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Near-threshold production of antihydrogen positive ion in positronium–antihydrogen collision

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Abstract

Near-threshold production of antihydrogen ion (H+) in positronium–antihydrogen collisions is predicted by a rigorous four-body scattering calculation. The convergence of the cross sections for the rearrangement and all competing reactions (elastic scattering, de/excitation and de/polarization of positronium) is carefully examined against partial waves. Multi-channel scattering solutions are composed of functions that diagonalize the four-body Hamiltonian, and scattering functions that satisfy the correct asymptotic boundary conditions. The production rates of H+ show large discrepancies compared to more approximate calculations.

1. Introduction

The simplest antiatom (antihydrogen H) consists of an antiproton (p) and a positron (e+). The development of sources of cold antihydrogen [1–7] was motivated by the prospects of using it as a probe of fundamental physics. In particular, precise spectroscopy of antihydrogenic energy levels can provide a test of CPT symmetry [8–11], whereas ballistic measurements can probe the gravitational interaction between matter and antimatter [12–22]. In the GBAR project [14–17], the ultracold antihydrogen for free-fall experiments is to be obtained via sympathetic cooling of antihydrogen ions (H− = p+e+) and antihydrogen (H). In the present paper, we consider the H(1s1) formation cross sections at energies close to the threshold, where these cross sections are most appreciable.

The H+ production channel from the collision between Ps and H(1s),

Ps(nl) + H(1s) → e− + H+,

opens at 6.05 eV in center-of-mass energy for Ps(n = 1), 0.95 eV for Ps(n = 2) and 0.0017 eV for Ps(n = 3). Theoretical treatment of the reaction (1) involves considerable challenges; e.g., it is a rearrangement process where the particle configuration drastically changes from initial channel to final channel. Besides, the slow collision between Ps and H requires a simultaneous treatment of all constituent particles and would not allow the semi-classical approximations. It should be also stressed that the reaction (1) competes with several other inelastic processes. Below the threshold energy of e− + H+, there are fragmentation channels of Ps(nl) + H(1s) (n ≤ 3). The reaction (1) competes with Ps excitation and/or deexcitation.

Due to the charge-conjugation symmetry, Ps + H collisions (1) are equivalent to Ps + H collisions. Low-energy scattering of Ps(1s) and H has been studied in a number of works before as a fundamental example of positronium–atom interaction [23–26]. So far, theoretical studies revealed the Ps(1s) + H(1s)
total/differential elastic cross sections and scattering length [27–36], but the understanding of inelastic scattering still remains. The Born-based approximations and eikonal-based approximations have been adopted to predict \( H^+ \) production cross section; however, such approximations assume intermediate to high energy collisions, and may not be appropriate for low-energy scattering. Although the close-coupling method [32, 37, 38] and a coupled pseudo-state approach (CPA) [39] can be applied to low-energy scattering, these methods have so far not been applied to collisions with excited positronium. Comini and Hervieux have adopted a continuum distorted wave final state approximation (CDW-FS) [40–42] to calculate the cross sections for \( H^+ \) production in collisions of \( H \) and \( Ps \) in excited states. However, the CDW-FS involves perturbative nature of the formulation. The suitability of this approach to the near-threshold production of \( H^+ \) remains to be tested by more rigorous calculations.

A quantitative prediction of \( H^+ \) production rate in \( Ps(nl) + H(1s) \) slow collision requires a rigorous theoretical treatment of the four-body non-adiabatic multi-branch scattering including a rearrangement reaction. In this communication we predict elastic/inelastic cross sections of these collisions in the vicinity of \( e^- + H^+ \) threshold energy by a rigorous four-body scattering calculation. We describe the four-body correlation during the scattering by means of orthogonal finite space basis functions that diagonalize the full four-body Hamiltonian, \( H \). We augment this description with the channel functions that satisfy the asymptotic boundary conditions, and calculate the complete multi-channel scattering states by solving the coupled channel equations. This procedure delivers the full scattering matrix \( S \) whose elements determine the elastic and inelastic cross sections.

2. Theory

We consider the Schrödinger equation for the non-relativistic time-independent scattering wavefunction [43],

\[
(H - \varepsilon)\psi = 0, \tag{2}
\]

where the Hamiltonian \( H \) includes kinetic energy operators in center-of-mass system and all inter-particle Coulomb potential operators. We construct the total wavefunction \( \Psi \) as

\[
\Psi = \sum_{\alpha} \psi_\alpha + \sum_{\upsilon} b_\upsilon \Phi_\upsilon, \tag{3}
\]

where \( \Phi_\upsilon \) are square integrable four-body functions that describe the ‘intermediate state’ during the scattering with constants \( b_\upsilon \), and \( \psi_\alpha \) are open channel functions that describe the asymptotically non-vanishing component.

Construction of \( \{ \Phi_\upsilon \} \) plays a primary role in accurate determination of the cross section. In this work we construct \( \{ \Phi_\upsilon \} \) using a Gaussian expansion method (GEM) [44–46]. \( \Phi_\upsilon \) is described in terms of finite range Gaussian functions written in the five sets of Jacobian coordinates \( \{ r_c, R_c, \rho_c \} \) in figure 1 and their positron-permutated sets. \( \{ \Phi_\upsilon \} \) are eigenfunctions of the four-body Hamiltonian \( H \) and corresponding eigenenergies \( E_\upsilon \) are given by

\[
\langle \Phi_\upsilon | H | \Phi_\upsilon \rangle = E_\upsilon \delta_\upsilon, \tag{4}
\]

The use of the basis functions written in several coordinate systems facilitates the description of the four-body interactions and multi-channel character of the scattering. It should be stressed that \( \{ \Phi_\upsilon \} \) provides the explicit description of virtual \( H \) excitation, virtual \( Ps \) excitation, virtual \( Ps^+ \) formation (mainly described by \( c = 4, 5 \) coordinate sets) and transient formation of \( H^+ \) during the scattering. They describe also the mutual polarization of the atoms which is important in the description of their collisional interaction. The \( \bar{p} - e^+ \) and \( e^+ - e^- \) correlations are expanded in terms of Gaussian functions whose maximum ranges are around 20 \( a_0 \) and 50 \( a_0 \), respectively. In the present calculation, \( \Phi_\upsilon \) are expanded in terms of 40 000–65 000 basis functions.

The channel function \( \psi_\alpha \) of \( Ps(nl) + H(NL) \) is written in the \( c = 1 \) coordinate system and its positron-exchanged coordinate system as

\[
\psi_\alpha (r_1, R_1, \rho_1) = \frac{1}{\sqrt{2}} (1 + P) R_{\alpha}^H (r_1) R_{\alpha}^{nl} (R_1) R_{\omega} (\rho_1) \left[ Y_1 (r_1) Y_L (R_1) \right] Y_{\lambda} (\rho_1), \tag{5}
\]

where \( [\cdots] \) denotes linear combination of the spherical harmonics with Clebsh–Gordan coefficients as defined in reference [47]. \( P \) is a permutation operator for two positrons. \( R_{\alpha}^H (r_1), R_{\alpha}^{nl} (R_1) \) and \( R_{\omega} (\rho_1) \) are radial functions of \( Ps(nl) \), \( H(NL) \), and the relative motion between them, respectively. In this communication we consider \( N = 1 \) and \( L = 0 \) for the ground state \( H \) atom. Then the quantum number \( \Lambda \) of composite angular momentum \( \Lambda = L + \Omega \) coincides with \( l \).
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\[ \psi_\alpha (r_2, r_3, \rho_2) = \left[ \phi_{L=0}^{\bar{H}^+} (r_3, r_2) R_\alpha (\rho_2) Y_\lambda (\hat{\rho}_2) \right]_{JM}, \]

where \( \phi_{L=0}^{\bar{H}^+} \) is a three-body wavefunction of \( \bar{H}^+ \) (it is numerically calculated using the same Gaussian basis functions and corresponds to binding energy \( E_0 = 0.027718 \) hartrees). The radial function \( R_\alpha (\rho_2) \) of the relative motion in equations (5) and (6) are determined by numerical integration during the process of solving the integro-differential equations that are part of the coupled-channel procedure.

The whole system can be characterized by its parity \( P \), a total angular momentum \( J \) and its projection onto the \( z \)-axis \( M \), where the \( z \)-axis can be chosen to be in an arbitrary direction. In collision between \( \text{Ps}(nl) \) and \( \bar{H}(NL) \), the parity is defined by \( I \), \( L \) and the angular momentum of relative motion \( \lambda \), that is, in the initial channel, \( P = (-1)^{I+L+\lambda} \). Turning to the final channel of the rearrangement process, the ground state of \( H^+ \left( ^1S^+ \right) \) possesses two positrons with singlet spin. As a consequence, the spatial part of its wavefunction has positive permutation parity. In the final channel, the parity of the whole system, \( e^- + H^+ \), is determined by the angular momentum of relative motion \( \lambda \). Therefore, noticing the vector sum of \( L \) and \( \lambda \) configurations \( J \), the parity of \( H^+ + e^- \) is \( P = (-1)^{L+\lambda} = (-1)^J \). Thus \( J = \lambda \) (since \( L = 0 \)). Since we consider spin-independent interaction throughout this paper, the parity conservation between the initial and final channels induces constraints on the partial waves contributing to \( H^+ \) production. Considering for the example, the \( \text{Ps}(2p) + \bar{H}(1s) \rightarrow H^+ + e^- \) reaction, \( J = 1 \) allows only \( s \)-wave and \( d \)-wave collisions where \( (-1)^J = (-1)^{L+\lambda} \), but not \( p \)-wave collision where \( (-1)^J \neq (-1)^{L+\lambda} \).

So far the channel \( \alpha \) is not defined rigorously. The radial component of scattering function \( R_\alpha (\rho_1) \) in equation (5) depends on the fragments \( \text{Ps}(nl) \) and \( \bar{H}(NL) \) and \( (\lambda, \Lambda, J, M) \). Similarly, \( R_\alpha (\rho_2) \) in equation (6) depends on \( J \) and \( M \). Hereafter, we call \( \alpha \) a ‘detailed’ channel that specifies the fragments and the angular momentum of its partial wave while a channel \( \mathcal{F} \) specifies only the fragments. For example, \( \mathcal{F} \) defines only a collision between \( \text{Ps}(1s) \) and \( \bar{H}(1s) \) whereas \( \alpha \) specifies also the partial waves and intermediate couplings.

Table 1 displays \( \alpha \) that access the final \( e^- + H^+ \) channel together with the associated \( \lambda \) and \( J \) quantum numbers. We denote the initial detailed channel as \( \alpha_l \) and the angular momentum of its partial wave as \( \lambda_l \). Since we consider all energetically open channels above the \( e^- + H^+ \) threshold energy, the scattering in \( J = 0 \) has 7 branches, \( J = 1 \) has 10 branches, and \( J \geq 2 \) has 11 branches. We denote the number of branches as \( \alpha_{\text{max}} \). For a given \( J \), the dimension of the \( S \)-matrix is \( \alpha_{\text{max}} \times \alpha_{\text{max}} \).
This representation of the scattering state was adopted to three-body muonic atom collisions [48, 49] and recently used in four-body antihydrogen atom collisions [50, 51]. The Schrödinger equation is converted to a set of coupled equations with the following conditions,

\[ \langle \psi_\alpha | (r, r', \rho) / R_{\alpha}(\rho) | H - E | \psi \rangle_{r, r', \rho} = 0, \]  

(7)

and

\[ \langle \Phi_{\alpha} | H - E | \psi \rangle = 0. \]

(8)

Here, \( \langle \cdot \cdot \cdot | r, r', \rho \rangle \) means the integration over the indicated coordinates leaving out integration over \( \rho \). Expressing the radial functions of the relative motion in the initial and final channels as \( R_{\alpha}(\rho) = \chi_{\alpha}(\rho) / \rho \), we get a set of coupled integro-differential equations for \( \chi_{\alpha} \). We solve it using a compact finite difference method [52] under proper boundary conditions at \( \rho \rightarrow \infty \).

\[ \chi_{\alpha}(\rho) \rightarrow \rho^2 u^{(-)}_{\chi}(k_{\alpha} \rho) \delta_{\alpha\alpha} - \sqrt{\frac{\mu_{1\alpha}}{\mu_{\alpha}}} \sigma_{\alpha\alpha}^{(JM)} \rho^2 u^{(+)}_{\chi}(k_{\alpha} \rho), \]

(9)

where \( u^{\pm}_{\chi} \) is an incoming/outgoing spherical Hankel function for channels with fragmentation into \( Ps(nl) \) and \( H(1s) \), and a spherical Coulomb–Hankel function for the final channel with fragmentation into \( e^- + \bar{H}^+ \). \( v_{\alpha} \) denotes speed of relative motion between the fragments in channel \( \alpha \). \( \chi_{\alpha}(\rho) \) is computed up to 800 \( a_0 \) for \( \rho_{1} \) and 1200 \( a_0 \) for \( \rho_{2} \), and above these values \( S \)-matrix elements are well converged.

The \( S \)-matrix elements \( S_{\alpha\alpha}^{(JM)} \) for each \( J \) and \( M \) give cross sections from an initial detailed channel \( \alpha_1 \) to other detailed channel \( \alpha \) as

\[ \sigma_{\alpha\alpha}^{JM} = \frac{\pi}{k_{\alpha}} | S_{\alpha\alpha}^{(JM)} |^2. \]

(10)

Since the initial wave involves all partial waves, the scattering cross section from \( F_1 \) to \( F \) can be expressed as

\[ \sigma_{\alpha\alpha} = \sum_{\lambda} \delta^{(\lambda)}_{\alpha\alpha}, \]

(11)

where \( \delta^{(\lambda)}_{\alpha\alpha} \) is a partial wave cross section of \( \lambda \) angular momentum. In the present framework, \( \delta^{(\lambda)}_{\alpha\alpha} \) can be calculated by gathering the \( \sigma_{\alpha\alpha}^{JM} \). Since the scattering process does not depend on \( M \), the partial wave cross sections are written as

\[ \delta^{(\lambda)}_{\alpha\alpha} = \frac{1}{(2I + 1)(2L + 1)} \sum_{\alpha_1} \sum_{\lambda_1} (2I + 1) \sigma_{\alpha_1}^{JM}, \]

(12)

where the summation over \( \alpha \) and \( \alpha_1 \) runs over all detailed channels belonging to \( F \) and \( F_1 \), respectively. Note that the allowed \( \alpha_1 \) should be compatible with \( \lambda_1 \). For example, \( Ps(3s) + H(1s) \) scattering (\( F_1 = 4 \)) in \( p \)-wave (\( \lambda_1 = 1 \)) is simply given by \( \alpha_1 = 4 \) for \( J = 0 \). On the other hand, \( Ps(3p) + H(1s) \) scattering (\( F_1 = 5 \)) in \( p \)-wave is given by the summation of \( \alpha_1 = 5 \) of \( J = 0 \) and \( \alpha_1 = 6 \) of \( J = 2 \) (these two detailed channels have the same \( \lambda \) but different internal coupling).

Our calculation does not assume the principle of detailed balance, and the \( S \)-matrix is not symmetric by the construction. Thus, we can use its symmetry as a check of the accuracy of our calculation. In this communication we evaluate the cross section with error \( \sigma_{\alpha\alpha} \pm \Delta \sigma_{\alpha\alpha} \) by the difference between \( S_{\alpha\alpha}^{JM} \) and \( S_{\alpha\alpha} \). In addition to the symmetry of \( S \)-matrix, the unitarity condition can also be an indicator of calculation accuracy. If the solution of the Schrödinger equation were exact, the value \( U_{\alpha_1} = \sum_{\alpha_1} | S_{\alpha_\alpha} |^2 \) would be unity due to the conservation of probability. The deviation, \( |1 - U_{\alpha_1}| \), can be used to estimate the error of scattering cross sections from a detailed channel \( \alpha_1 \). Throughout the presented calculations, the errors estimated from the unitarity condition are kept smaller than the accumulated errors from the symmetry condition of the \( S \)-matrix (\( U_{\alpha_1} = 1.001 \) in average with the standard deviation 0.003 for all calculated energy values).

3. Partial wave convergence of \( \bar{H}^+ \) production cross section

We investigate the \( \bar{H}^+ \) production as function of collision energy \( E_1 \) in the initial channel. Denoting the kinetic energy of relative motion in the final channel as \( E_2 \), we concentrate on the near-threshold \( \bar{H}^+ \) production, \( 0 < E_2 \leq 0.15 \) eV. Table 2 lists the partial wave cross sections of \( \bar{H}^+ \) production, \( \delta^{(\lambda)}_{\alpha_\alpha} \), for \( E_2 = 0.01 \) and 0.1 eV. Each of the cross sections converge against the number and chosen forms of \( \{ \Phi_{\alpha} \} \), and the choice of radial grid for finite difference method.

In \( Ps(1s) + H(1s) \) scattering, the dominant contribution comes from \( d \)-wave collision (\( \lambda_1 = 2 \)) with cross section \( \delta^{(2)}_{\alpha_\alpha} \sim 9a_0^2 \). The total cross section of \( \bar{H}^+ \) production almost converges up to \( \lambda_1 = 4 \). The cross
Table 2. Partial wave cross sections of $\bar{H}^+$ production, $\sigma^{H+}_{\lambda_i^J}$, at 0.01 eV and 0.1 eV in kinetic energy between $\bar{H}^+$ and $e^-$. The cross sections are in atomic unit ($a_0^2$). $\lambda_i$ is angular momentum of relative motion between Ps and $\bar{H}$. Digits in parentheses denote the uncertainty in the last digit estimated by the difference of $S_{\text{ex}}$ and $S_{\text{ex}}$.

| $\lambda_i$ | $\psi(1s) + \bar{H}(1s)$ | $\psi(2s) + \bar{H}(1s)$ | $\psi(3p) + \bar{H}(1s)$ | $\psi(3d) + \bar{H}(1s)$ |
|-------------|-----------------|-----------------|-----------------|-----------------|
|             | 0.01 eV | 0.1 eV | 0.01 eV | 0.1 eV | 0.01 eV | 0.1 eV |
| 0           | 1.23(9)  | 1.14(5)  | 3.96(8)  | 3.9(1)  | 10.13(2)  | 8.6(1) |
| 1           | 3.409(9) | 3.419(3) | 7.73(4)  | 6.96(2) | 3.89(1)  | 4.48(2) |
| 2           | 9.6(1)  | 9.42(6)  | 22.0(2)  | 17.5(1) | 13.1(5)  | 12.4(3) |
| 3           | 4.6(2)  | 4.7(1)   | 9.8(1)   | 8.5(1)  | 28.7(4)  | 25(1)   |
| 4           | 0.88(3) | 0.87(6)  | 2.7(3)   | 1.7(1)  | 21.7(2)  | 20.8(2) |
| 5           |         |          |         |         | 6.9(3)   | 8.4(8)  |
| 6           |         |          |         |         | 1.666(2) | 1.08(1) |
| Sum         | 19.7(6) | 19.7(3)  | 45.8(7)  | 38.2(4) | 84(2)    | 80(3)   |

| $\lambda_i$ | $\psi(3s) + \bar{H}(1s)$ | $\psi(3p) + \bar{H}(1s)$ | $\psi(3d) + \bar{H}(1s)$ |
|-------------|-----------------|-----------------|-----------------|
|             | 0.01 eV | 0.1 eV | 0.01 eV | 0.1 eV | 0.01 eV | 0.1 eV |
| 0           | 1.97(9)  | 0.68(7)  | 10.7(1)  | 5.9(2)  | 9.9(2)   | 3.28(4) |
| 1           | 1.121(2) | 2.46(8)  | 0.50(2)  | 1.35(5) | 0.063(4) | 0.42(2) |
| 2           | 0.003(1) | 0.41(2)  | 0.01(1)  | 0.008(2) | 0.02(4)  | 0.07(1) |
| Sum         | 3.29(5)  | 3.6(1)   | 11.2(2)  | 7.3(3)  | 10.0(2)  | 3.8(1)  |

section at 0.01 eV is similar to that at 0.1 eV for all partial waves. This is because the change of collision energy, i.e. $\Delta E_i / E_i$ is small. $\psi(2s) + \bar{H}(1s)$ scattering also has the largest contribution of the $d$-wave collision in $\bar{H}^+$ production. The $\bar{H}^+$ production cross section from $\psi(2s)$ is much larger than that from $\psi(1s)$. On the other hand, $\psi(2p) + \bar{H}(1s)$ scattering has the largest contribution of the $f$-wave collision ($\lambda_i = 3$) in $\bar{H}^+$ production while the $g$-wave contribution is the second dominant in the total $\bar{H}^+$ production cross section. The total cross section of $\bar{H}^+$ production from $\psi(2p)$ tends to converge with increasing $\lambda_i$.

Comparing to the case of $\psi(n = 1, 2)$, fewer partial waves are needed to converge the $\psi(n = 3)$ cross sections which is understandable in view of lower collision energy. Each partial wave cross section changes substantially between $E_i = 0.01$ and 0.1 eV, since in this case $\Delta E_i / E_i$ is large.

4. $\bar{H}^+$ production and the elastic/inelastic branches

Figure 2 shows the $\bar{H}^+$ production (rearrangement) cross section $\sigma_{\text{ex}} = \sigma_{\gamma, F_i}$ against the collision energy $E_i$ together with elastic/inelastic scattering cross sections. For $\psi(1s) + \bar{H}(1s)$ collision ($F_i = 1$), the $\bar{H}^+$ production cross section is given by $\sigma_{\text{ex}} = \sigma_{\gamma, F_1}$, the elastic scattering cross section by $\sigma_{\text{ela}} = \sigma_{\gamma, F_1}$, and Ps excitation cross section by $\sigma_{\text{ex}} = \sigma_{\gamma, F_1} + \sigma_{\gamma, F_2} + \sigma_{\gamma, F_3}$, $\ldots$. The zero-energy limit of $\sigma_{\text{ex}}$ is also confirmed to give the scattering length 4.329 $a_0$, in agreement with the results in references [33, 36, 38]. The $\bar{H}^+$ production whose channel opens at 6.0486 eV is the second dominant process after the elastic scattering. In the present energy region, these cross sections are nearly constant. $\sigma_{\text{ex}}$ is dominated by the excitation to $n = 2$ states followed by the $n = 3$ states whose channel opens at 6.0469 eV; the latter is smaller by one order of magnitude. The $\sigma_{\text{ex}}$ starts at the finite value and is also constant in agreement with Wigner’s threshold law [34] for the case when the final fragments are Coulomb attractive and when their relative velocity is much smaller than the velocity of the initial fragments.

Figures 2(b) and (c) shows the results of $\psi(n = 2) + \bar{H}(1s)$ collisions ($F_i = 2, 3$). Again, we find that $\sigma_{\text{ex}}$ is finite at the threshold energy. For the case of $\psi(2s)$ collision ($F_i = 2$), the $\bar{H}^+$ production cross section $\sigma_{\text{ex}} = \sigma_{\gamma, F_2}$ should be compared with Ps excitation cross section $\sigma_{\text{ex}} = \sigma_{\gamma, F_2} + \sigma_{\gamma, F_3} + \sigma_{\gamma, F_2}$ and deexcitation cross section $\sigma_{\text{dec}} = \sigma_{\gamma, F_2}$. Like the $\psi(1s)$ collision, $\psi(n = 2) + \bar{H}(1s)$ collisions produce $\bar{H}^+$ as the dominating inelastic process in scattering. One also finds that $\sigma_{\text{ex}}$ is zero at threshold and grows in agreement with Wigner’s threshold law for neutral fragments (each partial wave growing as $E_i^{\lambda_i+1/2}$). The behaviour of cross sections for $\psi(2p)$ collision is similar to that for $\psi(2s)$ collision, although the $\sigma_{\text{ex}}$ from $\psi(2p)$ is slightly larger than that from $\psi(2s)$.

Turning to $\psi(n = 3)$ the results for the $I = 0, 1, 2$ ($F_i = 4, 5, 6$) are shown in figures 2(d), (e) and (f). $\sigma_{\text{ex}}$ decreases rapidly just above the threshold energy, and is almost constant at higher energies. The deexcitation of $\psi(3l)$ states is seen to increase with $\lambda$. $\sigma_{\text{ex}} = \sigma_{\gamma, F_1} + \sigma_{\gamma, F_2} + \sigma_{\gamma, F_3}$ obey Wigner’s threshold law
Elastic and inelastic scattering cross sections $\sigma_{FF}$ for Ps$(nl)$ + $\bar{H}(1s)$ collision in positronic spin singlet state are displayed. $\bar{H}^+$ production cross section (red lines) are compared with previous results indicated by black lines: CDW-FS(UC) [40], DWBA and FBA [53] and CPA [39]. The light-blue vertical arrows indicate the threshold energies of $\bar{H}^+$ production in our calculation. For comparison with our data, the results of references [39, 53] have been multiplied by factor 4 as to account for the spin statistics of the positronic spin singlet scattering. The right-head arrows indicate the $\bar{H}^+$ production cross section of CDW-FS(UC) at the lowest energy considered in reference [40].

for the case where the final fragments move fast and the initial fragments collide slowly, that is, the partial wave cross sections are proportional to $E^{\lambda_i-1/2}$, and thus $\sigma_{\text{deexc}}$ are finite at the threshold of $\bar{H}^+$ formation. The major difference between the Ps$(n=3)$ collision and Ps$(n=2)$ collision is that the former results in smaller $\bar{H}^+$ formation and larger Ps deexcitation. In the considered energy interval, the $\bar{H}^+$ formation in Ps$(3d)$ collisions is on average an order of magnitude smaller than in Ps$(2p)$ collisions. At the same time, the cross section for Ps$(n=3)$ deexcitation is more than one order of magnitude larger than that for $\bar{H}^+$ production [whereby the deexcitation to Ps$(n=2)$ occurs faster than to Ps$(n=1)$]. The branches of rapid inelastic scattering may suppress the flux into the $e^- + \bar{H}^+$ branch due to the conservation of probability.

Our results are compared with $H^+$ production cross sections in previous works. CDW-FS calculations [40] were performed with several different wavefunctions of $\bar{H}^+$ and predicted monotonically decreasing $\bar{H}^+$ production cross sections. CDW-FS(UC) uses an uncorrelated Chandrasekhar wavefunction that reproduces $\bar{H}^+$ three-body energy with error of binding energy, 0.38 eV. In the present work, we have used a more precise $H^+$ wavefunction that reproduces $H^+$ three-body energy with more than 6 digits accuracy. That, together with very careful four-body description and coupling of all open channels, enabled us to predict the cross sections very close to the $H^+$ formation threshold. Comparing our results with previous works, CDW-FS overestimated the $\sigma_{\text{deexc}}$ for Ps$(2s, 2p, 3p$ and $3d)$. In contrast, CPA underestimated $\sigma_{\text{deexc}}$ for Ps$(1s, 2s)$. Our results for $H^+$ production in Ps$(n=3) + H(1s)$ scattering are much smaller than those calculated by FBA [53].

In relating the present results to the experiments one should bear in mind the particular experimental conditions. For instance, in the conditions of the GBAR experiment, with an almost stationary laser-excited Ps target, most of the center-of-mass energy comes from the $H$ (or $\bar{p}$ colliding with the Ps target) impact energy, which means that the $H^+$ production requires $1 + m_1/m_{Ps} = 919.6$ times larger kinetic energy of $H$ in the laboratory frame. In addition, since the $H^+$ production is allowed when the two positrons (i.e. one in
the Ps and the other in the H̅) couple to the singlet state and is not allowed for coupling in the triplet state, the net cross section of $\sigma_{7F_i}$ in figure 2 should be reduced by the spin weight $1/4^2$.

5. Conclusion

In conclusion, the near-threshold production of H̅+ in the collision of Ps(nl) + H(1s) occurs as the most dominant inelastic process when $n = 1, 2$, and the second dominant one when $n = 3$. Close to the threshold energy, the largest H̅+ production cross section is predicted for $n = 2$, followed by $n = 1$ and $n = 3$. We also find that the depletion of Ps($n = 2$) population by the reactions competing with H̅+ formation is smaller than the similar depletion of Ps($n = 3$). While our results are limited to lower energies, we find H̅+ production cross sections significantly smaller than previous calculations based on high-energy approximations. The presented results have been obtained by an ab initio calculation that does not contain any modeling approximations and rigorously deals with the non-adiabatic, multi-channel character of the composite-particle scattering. The numerical accuracy is reported in terms of the unitarity of the scattering matrix, and the scattering cross sections are seen to follow the trends predicted by the general scattering theory.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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7 In the arrangement of ħ beam impinging on the stationary Ps cloud, the basic formation rates of H̅+ are $n_{\text{Ps}} v_{\text{H}} \sigma_{7F_i}/4$, where the velocity $v_{\text{H}}$ of H̅ is similar to the velocity of antiprotons in the beam, and $n_{\text{Ps}}$ is the density of positronium. These rates are to be compared to the annihilation rates of e–Ps($n = 1, 2, 3$), the spontaneous deexcitation rates of Ps($n = 2, 3$) and the collisional deexcitation rates of Ps($n = 2, 3$). It is important to note that, unlike the formation rate of H̅+, the deexcitation rates of Ps($n = 2, 3$) are also contributed from the positronic triplet scattering.
