Positronium and Antihydrogen Formation in the e^+-H and Ps-$\bar{p}$ Systems

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The close coupling equations for the e^+-H and Ps-$\bar{p}$ systems are solved for a model calculation comprising three hydrogen H($1s$,$2s$,$2p$) and three positronium Ps($1s$,$2s$,$2p$) states. The summed cross section for Ps formation in the Ps($1s$), Ps($2s$), and Ps($2p$) states for $e^+ + H \rightarrow Ps + p$ reaction achieves a peak of $2.7\pi a_0^2$ and is smaller than the only existing set of experimental data. The cross section for antihydrogen formation in the $Ps + \bar{p} \rightarrow e^+ + \bar{H}$ reaction reaches a maximum of $(13\text{-}14)\pi a_0^2$ for incident antiproton energies between 6.5 and 11 keV.

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The e^+-e^--p system is one of the fundamental three body systems of physics, and one of the simplest systems to admit a rearrangement reaction, viz.,

$$e^+ + H \rightarrow Ps + p\,.$$

The calculation of cross sections for the rearrangement transition is a formidable theoretical proposition because of the difficulties inherent in treating a collision system which has a moving projectile with internal structure. Since the pioneering work of Massey and Mohr [1], there have been a number of calculations of the charge transfer process [2-4]. At low energies the Kohn variational calculations of Humberston and collaborators [5] are the most precise. In the intermediate energy region, a number of different variants of perturbation theory have been applied and some small basis close coupling calculations have also been performed [6]. The recent calculations of the Daresbury group are the most sophisticated of those using the close coupling formalism [7]. Recently, a completely general expression for the charge transfer matrix element, suitable for large scale computation, has been derived [8]. Hence, calculations which explicitly couple the hydrogen and positronium states in the coupled channels ansatz can now be performed routinely.

In this work we use six state model of the e^+-H system, including three hydrogen H($1s$,$2s$,$2p$) and three positronium Ps($1s$,$2s$,$2p$) states. In an obvious notation we refer to this as the close coupling CC(3,3) calculation. The momentum space Lippmann-Schwinger equation, viz.,

$$\langle \mathbf{k}'\Psi_{\alpha'}|T|\mathbf{k}\Psi_\alpha\rangle = \langle \mathbf{k}'\Psi_{\alpha'}|V|\mathbf{k}\Psi_\alpha\rangle + \sum_{\alpha''}\int d^3k'' \frac{\langle \mathbf{k}'\Psi_{\alpha'}|V|\mathbf{k}''\Psi_{\alpha''}\rangle\langle \mathbf{k}''\Psi_{\alpha''}|T|\mathbf{k}\Psi_\alpha\rangle}{(E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2}k''^2)}$$
$$+ \sum_{\beta''}\int d^3k'' \frac{\langle \mathbf{k}'\Psi_{\alpha'}|V|\mathbf{k}''\Phi_{\beta''}\rangle\langle \mathbf{k}''\Phi_{\beta''}|T|\mathbf{k}\Psi_\alpha\rangle}{(E^{(+)} - \epsilon_{\beta''} - \frac{1}{4}k''^2)},$$
$$\langle \mathbf{k}'\Phi_{\beta'}|T|\mathbf{k}\Psi_\alpha\rangle = \langle \mathbf{k}'\Phi_{\beta'}|V|\mathbf{k}\Psi_\alpha\rangle + \sum_{\alpha''}\int d^3k'' \frac{\langle \mathbf{k}'\Phi_{\beta'}|V|\mathbf{k}''\Psi_{\alpha''}\rangle\langle \mathbf{k}''\Psi_{\alpha''}|T|\mathbf{k}\Psi_\alpha\rangle}{(E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2}k''^2)}$$
$$+ \sum_{\beta''}\int d^3k'' \frac{\langle \mathbf{k}'\Psi_{\beta'}|V|\mathbf{k}''\Phi_{\beta''}\rangle\langle \mathbf{k}''\Phi_{\beta''}|T|\mathbf{k}\Psi_\alpha\rangle}{(E^{(+)} - \epsilon_{\beta''} - \frac{1}{4}k''^2)}$$

is solved by the method of numerical quadrature [8]. In the above equation, Ψ_α and Φ_β refer to the hydrogen and positronium states, ϵ_α and ϵ_β are their respective energies, and the generic interaction, V, is different for the different classes of channels. For most of the calculations undertaken as part of this research, 40 or 48 point Gaussian meshes were used in the discretization of the integral equation. Convergence tests indicate that the charge transfer cross sections reported in this Letter should have a numerical accuracy of better than 5%. Partial cross sections for charge transfer reactions are explicitly computed for $J=0$ to $J=12$. The partial wave sum was then extrapolated to infinite J by assuming the partial cross sections scale like a power series. The size of the correction made to the cross section by extrapolation was generally less than 5%. Calculations were performed at a large number of energies. At incident positron energies below 1.5 Ry, an energy step of 0.01 or 0.02 Ry was generally used between adjacent energies. At higher energies, an energy step of 0.05 or 0.10 Ry was used.

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An exhaustive series of checks have been made to validate the program used for the calculation. Cross sections for positronium formation to the Ps(1s), Ps(2s), Ps(2p), Ps(3s), Ps(3p), and Ps(3d) levels computed in the Born approximation agree with previous calculations [8–10]. Cross sections computed in the coupled static model, i.e., the H(1s)+Ps(1s) channel space, also agree with earlier calculations [8,11]. Finally, a large basis pseudostate calculation [12] is in good agreement with the variational calculations [5].

Cross sections for the excitation of hydrogen and positronium formation in the Ps(1s), Ps(2s), and Ps(2p) states are depicted in Fig. 1. The charge transfer cross section is roughly equal to the geometric area of the hydrogen atom (i.e., πa_0^2) over the entire energy range to 60 eV. The dominant contribution to the charge transfer cross section comes from the formation of positronium in the ground state. The summed Ps(2s) and Ps(2p) cross sections are less than 15% of the Ps(1s) cross section.

While the calculations of the Daresbury group use essentially the same basis to model the e^+-H system, their results cannot be sensibly compared with the present cross sections. They did not compute the off-diagonal matrix element connecting the different positronium channels correctly [13], and this caused some of their cross sections to be in error by as much as 50%.

The summed positronium formation cross section is computed by adding the cross sections to individual states and this can be compared with experimental cross sections of the Bielefeld-Brookhaven collaboration [14,15] in Fig. 1. The experimental data represent the cross section for positronium formation in all possible states. The present calculation underestimates the empirical data at low energies near the cross section peak, but agrees with experiment at higher energies. At the lower energies, we would expect the cross section to be more sensitive to the limited size of the channel space used in the close coupling expansion. Below the ionization threshold, our calculation can be compared with variational calculations [5] and also with a large basis pseudostate calculation, referred to as the CC(6,6) calculation, including three H and Ps physical states and three H and Ps pseudostates [12]. Both of these calculations give larger Ps formation cross sections than the present calculation. For example, at an incident energy of 9.8302 eV, the CC($\bar{6}$,$\bar{6}$) calculation gave $2.46\pi a_0^2$ for the Ps(1s) cross section, whereas the CC(3,3) cross section is $1.812\pi a_0^2$. Because of this, the calculations in the CC(6,6) model have been extended to higher energies. The pseudostate cross sections are compatible with the experimental cross section at the peak. Extending the pseudostate calculation into the intermediate energy region is more problematical since both physical resonances [16,17] (discussed later) and pseudoresonances exist in this energy region and there is no procedure to distinguish between the two classes of resonances.

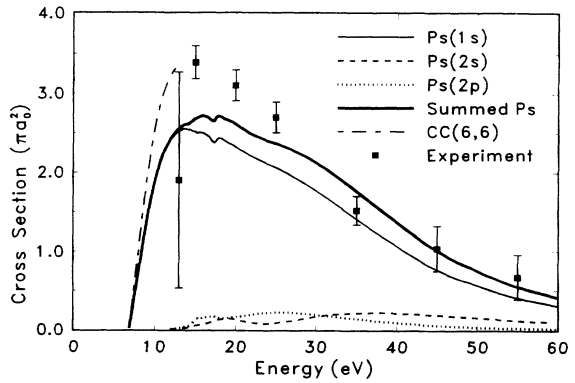

FIG. 1. Cross sections (in πa_0^2) for positronium formation to the Ps(1s), Ps(2s), and Ps(2p) states computed in the CC(3,3) model for the e^+-H(1s) entrance channel. The summed cross sections for both the CC(3,3) and CC(6,6) models are shown as well as the experimental data of the Bielefeld-Brookhaven collaboration [13,14].

The increase in cross section can be expected to be maintained at energies above the ionization threshold, although becoming smaller as energy increases, and this would remove most of the discrepancy with experiment. Positronium formation in the $n=3$ and higher levels can also be expected to increase the summed Ps formation cross section, most likely by an amount not exceeding 5%. To summarize, an improved model of the reaction can be expected to lessen the differences with experiment.

A unique feature of the graph depicted in Fig. 1 is the presence of structures in the cross section at incident energies near 15 and 18 eV. These features are the result of resonances that occur in the $J=0$, 1, 2, and 3 partial waves. The energy resolution of the Bielefeld-Brookhaven experiment [14,15] was 2.8 eV, and so cannot be expected to resolve these resonances. The details of these resonances, which are unlike anything occurring in electron hydrogen scattering, are beyond the scope of this Letter and are reported elsewhere [16,17].

The calculation of the cross section for the reaction

$$\mathrm{Ps}(1s)+\bar{p}\rightarrow e^+ + \bar{\mathrm{H}}(nl) \qquad (1)$$

is of interest since the antihydrogen system is a preferred system for high precision studies of the charge conjugation symmetry of physics [18]. Antihydrogen is different from other exotic atoms such as muonium, positronium, and protonium because it would be stable provided it was isolated from ordinary matter in an ion trap. The availability of a suitable antiproton beam from the Low-Energy Antiproton Ring (LEAR) at CERN means that antihydrogen can be formed by directing the antiproton beam through a chamber containing positronium and using the charge transfer process, Eq. (1), to make antihydrogen [19–21].

Among the considerations that influence the rate of antihydrogen production and hence the viability of any experiment are factors like the antiproton current, the posi-

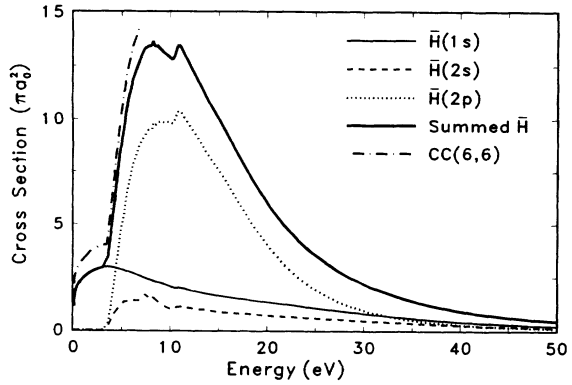

FIG. 2. Cross sections (in πa_0^2) for electron transfer to the $\bar{H}(1s)$, $\bar{H}(2s)$, and $\bar{H}(2p)$ states computed in the CC(3,3) model for the $\bar{p}$-Ps($1s$) entrance channel. The summed electron transfer cross sections are shown for both the CC(3,3) and CC(6,6) models.

tronium production rate and density, and the cross section for the charge transfer reaction. Apart from variational cross sections available below the ionization threshold [22], the only calculations of this charge transfer process use approximations of limited accuracy [23–25]. These limitations in accuracy are expected to be especially severe at incident energies just above the ionization threshold where the charge transfer cross section is largest. The present calculations can therefore be used to assist in the design of experimental conditions to maximize antihydrogen production.

The antihydrogen formation cross sections for Ps($1s$)-$\bar{p}$ collisions in the antiproton rest frame are shown in Fig. 2. The antihydrogen $n=2$ states are preferentially populated in the charge transfer process. In particular, the H($2p$) cross section is much larger than the H($1s$) and H($2s$) cross sections for energies less than 20 eV. For incident energies less than 40 eV, more antihydrogen is formed in the excited states than it is in the ground state.

The charge transfer cross section summed over the individual antihydrogen states is also depicted in Fig. 2. At energies below the ionization threshold, the summed antihydrogen cross section computed in the CC(6,6) model is depicted to give an indication of the accuracy of the present CC(3,3) cross section. The charge transfer cross section is greater than $13\pi a_0^2$ for incident positronium energies between 7 and 12 eV. This is equivalent to antiproton beam energies of 6.5 and 11 keV. We have also performed calculations in a model containing the H($n=1,2,3$) and Ps($n=1,2$) states at a few selected energies to estimate the contribution of the charge transfer cross section to the antihydrogen $n=3$ levels. The summed charge transfer cross section near the maximum is increased by about 10% and the position of the cross section maximum is not altered. The present results indicate that there would be little point in decreasing the energy of an antiproton beam in a circular ion trap below these energies, with a consequent degradation in beam intensity, unless it is planned to use lasers to pump a significant fraction of the positronium into an excited state [26,27].

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