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Heating due to momentum transfer in low-energy positronium-antiproton scattering

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We investigate the consequences of unexpectedly large elastic cross sections for the scattering of low energy antiprotons from $n \leq 3$ positronium (Ps) on the experimental implementation of antihydrogen formation via Ps-antiproton collisions. The integrated elastic cross sections, obtained using the two-center convergent close-coupling theory, can be up to three orders of magnitude greater than their counterparts for antihydrogen formation. The differential momentum transfer cross sections, which suppress the large cross sections at forward scattering angles, show remarkably rich behavior across all scattering angles. We discuss the implications of these findings for the heating, via momentum transfer, of clouds of trapped antiprotons that are typically used for the creation of antihydrogen.

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Positronium, the two-body bound state of an electron (e^-) and a positron (e^+) , continues to be of interest more than six decades after its discovery [\[1](#page-4-0)]. Current work includes studies of its collision physics (see e.g., [\[2](#page-4-1)[–6\]](#page-4-2)) and the production of excited, including Rydberg, states [\[7](#page-4-3)[–13\]](#page-4-4). The latter will find use as a probe of antimatter gravity $[14–16]$ $[14–16]$ and in the production of antihydrogen, H, via charge exchange with an antiproton (\bar{p}) [\[17](#page-4-7)[–21\]](#page-4-8).

In this respect, it is only recently that accurate cross sections for important collision processes involving excited state Ps, which require the two-centre convergent close-coupling (CCC) method [\[22](#page-5-0), [23\]](#page-5-1), have been obtained. Kadyrov et al. [\[24\]](#page-5-2) and Rawlins et al. [\[25](#page-5-3)] presented data for $\bar{H}(n'l')$, formation with $n' \leq 4$ upon $Ps(nl)+\bar{p}$ scattering with $n \leq 3$. Fabrikant *et al.* [\[26](#page-5-4)] analysed the threshold behavior in each partial wave L, and addressed issues associated with the degeneracy of the energy levels. This theoretical work was motivated by recent experimental progress. In particular, the AEgIS collaboration [\[21,](#page-4-8) [27\]](#page-5-5) plan to excite Ps atoms to highlying states to use the charge transfer reaction to pro-duce, by Stark acceleration [\[28](#page-5-6), [29](#page-5-7)], a beam of \overline{H} atoms. This will be used for studies of the gravitational interaction of antimatter using a moiré deflectometry method. It is also foreseen that an antihydrogen beam will be used to measure the ground state hyperfine splitting of the antiatom [\[30\]](#page-5-8), and although the ASACUSA group attempting this is currently applying trapped e^{\pm} - \bar{p} interactions to form antihydrogen [\[31](#page-5-9)[–34\]](#page-5-10), in principle there is no reason why this could not be replaced by a beam from the Ps- \bar{p} reaction. Such a beam is to be employed by the GBAR group [\[20,](#page-4-9) [35](#page-5-11)] in an antimatter gravity experiment in which the nascent \overline{H} collides with the same Ps target where it was produced to form an antihydrogen positive ion. This is then caught, cooled and photoionized to allow the remnant ultra-cold H to fall in the Earth's gravitational field [\[36\]](#page-5-12). It is also possible to envisage using Ps to create \bar{H} in an ion trap environment

[\[19,](#page-4-10) [25,](#page-5-3) [37](#page-5-13), [38](#page-5-14)] to promote capture of the antiatom in a magnetic minimum neutral atom trap [\[39](#page-5-15)[–42\]](#page-5-16). Thus, understanding the low-energy behavior of $Ps-\bar{p}$ scattering cross sections is of considerable current experimental and theoretical interest.

Key to further progress is to understand energy transfer to trapped antiprotons used to create antihydrogen via collisions with Ps, irrespective of whether the antiatom is to be formed into a beam or to be held in a magnetic minimum trap, as it has a major, and possibly limiting, influence on the experimental outcome. In particular, this will arise via the angular divergence of a beam, or the temperature of a trapped ensemble. To be able to fully assess the influence of Ps interactions, accurate partial and differential scattering cross sections (DCS) are needed for several processes. In this work we address the behavior of the elastic scattering and statechanging processes,

$$
Ps(n_i, l_i) + \bar{p} \to Ps(n_f, l_f) + \bar{p}, \tag{1}
$$

alongside the charge-transfer reaction of antihydrogen formation. Again, the n and l refer to the Ps principal and orbital angular momentum quantum numbers, and i and f denote the initial and final states respectively. For $i = f$ we have elastic scattering, and due to the degeneracy of the Ps energy levels, whenever $n_f = n_i$ with $l_f \neq l_i$ it is referred to as quasi-elastic scattering. The integrated cross section of the latter is infinite (assuming degeneracy of the l-states) due to the behavior of the partial cross section contributions, which go as $1/L$ [\[26](#page-5-4)]. In terms of the DCS this means that they are extremely forward peaked so that their integral over the scattering angle θ (with the inclusion of $\sin \theta$) does not exist. In reality, however, (hyper)fine structure splitting and the Lamb shift ensure that there is no pure degeneracy and so the quasi-elastic cross sections are finite [\[26](#page-5-4)], but are particularly large and highly forwardpeaked. The CCC calculations of Rawlins et al. [\[25](#page-5-3)] con-

FIG. 1. Integrated cross sections for elastic, momentum transfer (MTCS), and H formation (in all states) for $Ps(n, l)$ -p scattering calculated using the CCC theory, see text. Note, the same results apply to the charge-conjugated reactions.

centrated only on the charge-exchange transitions, which are rapidly convergent with increasing L. By contrast, the elastic-scattering results of interest here have been obtained by extending those calculations to $L \leq 80$. The large L are necessary due to the large dipole polarizability of Ps.

Results of the CCC theory for $Ps(n, l)$ - \bar{p} cross sections for integrated elastic scattering, σ_{el} , momentum transfer $\sigma_{\rm mt}$, and charge transfer ($\sigma_{\bar{H}}$ to all final states) are shown in figure [1](#page-2-0) for Ps kinetic energies E ranging from 10^{-5} eV to 10 eV. There are a number of notable features: (i) σ_{el} dominates its charge-transfer counterpart in all cases, typically by 2-3 orders of magnitude, though (ii) for the excited states, this enhancement is lower for the $n = 3$ levels. (iii) The threshold behavior, discussed in detail by Fabrikant *et al.* [\[26\]](#page-5-4), is $1/E$ for all cases except for $\text{Ps}(1s)$, where it is $1/\sqrt{E}$ for the (anti)H-formation cross section, and constant for the elastic cross section due to the dominant $L = 0$ partial wave. This is also the reason

FIG. 2. Elastic $Ps(n, l)$ -p differential cross sections at 25 meV calculated using the CCC theory, see text.

that (iv) $\sigma_{\rm mt}$ tends to $\sigma_{\rm el}$ for Ps(1s), though otherwise it is much lower, an effect that seems to diminish with increasing l for $n = 3$. Finally, though not shown here, the cross sections for reaction [1](#page-1-0) involving changes of n are found to be several orders of magnitude lower than those presented. Accordingly, we neglect these processes in the discussion below.

The remarkably large magnitude of the elastic cross sections at low energies means that, though energy exchange in Ps- \bar{p} interactions is small due to the low Ps mass, it may be sufficient to cause heating of the trapped antiparticles, and that deflection of the Ps (which could lead to a reduced overlap with the collision target) may take place before a charge transfer reaction occurs. Thus, consideration must be given to the relevant DCS, $d\sigma_{el}/d\Omega$. From an experimental perspective the key Ps kinetic-energy range is currently 10-100 meV, as suitable vacuum compatible sources are routinely available (see e.g., [\[43\]](#page-5-17)). Thus, we select DCS data for presentation in figure [2](#page-2-1) for the single value of $E = 25$ meV for each of the 6 Ps states $(1s, 2s, 2p, 3s, 3p \text{ and } 3d)$.

The elastic DCS for the Ps excited states are all very strongly forward-peaked, a feature which is shared across the 10-100 meV range, and with the outcome being dominated by scattering through angles below 10◦ in most cases. This is an important finding, as it implies that the colliding Ps will be essentially undeflected on its passage through the \bar{p} cloud. The angular distributions broaden somewhat as l increases at fixed n , and are more narrowly forward-peaked at fixed l for $n = 3$ when compared to $n = 2$. The origin of the large magnitudes and the forward-peaking is the contribution of the large- L partial waves, where dipole coupling between degenerate states diminishes slowly with increasing L. Furthermore, the excited-state DCS exhibit remarkable oscillatory features, which originate from the low partial waves. Note that the oscillations in energy reported by Fabrikant et al. [\[26\]](#page-5-4) should not be confused with the structures presented here. The latter arise at a single energy from the out-of-phase oscillations in the low partial waves. When summed over all $L \leq 80$ partial waves smooth integrated cross sections are obtained as a function of energy, as presented in Fig. [1.](#page-2-0) The behavior presented in Fig. [2](#page-2-1) is representative of all of the energies given in Fig. [1.](#page-2-0)

To assess the influence of elastic scattering on collisional energy transfer, we consider an angularaveraged (Ps) energy loss $\langle \Delta E \rangle = \langle P(\theta) \Delta E(\theta) \rangle =$ $(8\pi E m_e/M\sigma_{\rm el})\langle\sin\theta(1 - \cos\theta)(d\sigma_{\rm el}/d\Omega)\rangle$, with the probability of elastic scattering at an angle θ as $P(\theta) = 2\pi \sin \theta (d\sigma_{\rm el}/d\Omega)/\sigma_{\rm el}$ and with $\Delta E(\theta)/E =$ $(4m_e/M)(1-\cos\theta)$, where m_e and M are the electron and proton masses respectively. These standard relations [\[44\]](#page-5-18) show that $\langle \Delta E \rangle = 4E m_e \sigma_{\rm mt}/M \sigma_{\rm el}$, though the analysis reveals that the angular factor $\sin \theta (1 - \cos \theta)$ has a profound modulating influence on the scattering angles at which energy transfer occurs, as illustrated in fig-ure [3.](#page-3-0) Whilst the data for $Ps(1s)$ display a single broad maximum near the angle (120°) at which $\sin \theta (1 - \cos \theta)$ is peaked, the distributions for the excited states exhibit features derived from the oscillatory structures in $d\sigma_{el}/d\Omega$. It is notable that $\sin \theta (1 - \cos \theta) \sim \theta^3$ at small θ , an effect which dramatically suppresses the influence of the small-angle scattering such that the Ps energy loss is governed by the DCS across the full angular range, and is concentrated in peaks.

To gauge possible experimental impact, we consider a scenario in which low-energy Ps emanating from an appropriate source crosses a cloud of trapped antiprotons (which for simplicity is taken to be stationary) of total number $N_{\bar{p}}$ at a density $\rho_{\bar{p}}$ and characterised by a length dimension d. We assume that the Ps atoms are in a single (n, l) state, produced for instance by laser excitation from the ground state, though this can easily be relaxed if appropriate. The total number of elastic collisions involving N_{Ps} Ps atoms crossing the antiproton cloud is $N_{\text{Ps}}\rho_{\bar{p}}\sigma_{\text{el}}d$, such that the average temperature increase per antiproton is

$$
\langle \Delta T_{\bar{p}} \rangle = \frac{\langle \Delta E \rangle}{N_{\bar{p}} k_B} N_{\rm Ps} \rho_{\bar{p}} \sigma_{\rm el} d = \frac{4 m_e E}{M k_B} \frac{N_{\rm Ps}}{N_{\bar{p}}} \rho_{\bar{p}} \sigma_{\rm mt} d,\tag{2}
$$

FIG. 3. Elastic $Ps(n, l)$ -p differential cross sections of Fig. [2](#page-2-1) multiplied by the factor $\sin \theta (1 - \cos \theta)$.

with k_B being Boltzmann's constant. By noting that the number of H formation collisions is $N_{\overline{H}} = N_{\text{Ps}} \rho_{\overline{p}} \sigma_{\overline{H}} d$ we find that

$$
\langle \Delta T_{\bar{p}} \rangle = \frac{4m_e E}{M k_B} \frac{N_{\bar{\mathcal{H}}}}{N_{\bar{p}}} \frac{\sigma_{\text{mt}}}{\sigma_{\bar{\mathcal{H}}}}.
$$
(3)

Inserting values results in

$$
\langle \Delta T_{\bar{p}} \rangle \approx 25 E \frac{N_{\bar{\mathcal{H}}}}{N_{\bar{p}}} \frac{\sigma_{\text{mt}}}{\sigma_{\bar{\mathcal{H}}}},\tag{4}
$$

in units of mK, where E is in units of meV.

In studies of charge-transfer reactions involving Ps, we assume that $N_{\bar{H}}/N_{\bar{p}}$ is optimised to be of order unity by appropriate choice of Ps state. Thus, aside from kinematic factors, $\langle \Delta T_{\bar{p}} \rangle$ is governed by the behaviour of $\sigma_{\rm mt}/\sigma_{\rm H}$. This quantity can be derived from our work, and tends to a constant at low energies for $n > 1$, with approximate values of 15 (for 2s), 50 $(2p)$, 1.4 $(3s)$ 3 $(3p)$ and 7 $(3d)$. As such, with Ps kinetic energies of the order of 10's of meV, it is clear that \bar{p} temperature increases of the order of 100's of mK may ensue. Whilst

we cannot presently calculate accurate cross sections for states with $n > 3$, which are those likely to be involved in experiments, our work suggests that a minimum temperature gain of $25E$ (meV) mK should be conservatively assumed when analysing the possible outcomes of antihydrogen formation using the $Ps-\bar{p}$ system (see below). Thus, temperature gains may be of a similar order to the depths of the neutral atom traps used for H capture [\[39](#page-5-15)– [42\]](#page-5-16). Furthermore, in the AEgIS experiment it is thought that in order to provide a sufficiently well-defined \bar{H} beam for their measurement of antimatter gravity, a cloud of antiprotons at a temperature equivalent of 100 mK is required [\[27\]](#page-5-5). Our work shows that this may be challenging due to Ps collisional heating. It is also worth noting that whatever laser excitation scheme is used to promote efficient charge transfer, a significant fraction (typically 70%) of the Ps crossing the ion cloud will remain in the 1s state. It is straightforward to show using the cross section data in figure [1](#page-2-0) that the momentum transfer imparted from $Ps(1s)$ collisions is negligible in comparison to that from the excited states.

Our findings imply that elastic collisions may be a source of significant temperature rise of a trapped antiproton cloud, which will be cumulative throughout an experiment if there is no active means of cooling. Thus, collision cross sections should be carefully manipulated via appropriate choice of Ps state to minimise this effect. Another implication of our discovery that $\sigma_{el} \gg \sigma_{\bar{H}}$ is that the quasi-elastic (i.e., the l-changing processes from reaction [1\)](#page-1-0) cross sections are likely to be enhanced by at least the same factor. For instance, at around 25 meV the $Ps(2s)$ - $Ps(2p)$ cross section is expected to be an order of magnitude higher than either of the σ_{el} for $n = 2$ [\[26\]](#page-5-4).

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Thus, (i) the potential importance of l-changing processes mean that estimates of heating due to momentum transfer using the current values of σ_{el} should be viewed as the minimum of what will occur in practise and (ii) that an initial Ps ensemble involving a single excited state is liable to be collisionally mixed across the relevant lmanifold before an \bar{H} -formation event. Whilst this will have only a minor effect on the overall H-formation rate, it will alter the distribution of states produced, and the resultant decay pathway to the ground state.

In conclusion, we have presented accurate data for $Ps(n)$ - \bar{p} elastic scattering for $n \leq 3$ that have revealed very large integrated cross sections, with some orders of magnitude greater than for antihydrogen formation. The experimental implications of this have been explored, and we find that antiproton temperature rises of several hundred mK are possible. Thus, the heating by momentum transfer of antiproton clouds used for antihydrogen formation via the Ps- \bar{p} system must be taken into account. Our work has also highlighted an urgent need for theoretical guidance for $Ps(n)$ - \bar{p} scattering for $n > 3$.

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