Threshold effects in positron scattering on noble gases

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The energy dependence of the positronium (Ps) formation cross section for positrons colliding with all the stable inert atoms is analyzed near threshold. Using R-matrix and threshold theories, the corresponding variations with energy of the elastic-scattering and total cross sections are predicted and compared to experiment where possible. As the target atomic number increases from He to Xe, Wigner cusps are predicted to develop in the elastic cross section near the Ps formation threshold, reflecting the progressive increase of the interaction strength between the positron and the atoms.

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I. INTRODUCTION

Effects which have been attributed to coupling between various scattering channels have recently been observed in a number of studies with positron (e^+) scattering on atoms and molecules [1–3]. Despite earlier surmises [4,5], however, the cross sections for e^+ elastically scattered from He and H_2 do not manifest an anomalous energy dependence near the threshold for positronium (Ps) formation [6,7]. Anomalies of this type, often referred to as Wigner cusps [8], have been found to arise near thresholds for nonelastic processes in atomic and nuclear collisions [9,10], and are usually expected to occur if the nonelastic cross section starts at threshold with an infinite slope [11–14].

We show that threshold theory [11–16] can explain the negative findings in the case of He [6,7]. Furthermore, it predicts that a pronounced Wigner cusp should exist in the elastic-scattering cross section ($\sigma_{\rm el}$) of positrons on Xe. The theory requires knowledge of the partial-wave components of the Ps-formation cross section ($\sigma_{\rm Ps}$) near threshold, which we obtain from an R-matrix theory [8,11,16] fit to this cross section, using new measurements [17]. The theory also requires knowledge of positron pure elastic- (uncoupled) scattering phase shifts, computed without consideration of the nonelastic (Ps-formation) channel. We use calculations of McEachran and coworkers [18–20]. We first sketch the relevant theoretical information and then apply it to experiment.

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II. THEORETICAL CONSIDERATIONS

We consider the following simple collision:

$$e^+ + A \to e^+ + A \quad \text{(elastic channel)}\,,$$
$$\to \mathrm{Ps} + A^+ \quad \text{(nonelastic channel)}\,, \tag{1}$$

where A is a noble-gas atom in its ground state. Assuming the intrinsic spin of the positron does not play an important role in these processes, we can write angular momentum and parity conservation as

$$l = l' + l_{A^+}\,, \quad (-1)^l = (-1)^{l' + l_{A^+}}\,, \tag{2}$$

where l and l' are the incoming positron and outgoing positronium orbital angular momenta, and l_{A^+} is the orbital angular momentum of the captured electron. For He, $l_{A^+}=0$; for all the other noble gases, $l_{A^+}=1$ is dominant.

For later purposes, we note that for all the noble gases Ps formation is endothermic and the threshold energy $E_{\rm th}$ is related to the atomic ionization energy I by $E_{\rm th} = I - B_{\rm Ps}$, where $B_{\rm Ps} = 6.80$ eV is the Ps binding energy [21]. Also, the total cross section is given by $\sigma_{\rm tot} = \sigma_{\rm el}$ for $E < E_{\rm th}$ and $\sigma_{\rm tot} = \sigma_{\rm el} + \sigma_{\rm Ps}$ for $E_{\rm ex} > E \ge E_{\rm th}$, where E is the positron energy and $E_{\rm ex}$ is the first excitation energy of the target atom.

R-matrix theory predicts the energy dependence of the nonelastic cross section near threshold as follows [16]:

$$\sigma_{\rm Ps} \equiv \sum_l \sigma_{\rm Ps}^{(l)}$$
$$= \sum_{l,l'} (4\pi/k^2)(2l+1) P^{(l)}(ka) P^{(l')}(k'a) r^{(l,l')}\,, \tag{3}$$

where k is the incoming and k' the outgoing (c.m.) wave number [$E = \hbar^2 k^2/(2m_{e^+})$; $E - E_{\rm th} \equiv E' = \hbar^2 k'^2/(2m_{\rm Ps})$ is the outgong positronium energy]. The quantity a is a radius (which can be channel dependent [22]), characteristic of R-matrix theory, beyond which all wave functions assume their asymptotic behavior. The quantity $r^{(l,l')}$ is essentially the square of an R-matrix element, which depends on the coupling strength between the entering and nonelastic channels. In the present case, where both channels are without a pure $(1/r)$ Coulomb potential, the (barrier) penetration factors P have the form [22]

$$P^{(0)}(\rho)=\rho\ ,\quad P^{(1)}(\rho)=\rho^3/(1+\rho^2)\ , \tag{4}$$

where $\rho=ka$ or $k'a$. In general,

$$P^{(l)}(\rho)\propto\rho^{2l+1}\quad(\rho\ll1)\ , \tag{5}$$

$$=\rho\quad(\rho\gg1)\ . \tag{6}$$

These expressions ignore any polarization potentials, such as a $1/r^4$ term, in the asymptotic region.

The main energy dependence of $\sigma_{\rm Ps}$ near threshold is determined by the second penetration factor in Eq. (3), leading to

$$\sigma_{\rm Ps}^{(l)}\propto(E')^{l'+1/2}\ , \tag{7}$$

where the proportionality factor depends on l. In nuclear reactions, one needs to extend the sum in Eq. (3) only over the l value(s), which give $l'=0$ [11–13], but we show below that in the collisions (1) the $l'=1$ outgoing wave has to be included in some cases, even near threshold.

Having obtained the partial-wave components of $\sigma_{\rm Ps}$ by fitting Eq. (3) to experiment, threshold theory can be used to predict $\sigma_{\rm tot}$ and $\sigma_{\rm el}$ if also the partial-wave pure elastic-scattering phase shifts δ_l, neglecting the Ps-formation channel, for positron scattering on noble-gas atoms are known. In threshold theory, the cross sections of interest are decomposed as follows:

$$\sigma_{(\rm tot,el)}(E)=\sigma^0(E)+\Delta\sigma_{(\rm tot,el)}(E,|E|')\ , \tag{8}$$

where

$$\sigma^0(E)=\sum_l(4\pi/k^2)(2l+1)\sin^2\delta_l(E)\ , \tag{9}$$

is that part of the cross section which is uncoupled from the nonelastic channel and depends only on the positron energy E. Hence, it varies smoothly across the threshold. As shown below, the "threshold effects" $\Delta\sigma_{(\rm total,el)}$ depend mainly on the outgoing Ps energy E'. In Eq. (8), $\Delta\sigma$ is defined so that at threshold it is zero, from which it follows that $\sigma^0(E_{\rm th})$ is equal to the total (or elastic) cross section at threshold. From the definitions of $\Delta\sigma$ and $\sigma_{\rm tot}$, one sees that

$$\Delta\sigma_{\rm tot}=\Delta\sigma_{\rm el}+\sigma_{\rm Ps}\quad(E_{\rm ex}>E\geq E_{\rm th})\ , \tag{10}$$

whereas below threshold, $\Delta\sigma_{\rm tot}=\Delta\sigma_{\rm el}$.

The threshold effects are obtained from the unitarity of the scattering matrix and its analytic continuation across the threshold [11]. If the intrinsic spin of the positron does not play any role in the scattering processes, the expressions are [16]

$$\Delta\sigma_{\rm tot}=\sum_l\sigma_{\rm Ps}^{(l)}(|E'|)\begin{cases}\cos2\delta_l & (E>E_{\rm th})\\ (-1)^{(l'+1)}\sin2\delta_l & (E<E_{\rm th}),\end{cases} \tag{11}$$

$$\Delta\sigma_{\rm el}=\sum_l\sigma_{\rm Ps}^{(l)}(|E'|)\begin{cases}-1+\cos2\delta_l & (E>E_{\rm th})\\ (-1)^{(l'+1)}\sin2\delta_l & (E<E_{\rm th})\ .\end{cases} \tag{12}$$

In Refs. [11–14], it is assumed that the value of δ_l is to be taken at $E=E_{\rm th}$, but Ref. [16] shows that a more accurate approximation is obtained if δ_l is allowed to vary with E. From the derivation in Ref. [11] or footnote 16 in [15], it can be seen that the region of validity of the threshold expressions is limited by the requirement

$$\sigma_{\rm Ps}^{(l)}<(\pi/k^2)(2l+1)$$
$$\simeq[(2l+1)/(E\ \text{ in eV})]10^{-15}\ \text{cm}^2\ , \tag{13}$$

in which the right-hand side is the unitarity limit of the partial-wave cross section.

III. EXPERIMENTAL CONSIDERATIONS

Turning now to experiment, first we make a near-threshold partial-wave analysis of the $\sigma_{\rm Ps}$ data, which is required for the evaluation of Eqs. (11) and (12). Following Eq. (7), we plot $\log\sigma_{\rm Ps}$ versus $\log E'$ and try to determine the components with slopes $\frac{1}{2}$ $(l'=0)$, $\frac{3}{2}$ $(l'=1)$, etc. [23]. Figure 1 shows such a plot for all the noble-gas cross sections [17]. Using expressions (4) for the penetration factors, the data have been least-squares fitted to the partial-wave cross-section expressions $\sigma_{\rm Ps}^{(l)}(l'=0)$ or $\sigma_{\rm Ps}^{(l)}(l'=1)$ in Eq. (3). We assume (i) that only the $l'=0$ and 1 components need to be considered near threshold, and (ii) that a, $r^{(l,0)}$, and $r^{(l,1)}$ can be treated as adjustable, energy independent parameters [24].

Before proceeding with the fits, though, one has to determine from Eqs. (2) which l values are associated with $l'=0$ and 1, so that the proper $P^{(l)}$ values can be chosen in Eq. (3). One finds for He, $l=l'$, and for all the other noble gases, $l'=0\rightarrow l=1$, $l'=1\rightarrow l=0$ or 2. To minimize the number of fitting parameters, we assume in the latter case that near threshold the influence of the d-wave *cross-channel coupling parameter* $r^{(2,1)}$ can be neglected. We are aware that, in the relevant energy region, the d-wave *elastic-scattering* phase shift can be appreciable compared to the s- and p-wave phase shifts [18–20], but the phase shifts are not connected directly to the cross-channel coupling parameters. In R-matrix theory, the uncoupled elastic-scattering phase shifts depend on the squares of the reduced widths γ_λ for the entering channel, whereas the cross-coupling parameters depend on the products $\gamma_\lambda\gamma'_\lambda$ for the entering and emerging channels, which can be positive or negative. Here, λ is the R-matrix level index [22].

We see from Fig. 1(a) that within experimental error, $\sigma_{\rm Ps}$ for He can be fitted with a pure $l=1$, $l'=1$ partial wave. For the other noble gases, Ne and Xe can be fitted with pure $l=1$, $l'=0$ partial waves, but Kr, and possibly Ar, may need small $l=0$, $l'=1$ admixtures. The dominance of the $l=1$ entering partial wave for the near-threshold Ps formation, found here empirically, also

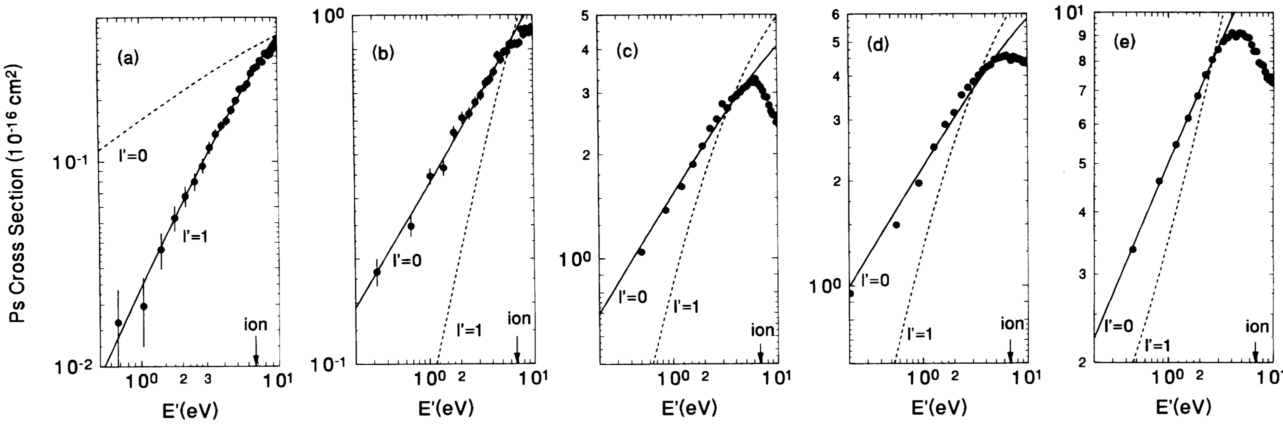

FIG. 1. Plots of σ_{Ps} as a function of the positron energy E' above threshold, (a) for He, (b) for Ne, (c) for Ar, (d) for Kr, and (e) for Xe. The ionization energy I is indicated by "ion," above which for Kr and Xe the measured cross section represents the Ps formation plus ionization cross sections. For He, Ne, and Ar, the ionization cross sections of H. Knudsen [J. Phys. B **23**, 3955 (1990)] were interpolated and subtracted. Relative errors are given. The absolute accuracy of the data is discussed in the text. Least-squares fits to the partial-wave cross sections, given in Eq. (3), are shown. The dashed curves are normalized arbitrarily.

occurs in calculations for a H target [25]. This is one of the interesting results, as yet not explained, which arises from the present analysis.

Proceeding now to the evaluation of Eq. (8), it is fortunte that McEachran and co-workers have calculated σ^0, as well as δ_l up to $l=6$, for all the noble gases. For the evaluation of Eqs. (11) and (12), we use the values of $\sigma_{\mathrm{Ps}}^{(0)}$ and $\sigma_{\mathrm{Ps}}^{(1)}$ obtained from the fits shown in Fig. 1 and the δ_0 and δ_1 values from Refs. [18–20]. The resultant predicted curves for $\sigma_{\mathrm{tot,el}}$ are shown in Fig. 2, as well as available data [6,26–31] (for clarity, some data for σ_{tot} listed in Ref. [32] has been omited).

Before we compare theory and experiment, a comment on the precision of the data is in order. The cross section σ_{Ps} is determined from the ion yield and needs normalization to other work in order to obtain absolute values [17]. For He and Ar, normalized to the cross sections of Ref. [33], we believe, our absolute values are accurate to $\pm 20\%$. For the normalization of the Ne, Kr, and Xe data, we found only preliminary measurements by Diana and co-workers [34–36]; we assign to our absolute values uncertainties between ± 30 and 50%. These experimental uncertainties are reflected directly as uncertainties in the $\Delta\sigma$ predictions. Uncertainties in the σ_{tot} measurements are discussed in detail in Ref. [32]; globally speaking, they lie between ± 5 and 20%, with the He measurements

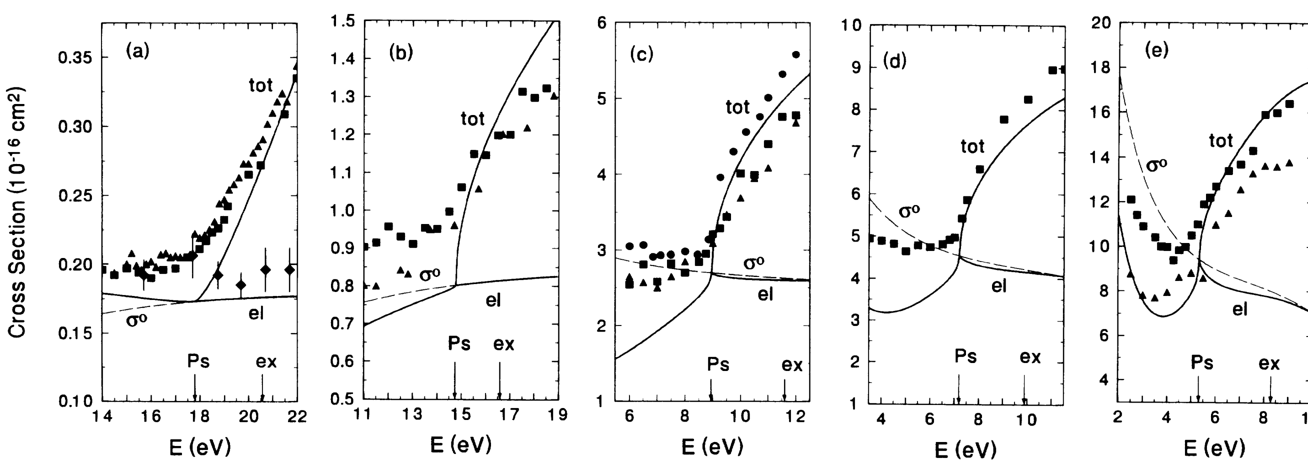

FIG. 2. Total (tot) and elastic (el) scattering cross sections for $e^+ +$(noble-gas atom) collisions near the Ps-formation threshold (Ps), as a function of the positron energy E. The first excitation potential of the noble-gas atom is indicated by "ex," beyond which the theoretical expressions begin to lose their validity. Data points for σ_{tot} are as follows. (a) He: Refs. [29] (squares) and [30] (triangles); (b) Ne: Refs. [27] (triangles) and [29] (squares); (c) Ar: Refs. [26] (squares), [27] (triangles), and [28] circles; (d) Kr: Ref. [31] (squares); (e) Xe: Refs. [27] (triangles) and [31] (squares). The accuracy of the data is discussed in Ref. [32] (see text). For He, the σ_{el} data are from Ref. [6] (diamonds). The broken curves are σ^0 from Refs. [18–20]. The solid curves give the predictions for σ_{tot} and σ_{el}. Below threshold, $\sigma_{\mathrm{tot}}=\sigma_{\mathrm{el}}$.

the most precise and with decreasing accuracy as Z increases. In the Ps-production measurements, the positron energy scale could be calibrated to approximately ± 0.1 eV by linearizing, as far as possible, a plot of the ion yield $N(E)$ as a function of E for each target. For He, this could be achieved by plotting $N^{2/3}$ versus E; for the other targets, N^2 versus E. [These powers of N are suggested by Eq. (7).] The intercept on the abscissa was set equal to E_{th}.

IV. RESULTS AND DISCUSSION

The energy region over which a comparison between theory and experiment in Fig. 2 is valid is subject to two restrictions: (i) condition (13) must be fulfilled; and (ii) excitation, either of the atom A, the ion A^+, or of the Ps atom, is not included in the theoretical expressions, so that E must not exceed the lowest of these excitation energies E_{ex}, the first excitation potential of atom A. Both of these restrictions limit a comparison between theory and experiment to a few eV around threshold.

Looking now at Fig. 2, one sees that, overall, threshold theory predicts the rapid rise found in σ_{tot} above threshold; Eq. (11) relates this effect to the small values of the relevant pure elastic-scattering phase shifts δ_l. In physical terms, the sharp cross-section rise reflects the fact that the weakness of the positron interaction with noble-gas atoms, due to the repulsion by the nucleus that is opposed by the attraction of the electron cloud, also weakens the coupling between the incident elastic and the nonelastic channels. For He, the interaction is weakest and the δ_l are the smallest, resulting not only in a relatively steep rise in σ_{tot} above threshold, but also in the near absence of any cusp feature in σ_{el} [Eq. (12)]. Indeed, one does not expect here a cusp anomaly because of the absence, within experimental errors, of the $l'=0$ outgoing wave indicated in Fig. 1(a) [12,13]. This predicted absence of a threshold cusp in the elastic scattering on He agrees with experiment [6]. As Z increases, the relevant phase shifts increase [19,20] because of the increasing strength of the interaction between a positron and a noble-gas atom, and a Wigner cusp develops; our calculations predict it to be most prominent in Xe. In fact, in this case the theory agrees well with the rounded shape of the below-threshold part of the cross section.

Below threshold, $\Delta\sigma_{\mathrm{tot}}$ is proportional to $\sin 2\delta_l$; above to $\cos 2\delta_l$ [Eq. (11)]. Hence, for small δ_l the below-threshold effect is more sensitive to the calculated values of δ_l. The below-threshold discrepancies apparent in Figs. 2(c) and 2(d) could be due to errors in the (small) calculated phase shifts δ_0, although these discrepancies are reduced considerably if the $l'=1$ components of σ_{Ps} are taken into account in the analysis, in addition to the $l'=0$ components. Also, we recall that the magnitude of the discrepancies is directly affected by any relative calibration error between the measured σ_{Ps} and σ_{tot} values and that six phase shifts contribute to σ^0. Hence an error in one of them, such as δ_1, would not necessarily determine the sign of any possible error in σ^0.

As noted in the discussion of Eq. (8), in principle, σ^0 should be exactly equal to the (measured) cross section at threshold. In fact, one sees from Fig. 2 that there are discrepancies between theory and experiment of the order of 10%, which is not unexpected. If these discrepancies could be removed, agreement between the predictions and the measurements would be improved. In view of the above uncertainties, the degree of agreement between the theoretical predictions and the measured cross sections, apparent in Fig. 2, is satisfactory.

One can contrast the interaction of positrons with noble gases with that occuring with alkali atoms. Here, $I < B_{\mathrm{Ps}}$, making the nonelastic channel exothermic ($E_{\mathrm{th}}=0$). The main low-energy dependence of σ_{Ps} then results from the first penetration factor in Eq. (3), leading to the relation $\sigma_{\mathrm{Ps}} \propto E^{l-1/2}$ [12,13]. At low energies, one expects $l=0$ to dominate because s-valence electrons are captured. One should then obtain a $1/v$ law for σ_{Ps} (v = positron velocity), but so far the experiments may not have been taken to a low enough energy to see this effect [37]. The $1/v$ law is well known for the nuclear capture of slow neutrons and for the annihilation of positrons, both of which also are exothermic reactions.

V. CONCLUSIONS

In conclusion, the energy dependence of the positronium-formation cross section for positrons colliding with all the stable inert-gas atoms has been analyzed near threshold. This dependence, in conjunction with R-matrix and threshold theories, has been used to explain the absence of a threshold cusp anomaly in the elastic scattering on He, but predicts progressively more pronounced Wigner cusps for the heavier inert atoms, reflecting the increasing strength of the interaction between the positron and the atoms. Experimental tests are in progress [38]. We have also found the interesting fact, as yet not understood, that near-threshold production of Ps in our targets occurs predominantly with entering p-wave positrons.

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