Antihydrogen formation by collisions of antiprotons with positronium in a magnetic field

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Using the classical trajectory Monte Carlo method, we calculated the charge-transfer cross section for antiprotons colliding with Rydberg positronium, leading to antihydrogen formation. The results show a significant influence of an externally applied magnetic field which causes a reduction of the cross section.

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The recent success of experiments to produce significant numbers of cold antihydrogen atoms has opened a new door to the test of fundamental symmetries in physics (cf. Refs. [1–3] and references therein). An accurate spectrometry of photon transitions in hydrogen and its antimatter counterpart could resolve the question if the Rydberg constants in both systems are identical, as required by the *CPT* theorem. In these experiments slow antiprotons interact with positrons stored in a "nested trap" and capture processes yield cold antihydrogen atoms; three-particle $\bar{p}$-$2e^+$ recombination as well as radiative $\bar{p}$-e^+ recombination are discussed as possible causes for antihydrogen formation. However, as an alternative route e^+ capture from positronium,

$$\bar{p}+(e^+e^-)\rightarrow\bar{\mathrm{H}}+e^-, \tag{1}$$

has recently received considerable attention (cf. Refs. [4–6] and references therein). Early work on process (1) has concentrated on capture from low-lying positronium (Ps) states, while Charlton's work [4] drew attention to the advantages offered by high-lying states (in particular, large cross sections, large Ps lifetime, and target density). For all these processes, a major problem in the quantitative interpretation lies in the unknown effect of the strong (≈ 5 T) magnetic field present in the trap. Therefore, in an extension of our previous classical trajectory Monte Carlo (CTMC) calculations [7,8] on p-H collisional charge transfer and ionization in a magnetic field, we present some preliminary results for the latter problem [Eq. (1)], namely, the effect of a strong magnetic field on $\bar{p}$-Ps collisions. Since high-n states (n being the principal quantum number) are of special interest, the Ps target is assumed to be in a Rydberg state. This has the additional advantage that these states are particularly suited for a classical description, which is the basis of our CTMC treatment. Our study may also provide a first-step model to estimate the influence of the external magnetic field on the $\bar{p}$-$2e^+$ system. Both situations deal with a three-body collision involving two weakly interacting light particles, trapped at large distances from each other about their respective magnetic-field lines.

The presence of a magnetic field in such calculations is by no means a trivial problem since in general the center-of-mass motion and the internal motion of the system cannot be separated. The first rigorous treatment of a two-body system in a magnetic field was published by Avron, Herbst, and Simon [9]. A new operator connected with the center-of-mass motion, the so-called pseudomomentum **K**, was introduced in their work. It represents a conserved quantity for the system, making it possible for neutral systems to perform a pseudoseparation of the center-of-mass motion. Later, a classical investigation of the highly excited hydrogen [10,11] and positronium [12,13] atoms in a magnetic field has been performed by Schmelcher and co-workers. The Coulomb potential is distorted by the magnetic field, and above a critical value K_c of the pseudopotential an additional well forms on the negative x axis, where x is the particle distance perpendicular to the field direction; it will be referred to as the outer well (OW). The outer well moves away from the magnetically distorted Coulomb potential and becomes broader and deeper with increasing K. Particles in this OW are trapped at large distances from each other, leading to delocalized states. Figure 1 shows examples of this potential for Ps, the case of interest in this work.

As in our previous work on p-H collisions in a magnetic field [7,8] we applied the CTMC method to calculate cross sections for the reaction (1). The target Ps atoms, embedded in magnetic fields of 4 T and 5 T, are in Rydberg states with binding energies corresponding to field-free principal quantum numbers $n=40$ and 50. Unfortunately, in contrast to a Rydberg hydrogen atom with an "infinitely heavy" proton nucleus, the center-of-mass of Ps in a magnetic field is unstable. This makes a direct application of our CTMC method to the system under study here more difficult.

First we have to create the proper initial e^+e^- target states. To this end, we follow the treatment proposed by Schmelcher and co-workers [12–14]. The nonrelativistic Hamiltonian of two particles with equal masses and opposite charges in a homogeneous static magnetic field is given by

$$H=\frac{1}{2}(\mathbf{p}_1+\mathbf{A}_1)^2+\frac{1}{2}(\mathbf{p}_2-\mathbf{A}_2)^2-\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}, \tag{2}$$

where $\mathbf{p}_1,\mathbf{p}_2$ and $\mathbf{r}_1,\mathbf{r}_2$ are the momenta and coordinates of the electron and positron, respectively. $\mathbf{A}_1=\frac{1}{2}\mathbf{B}\times\mathbf{r}_1$ and $\mathbf{A}_2=\frac{1}{2}\mathbf{B}\times\mathbf{r}_2$ are the symmetric gauge vector potentials of the

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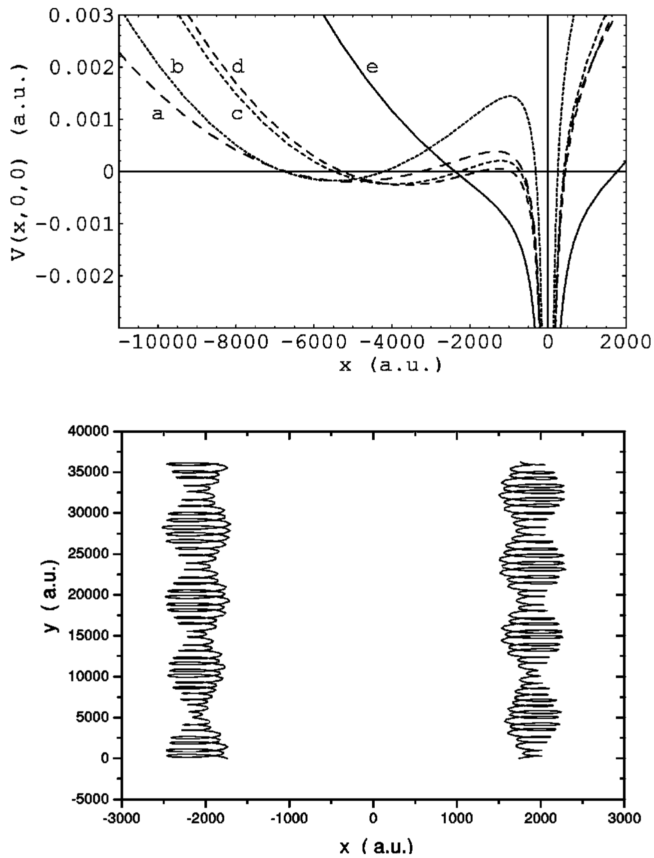

FIG. 1. Top: $V(x,0,0)$ for Ps in a magnetic field. (a) $B=4$ T, $K=0.09$; (b) $B=5$ T, $K=0.12$; (c) $B=5$ T, $K=0.09$; (d) $B=5$ T, $K=0.085$; and (e) $B=5$ T, $K=0.01$. Solid curve: $K<K_c$; for all other curves $K>K_c$. x is the particle distance perpendicular to the field direction. Bottom: an example of e^- and e^+ particle trajectories in the external magnetic field which points along the z direction. Note that the Ps center-of-mass moves along the y direction.

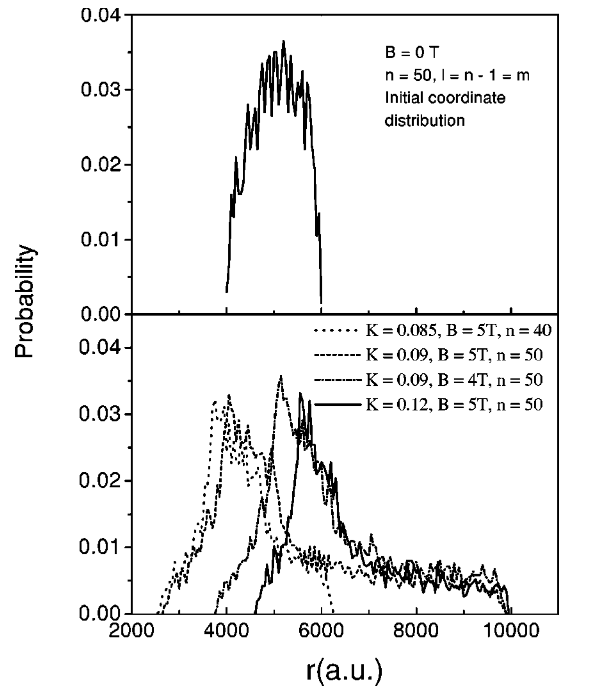

FIG. 2. Initial coordinate distribution of the positronium ensemble. Top: field-free condition ($B=0$ T), $n=50$, $l=n-1=m$. Bottom: external magnetic fields $B=4$ T and 5 T, $n=40$ and 50; $K=0.085$, 0.09, and 0.12.

two particles. All quantities are given in atomic units. As has been discussed in Ref. [12], the Hamiltonian of Eq. (2) is not translationally invariant and the total momentum is not conserved. However, the pseudomomentum

$$\mathbf{K}=\mathbf{p}_1+\mathbf{p}_2-\frac{1}{2}\mathbf{B}\times\mathbf{r}_1+\tfrac{1}{2}\mathbf{B}\times\mathbf{r}_2 \tag{3}$$

is a conserved quantity. For the special case of Ps, an effective Hamiltonian is given in Cartesian coordinates [cf. Eq. (6) in Ref. [13]] by

$$H_{Ps}=\frac{1}{2\mu}\mathbf{p}^2+\frac{\gamma}{4}(x^2+y^2)+\frac{\gamma K x}{2}+\frac{K^2}{4}-\frac{1}{|\mathbf{r}|}, \tag{4}$$

where $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ and $\mathbf{p}=\mathbf{p}_1-\mathbf{p}_2$ are the interparticle distance and momentum vectors. μ is the reduced mass. The magnetic-field vector is $\mathbf{B}=(0,0,\gamma)$, the pseudomomentum vector $\mathbf{K}=(0,K,0)$ is assumed to point along the y axis, and $\gamma=B$ in (T)/(2.35×10^5). For the field strengths $B=4$ T and 5 T of interest here, the critical values of the pseudomomentum can be calculated to be 0.061 and 0.066, respectively. In this work, we concentrate on K values around 0.1, which are above the critical values. Thus, an outer well is formed, which we approximate by an anisotropic harmonic oscillator [14] and expand around the minimum. The resulting long-lived delocalized OW states are the required initial target states. Figure 2 shows some internal coordinate distributions of the Ps ensemble, having randomly distributed starting conditions in coordinate/momentum space for different values of field strength and pseudomomentum. At the same magnetic-field strength B, the internal distance $\mathbf{r}$ of Ps increases with increasing K (cf. also Fig. 1), while a stronger field and a higher internal binding energy (i.e., smaller n) compress the internal distance, in agreement with Shertzer, Ackermann, and Schmelcher's work [13]. For comparison, a field-free situation is also shown.

For the incoming ensemble of projectile ions, we use a standard distribution [15]. The projectile velocity $\mathbf{v}$, its impact parameter b, and the initial distance z_0 from the target determine the initial condition of the projectile. The initial distance z_0 of the projectile ($\gtrsim 5\times10^4$ a.u.) is such that at this distance the projectile-Ps interaction is negligibly small compared to the electron-positron interaction. We assume that the projectile moves with a constant velocity along the z axis, parallel to the magnetic-field direction. The impact parameter of the projectile is chosen randomly by selecting b^2 in the interval $[0,b_{max}^2]$. Note that the center-of-mass motion of the Ps in the magnetic field depends on the target state. Therefore, the origin of the impact parameter $b=0$ is estimated by calculating the meeting point of the Ps and the projectile, taking into account the projectile velocity and the center-of-mass motion of the Ps. The maximum impact parameter b_{max} is chosen sufficiently large to ensure a vanishingly small capture probability outside this b value.

During the collision, the $\bar{p}$ projectile evolves with the approximation of a straight-line trajectory under the full three-body Hamiltonian,

$$H=\frac{1}{2}(\mathbf{p}_1+\mathbf{A}_1)^2+\frac{1}{2}(\mathbf{p}_2-\mathbf{A}_2)^2-\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}+\frac{1}{|\mathbf{r}_1-\mathbf{r}_3|}-\frac{1}{|\mathbf{r}_2-\mathbf{r}_3|}, \quad (5)$$

where $\mathbf{r}_3$ is the coordinate of the projectile. For a given set of initial positions, the integration of Hamilton's equations of motion is performed according to Eq. (5) by a standard Runge-Kutta method.

After the collision, the projectile proceeds to an asymptotic distance ($z_f=2\times10^5$ a.u.), sufficiently large to allow a clear energetic separation of the three particles into two-particle pairs. The resulting two-body e^+-e^- and e^+-$\bar{p}$ energies classify the outcome of the collision: excitation or ionization of the target Ps, or capture by the projectile ion. The required two-body Hamiltonians for the electron-positron and the positron-antiproton pair, $H_{e^+\text{-}e^-}$ and $H_{e^+\text{-}\bar{p}}$, are, respectively, defined by

$$H_{e^+\text{-}e^-}=\frac{1}{2}(\mathbf{p}_1+\mathbf{A}_1)^2+\frac{1}{2}(\mathbf{p}_2-\mathbf{A}_2)^2-\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}, \quad (6)$$

$$H_{e^+\text{-}\bar{p}}=\frac{1}{2}(\mathbf{p}_2-\mathbf{v})^2-\frac{1}{|\mathbf{r}_2-\mathbf{r}_3|}+\frac{1}{2}\gamma l_z+\frac{1}{8}\gamma^2(x_2^2+y_2^2), \quad (7)$$

where l_z is the z component of the e^+ angular momentum [7]. With Eqs. (6) and (7), the ionization thresholds of Ps as well as of $\bar{H}$ in the presence of a magnetic field are zero. Therefore, if $H_{e^+\text{-}e^-}$ is constant and less than zero, the positron remains bound to the e^-. If $H_{e^+\text{-}\bar{p}}$ is constant and less than zero, the positron is captured by the projectile. All other situations lead to ionization.

We now calculate the charge-exchange cross section for initial Ry states $n=40$ and 50 of the target Ps for magnetic-field strengths of 4 T and 5 T. The relative impact projectile velocities v_r are between 0.5 and 2.8 ($v_r=v/v_e$, with v_e the classical electron velocity in a circular Ps Bohr orbit). They correspond to collision energies between 0.62 and 19.6 eV ($n=50$) and between 0.98 and 30.6 eV ($n=40$).

The results of the charge-exchange cross section are displayed in Fig. 3. To further illuminate the influence of the magnetic field, two field-free cases are also included, namely, having angular momenta $l=n-1=m$ and $l=n-1,m=0$ (i.e., for circular Ry motion in planes perpendicular and parallel to the z direction, respectively) [16]. The influence of the magnetic field is quite substantial: it results in a cross section reduction of a magnitude similar to the one found for p-H collisions [7], the reduction being larger for increasing B. In addition, a smaller Ps binding energy (increasing n) and a larger geometrical extension of the target Ps atom (increasing K) yields a larger capture cross section. Due to the irregular motion of the Ps (cf. Fig. 1, bottom) the velocity matching effect is not expected to play an important role. Thomas capture [17,18], which happens in the collision plane in the field-free case [19], is foiled due to the magnetic field.

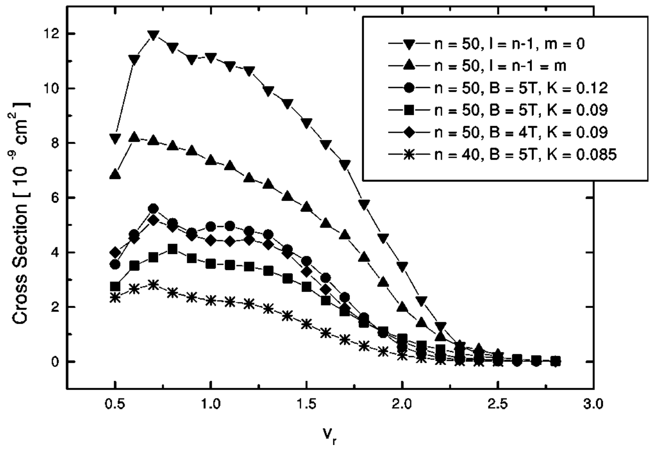

FIG. 3. Charge-exchange cross section as a function of the relative velocity v_r for collisions of $\bar{p}$ projectiles with Ps targets in the external magnetic fields $B=4$ T, 5 T for $n=40$, 50, and $K=0.085$, 0.09, 0.12 initial states, respectively. For comparison, the field-free $n=50$, $l=n-1=m$ and $l=n-1$, $m=0$ initial states are also included. The curves are drawn to guide the eye. Statistical uncertainty is 5%.

The observed behavior may be of interest for future experiments of the type $\bar{p}$-e^+e^- or $\bar{p}$-$2e^+$. Evidently, the magnetic field reduces the cross section, but this reduction remains within reasonable limits. Further explorations in the parameter space of cross section changes with K and binding energy would be worthwhile.

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