Antihydrogen Formation via Antiproton Scattering with Excited Positronium

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Utilizing the two-center convergent close-coupling method, we find a several order of magnitude enhancement in the formation of antihydrogen via antiproton scattering with positronium in an excited state over the ground state. The effect is greatest at the lowest energies considered, which encompass those achievable in experiment. This suggests a practical approach to creating neutral antimatter for testing its interaction with gravity and for spectroscopic measurements.

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For more than a decade, antihydrogen ($\bar{\mathrm{H}}$) atoms have been created in dedicated experiments (see, e.g., [1–3]) performed at the CERN Antiproton Decelerator facility [4,5]. Most of this work has entailed careful mixing of cold positrons (e^+) and antiprotons ($\bar{p}$) in purpose-built charged particle traps in which the antiatoms have been formed predominantly in loosely bound states via the three-body reaction $\bar{p} + e^+ + e^+ \to \bar{\mathrm{H}} + e^+$. It has also recently been demonstrated that some of the $\bar{\mathrm{H}}$ created in this manner is cold enough to be confined in sub-Kelvin deep magnetic minimum neutral atom traps for periods of up 2×10^3 s [6–9], an achievement that has allowed the first experiments on the properties of the antiatom to be conducted [10–12].

It has long been appreciated (see, e.g., [13–17], and references therein) that interactions of antiprotons with positronium (Ps, the $e^+ - e^-$ bound state) atoms can lead to antihydrogen formation via the reaction

$$\bar{p} + \mathrm{Ps} \to \bar{\mathrm{H}} + e^-. \tag{1}$$

There has been a resurgence of interest in this mechanism of late, and two experiments intend its use to facilitate investigations of the gravitational properties of $\bar{\mathrm{H}}$. The AEgIS Collaboration [18,19] plans to produce a beam of Rydberg $\bar{\mathrm{H}}$ atoms via reaction (1) (using excited Ps as a target), and the very small recoil energies imparted to the antiatom [15] are vital in providing beam fidelity for their proposed interferometric studies. Another route to tests of the weak equivalence principle for antimatter, originally proposed by Walz and Hänsch [20] and adopted by the GBAR group [21–23], involves using $\bar{\mathrm{H}}$ created by reaction (1) to form the antihydrogen positive ion (by collision with another Ps atom), which is then caught and cooled, before the positron is photoionized to leave the remnant ultracold $\bar{\mathrm{H}}$ in free fall in Earth's gravitational field.

Other antihydrogen groups also have the possibility to produce Ps atoms in the vicinity of trapped antiproton clouds, since most materials (and, in particular, here the metallic surfaces of the electrodes used to confine the antiprotons and positrons) will emit Ps atoms into vacuum when bombarded with low energy e^+ (see [24] for a review). Thus, the consideration of reaction (1) as a viable route to $\bar{\mathrm{H}}$ formation is both pertinent and timely. We note that the ATRAP Collaboration has already performed a proof-of-principle demonstration of $\bar{\mathrm{H}}$ formation using excited Ps [25] via a laser-controlled double charge exchange mechanism [26] involving first exciting Cs atoms, which on interaction with a cloud of cold e^+ produced the Ps which underwent reaction (1).

All the aforementioned experiments pose significant technical challenges, and the ability to make detailed computations and simulations of expected signal levels is crucial. Underpinning such analyses is a confidence in detailed cross sections, both integral and state selective, for reaction (1). However, in this respect, the only direct experimental evidence available is a few total transfer cross sections for the charge conjugate (proton-Ps) case [27] and the limited information that can be derived from the charge conjugate and time-reversed reaction, namely, Ps formation in e^+-H collisions (see, e.g., [28], Chap. 4). Further experimental progress in this area is unlikely in the near future. Thus, only theory can provide the level of detail required to guide the antihydrogen programs, in particular, for Ps in different principal quantum (n) states. It is this that has motivated our study in which we present the required cross sections for reaction (1), where the initial Ps may be in a $n \leq 3$ state.

In order to provide the necessary guidance to experiment, theory must be accurate to within a few percent over the entire energy range of interest. The problem under consideration is particularly challenging due to its two-center (Ps and atom) nature, with the rearrangement channel (charge transfer) being the one of explicit interest; see Surko, Gribakin, and Buckman [29] for a review of the field. Reaction (1) is equivalent to proton scattering on Ps resulting in atomic hydrogen formation. In turn, this is, as

mentioned above, the time-reversed case of positron scattering on atomic hydrogen resulting in Ps(n) formation, with the cross sections required at positron energies just above the thresholds.

This difficult task is able to be addressed by using the two-center convergent close-coupling (CCC) method [30]. For the problem of interest, it is without approximation [other than the center of mass is at the (anti)proton] but requires a careful study of convergence of the cross sections with variation in the near-complete expansions of the H and Ps states. An example of such a study has been given by Kadyrov *et al.* [31] in the case of the positron energy just above the Ps($1s$) threshold. There, a relatively small near-complete two-center Laguerre-based expansion yielded accurate results down to 10^{-5} eV above this threshold and showed that the Wigner threshold law [32] is strictly valid only at threshold. This is an important validation of the computational method, which is sometimes not satisfied [33]. Here we wish to extend this to $n \leq 3$ states, and so small Laguerre-based expansions are not possible, since the same expansions need to yield not only accurate $n \leq 3$ states but also have a sufficiently increased number of higher excited states and a discretization of the continuum necessary for convergence at the higher energies considered.

The details of the two-center CCC calculations for positron scattering on atoms have been given by Ref. [30]. The approach builds on the work of Mitroy [17,34,35]. Briefly, the total wave function is expanded in both the atomic and positronium target states with the resulting close-coupling equations solved in momentum space as coupled Lippmann-Schwinger equations. Convergence needs to be checked by variation of the number of atomic states N_{H} and positronium states N_{Ps} used in the expansions. The total number of states for each center is obtained from $\sum_{l=0}^{l_{\max}} N_l$, where l is the orbital angular momentum and N_l is the Laguerre basis size. In addition, there is the choice of the Laguerre exponential parameter λ_l. This results in a large number of parameters to check the convergence. However, since the Laguerre basis is complete, we can organize convergence studies in the following way. We begin by setting $\lambda_l^{(\mathrm{H})} = \lambda^{(\mathrm{H})} = 1$ and $\lambda_l^{(\mathrm{Ps})} = \lambda^{(\mathrm{Ps})} = 0.5$. These values are optimized for the corresponding $n = 2$ states, which allow for minimal N_l to also obtain accurately the $n = 1$ and $n = 3$ states. Furthermore, we set $l_{\max}^{(\mathrm{H})} = l_{\max}^{(\mathrm{Ps})} = 3$, which has been checked to be sufficiently large for the cross sections of interest. Last, we set $N_l = N_0 - l$ for both centers and set $N_0^{(\mathrm{H})} = N_0^{(\mathrm{Ps})} \equiv N_0$, leaving us with just this one parameter to vary. The completeness of the Laguerre basis ensures that as we increase N_0 the completeness is systematically approached for both centers. Taking N_0 arbitrarily high is not possible due to the ill conditioning associated with the use of two nonorthogonal expansions. This has been studied in some detail previously [36], and convergence may be able to be obtained prior to the onset of numerical instabilities. Internal consistency of the CCC approach may also be studied by varying the way each center is treated; see Bailey, Kadyrov, and Bray [37] for an example.

We performed a series of calculations for $N_0 = 4, 5, \ldots, 10$, with the $N_0 = 10$ being those presented in Fig. 1 converged to within $\pm 5\%$ at most energies. Such

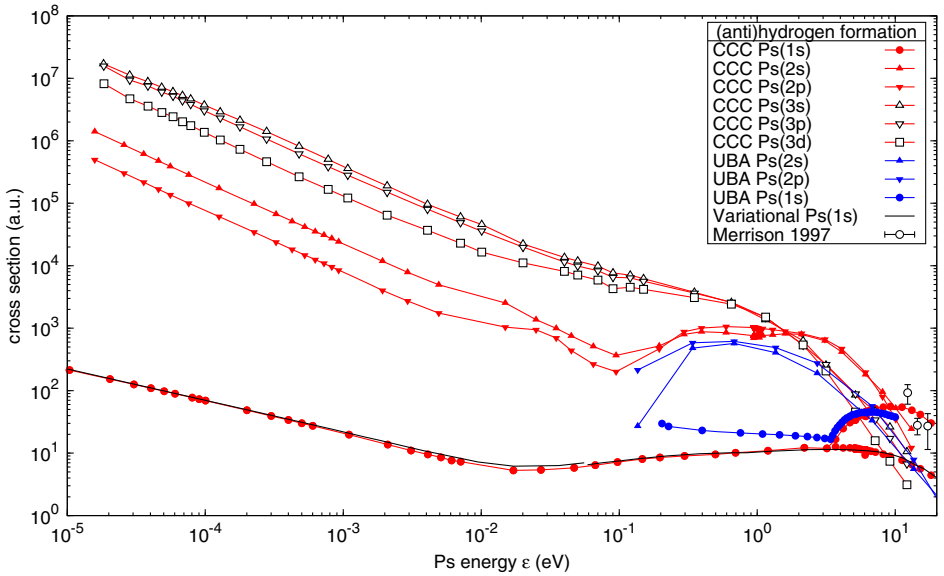

FIG. 1 (color online). Total cross sections for positronium atoms, in the specified initial state nl, scattering on (anti)protons to form (anti)hydrogen calculated by using the CCC method; see the text. For Ps($1s$), the variational calculations [13,38,39] are for (anti) hydrogen formation in the $1s$ state only (CCC-calculated unconnected points presented for comparison), while the UBA calculations of Mitroy [17] and Mitroy and Stelbovics [16], and the CCC calculations generally, are for (anti)hydrogen formation in all open states. The three experimental points are due to Merrison *et al.* [27].

calculations have a total of 68 states, 34 for each center. The cross sections are obtained for Ps(nl) transitions to all open H($n'l'$) states. This creates very many transitions, particularly at the higher energies. To make the presentation more manageable, we sum the (anti)atom-formation cross sections and present them for the Ps(nl) initial states, as shown in Fig. 1.

Beginning with the lowest energies presented, we see several orders of magnitude cross section increase in going from Ps($1s$) to Ps($n = 2$) initial states. A further order of magnitude increase is obtained by starting with Ps($n = 3$). This indicates that antihydrogen creation via interaction of Ps in excited states with relatively slow antiprotons is a very practical proposition, as we discuss below.

Within the $n = 2$ and $n = 3$ Ps states, we see the individual l components are of a commensurate magnitude, with a systematic reduction in the cross section at the lower energies with increasing l. The interplay of the formation of a specific (anti)hydrogen state is quite complex and energy dependent as various thresholds open up. Just at the Ps($n = 3$) threshold, there are six ($1s$, $2s$, $2p$, $3s$, $3p$, $3d$) final atomic states open, all contributing to the presented curves. The structures observed at the higher energies are a reflection of the opening of higher excited (anti)hydrogen states. A detailed presentation will be given elsewhere.

Here we wish to address the origin of the massive enhancement of the cross sections at low energies with increasing n of the Ps initial state. It is due not only to the size increase of excited Ps, but also to the formation of atomic states in preferentially excited levels. Numerically, this manifests itself in a somewhat unexpected way. At the lowest energies considered for the Ps($1s$) case, only the zeroth partial wave contributes to the atomic formation in the $n = 1$ state. However, for Ps($n = 2$) the first five partial waves are significant, with the dominant formation of the atom also having $n = 2$. Having five partial waves contribute at an energy of around 10^{-5} eV is rather unusual and is due to the degeneracy of the $n = 2$ energy levels in both the Ps and the atom. This degeneracy leads to long-range coupling (the polarizability behaves as r^{-2} rather than r^{-4}) and even infinite (nonrelativistic) cross sections involving the degenerate states. The energy degeneracy also affects the threshold behavior, as studied in detail by Fabrikant [40]. When we multiply the Ps($n > 1$) cross sections in Fig. 1 by the Ps energy ε, the result tends to a constant. This is in contrast to the Ps($1s$) cross sections, which behave as $1/\sqrt{\varepsilon}$, as was also determined previously [31]. The $1/\varepsilon$ threshold behavior for the excited states considerably enhances the cross section relative to the ground state.

In the figure, we also give comparison with some previous calculations and the only available experiment of Merrison *et al.* [27]. For Ps($1s$) the variational calculations of Humberston *et al.* [13] have been superseded by those of Humberston *et al.* [38], though the latter have not previously been published but kindly provided to us [39]. They only include atomic formation in the $1s$ state. The agreement with the CCC results is excellent across the 6 orders of magnitude energy variation. Above 4 eV, the full CCC results include (anti)hydrogen formation in excited states, as do the unitarized Born approximation (UBA) results of Mitroy [17], which are necessary to yield agreement with experiment. The CCC results for just the ground state (unconnected points) remain in excellent agreement with those of Humberston *et al.* [13]. We have also checked to have good agreement with the partial wave contributions given by Kuang and Gien [41]. Given that the close-coupling method is unitary and yields cross sections for all open transitions simultaneously, such a comparison just for Ps($1s$) gives us great confidence in all of the presented CCC-calculated cross sections.

There are few calculations involving Ps($n > 1$) as projectiles, and none as far as we are aware extend to low energies of interest here. Mitroy and Stelbovics [16] and Mitroy [17] performed a large number of UBA calculations involving Ps($n \leq 4$) initial states to within 0.1 eV of threshold. Such approximations are high energy approximations and so are unable to yield accurate results. Nevertheless, we see some qualitative agreement with the CCC calculations, in particular, the rise of the Ps($n = 2$) cross section past 0.1 eV, which is due to the opening up of the $n = 3$ atomic states.

On the experimental front, there has been much recent progress in the development of efficient, low energy (typically $\lesssim$100 meV; see, e.g., [42]), and pulsed Ps sources. This has led to the creation of dense samples [43,44], the observation and excitation of molecular Ps [45,46], and experiments involving laser excitation to a variety of Ps states [47,48]. Furthermore, the aforementioned AEgIS and GBAR antihydrogen collaborations have advanced plans to use excited state Ps reactions involving states in the $n = 2$ and $n = 3$ manifolds [23,49].

The cross sections presented here allow, for the first time, realistic estimates of antihydrogen formation rates for the interaction of very low energy Ps with trapped antiprotons, in kinematics applicable to most antihydrogen experiments. (It is also worth noting that the cross sections can be simply transformed for the antiproton-beam configuration to be employed by GBAR.) Without allowing for the antiproton-Ps overlap, or laser excitation efficiencies to excited states, which will be dependent upon detailed experimental factors, we estimate a reaction rate as $\lambda_{\bar{\mathrm{H}}} = n_{\mathrm{Ps}}\sigma_{\bar{\mathrm{H}}}v_{\mathrm{Ps}}$, with the relevant antihydrogen formation cross section of $\sigma_{\bar{\mathrm{H}}}$ and with n_{Ps} and v_{Ps} the Ps atom density and speed, respectively.

Assuming, for example, Ps($3p$) with kinetic energies in the 10–100 meV range, we find from Fig. 1 that $\sigma_{\bar{\mathrm{H}}}v_{\mathrm{Ps}}$ is around 1.2×10^{9} a.u. ms^{-1}, or approximately 3.6×10^{-12} m^3 s^{-1}. Assuming a Ps target density of $n_{\mathrm{Ps}} \approx 10^{15}$ m^{-3}, which is similar to the aspirations of the GBAR group, then $\lambda_{\bar{\mathrm{H}}} \approx 3.6 \times 10^{3}$ s^{-1}. For 10^5 antiprotons

interacting with Ps for 10^{-7} s, which is less than the ground state ortho-Ps lifetime, we find that about 36 antihydrogen atoms can be manufactured in this manner. Given the trends found as n is increased in Fig. 1, yields will increase dramatically for higher Ps levels. Thus, reaction 1 will quickly become competitive with the aforementioned three-body reaction, with the added advantages that the $\bar{H}$ states formed will be more deeply bound and thereby less susceptible to ambient fields.

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