead to significant changes in the measured magnitude and shape of the total scattering cross sections for certain targets. We have used both theoretical cross sections and experimental measurements to support these conclusions. This is not a new revelation by any means, and we do not claim it as such, but it is one which, in practice, has been acknowledged but largely ignored when presenting absolute scattering data. While most published works acknowledge the range of angles that are 'missed', most also have not corrected for this effect. Recent measurements, for the most part with better forward angle discrimination than previously achieved, have revealed considerably higher total cross-section values than earlier experiments. Clearly, care must be taken when

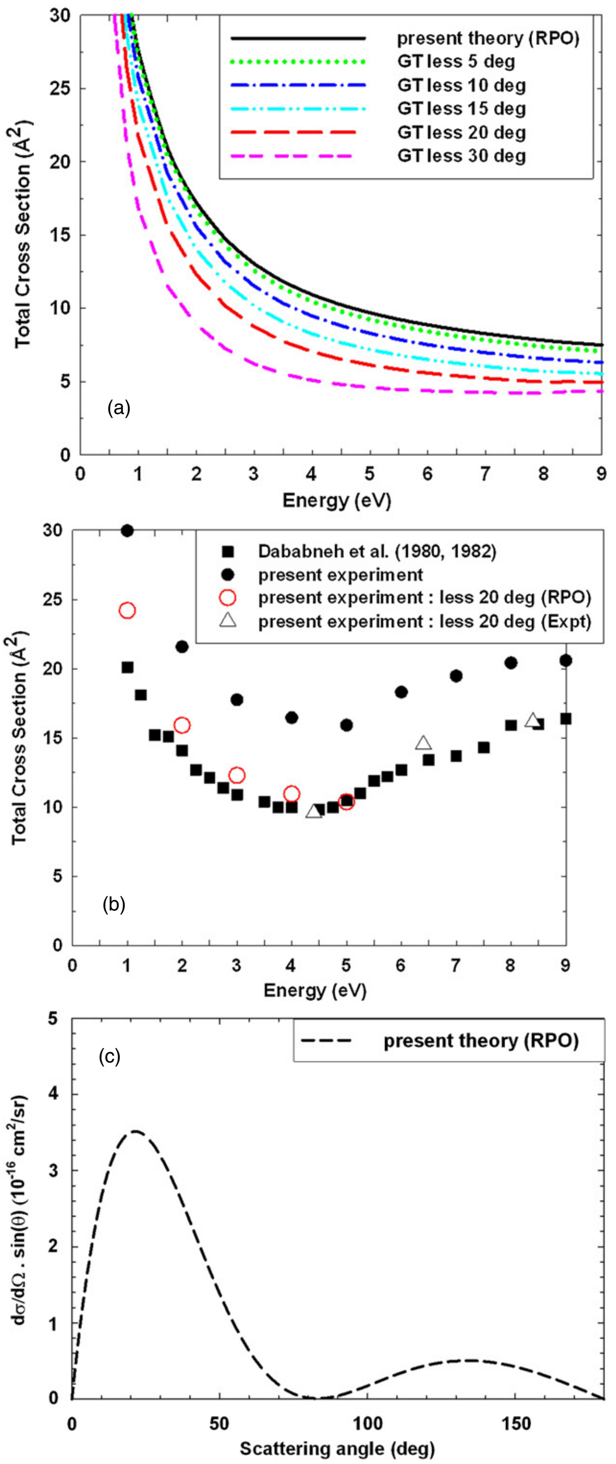

Figure 2. (a) Relativistic polarized orbital calculation of the total positron scattering cross section from xenon (—) and with 5°, 10°, 15°, 20° and 30° excluded from the integration of the DCS (curves descending with increasing missing angle.) (b) (●) present corrected data for the xenon total cross section, (○) present data with the forward 20° of scattering omitted using the RPO cross sections, (Δ) present data with the angular discrimination experimentally degraded by 20°, (■) data of Dababneh *et al* [14]. (c) The present elastic DCS for 2 eV scattering from xenon calculated in the RPO approximation and weighted by $\sin\theta$.

comparing results between different experimental groups as well as between experiment and theory, which is unaffected by the problems of limited angular discrimination. No experimental technique can provide ‘complete’ total elastic scattering cross sections and all will suffer from some lack of discrimination against forward scattering. It is probable that such effects are at least partly responsible for the apparent broad disagreement in measurements of positron total scattering cross sections in the noble gases and some molecular systems. A careful estimation of the degree of angular discrimination, combined with an input from theory, can help to both better define what is being presented as the total cross section, and potentially improve the level of agreement between various measurements. It would appear that for the rare gases and for contemporary scattering calculations, the percentage of missing forward angle scattering is rather insensitive to the theoretical approach used.

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References

[1] Stein T S and Kauppila W E 1982 *Adv. At. Mol. Phys.* **18** 53
[2] Makochekanwa C *et al* 2009 *New J. Phys.* **11** 103036
[3] Kimura M, Sueoka O, Hamada A and Itikawa Y 2000 *Adv. Chem. Phys.* **111** 537
[4] Murphy T J and Surko C M 1992 *Phys. Rev.* A **46** 5696
[5] Sullivan J P, Gilbert S J, Marler J P, Greaves R G, Buckman S J and Surko C M 2002 *Phys. Rev.* A **66** 042708
[6] For example, see Sinapius G, Raith W and Wilson W G 1980 *J. Phys B: At. Mol. Phys.* **13** 4079
Kauppila W E, Stein T S, Smart J H, Dababneh M S, Ho Y K, Downing J P and Pol V 1981 *Phys. Rev.* A **24** 725
Sueoka O and Hamada A 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** 5055
[7] Canter K F, Coleman P G, Griffith T C and Heyland G R 1973 *J. Phys. B: At. Mol. Phys.* **6** L201
[8] Stein T S, Kauppila W E, Pol V, Smart J H and Jesion G 1978 *Phys. Rev.* A **17** 1600
[9] Kwan C K, Hsieh Y-F, Kauppila W E, Smith S J, Stein T S, Uddin M N and Dababneh M S 1984 *Phys. Rev. Lett.* **52** 1417
[10] Charlton M, Laricchia G, Griffith T C, Wright G L and Heyland G R 1984 *J. Phys. B: At. Mol. Phys.* **17** 4945
[11] Bray I 2010 private communication
[12] Sullivan J P, Jones A C, Caradonna P, Makochekanwa C and Buckman S J 2008 *Rev. Sci. Inst.* **79** 113105
[13] Kauppila W E, Stein T S and Jesion G 1976 *Phys. Rev. Lett.* **36** 580
[14] Dababneh M S, Kauppila W E, Downing J P, Lapierre F, Pol V, Smart J H and Stein T S 1980 *Phys. Rev.* A **22** 1872