

Three-body recombination for electrons in a strong magnetic field: Magnetic moment

F. Robicheaux

Department of Physics, Auburn University, Auburn, Alabama 36849-5311, USA

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Using a classical Monte Carlo method, we have computed the three-body recombination (two free electrons and a proton scattering into one free electron and a hydrogen atom, $e+e+p \rightarrow H+e$) in strong magnetic fields. The proton is fixed in space but the electrons are allowed their full, three-dimensional motion. We investigate recombination for temperatures and fields similar to those used in recent experiments that generated antihydrogen. The present rate is compared to that when the electrons' motion is given by the guiding center approximation, validating previous results at low temperature and demonstrating the breakdown of this approximation at higher temperature. Unlike the $B=0$ case, strong B gives preferential recombination to atoms with positive magnetic moment. Also, the canonical angular momentum in the field direction is often negative even when the magnetic moment is negative. Both results affect the trapping of antihydrogen using spatially dependent magnetic fields.

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I. INTRODUCTION

Recently, two groups [1,2] reported the formation of antihydrogen (\bar{H}) by having antiprotons (\bar{p}) traverse a positron (e^+) plasma. Presumably [3], the \bar{H} is formed through three-body recombination (TBR): two e^+ s scatter in the field of the \bar{p} so that one e^+ loses enough energy to become bound to the \bar{p} and the other e^+ carries away the excess energy. The theoretical treatment of this process is quite daunting due to the small cyclotron period of the e^+ : 36 ps in a 1 T field. TBR in a strong magnetic field was first treated in Ref. [4] where TBR in the $B \rightarrow \infty$ limit was obtained. In this limit, the light particles are pinned to the field lines and the heavy particle is fixed in space. Later, Ref. [5] treated the large, but not infinite, B limit by allowing the light particles to have $\vec{E} \times \vec{B}$ drift velocity for motion perpendicular to \vec{B} and allowing the heavy particle to have its full motion. The total rate was found to be approximately 60% larger than in the $B \rightarrow \infty$ limit. More importantly, Ref. [5] reported that the TBR rate did not decrease rapidly with increasing velocity of the heavy particle suggesting the \bar{H} 's would form with energies much greater than $k_B T$. More detailed simulations [6] and measurements [7,8] confirmed that the majority of \bar{H} had kinetic energy substantially larger than $k_B T$. By launching the \bar{p} through the e^+ plasma at lower energy, this problem can be averted.

Now that the goal of \bar{H} formation has been accomplished, the next step is to trap it. This will be attempted through the use of spatially varying magnetic fields. Multipole fields and mirror coils will be arranged so that the minimum of $B \equiv |\vec{B}|$ will be where the \bar{H} are formed. The B will increase toward the walls of the trap so that low-field-seeking \bar{H} atoms will experience forces pushing them away from the walls. Thus, the sign of $-\vec{\mu} \cdot \vec{B}$, where $\vec{\mu}$ is the magnetic moment, is crucially important. Naively, one might expect that the \bar{H} will be formed with random magnetic moments and that the magnetic moments will be very large since the \bar{H} are

in Rydberg states. Thus, one might expect to lose $\sim 1/2$ of the \bar{H} because they will be in high-field-seeking states, but the remaining atoms will be much more easily trapped because of the large magnetic moment compared to the ground state. This expectation is wrong.

The \bar{H} is formed in a *strong* magnetic field. Thus, the e^+ approaches the \bar{p} in a tight cyclotron orbit. A 4 K e^+ in a 1 T field has a cyclotron radius of ~ 60 nm. An \bar{H} with an energy corresponding to an $n=70$ state (~ 32 K binding energy) has a radius ~ 260 nm. The geometry of the motion in strong B means the cyclotron motion of the e^+ needs to overlap the \bar{p} in the plane perpendicular to \vec{B} to give a negative $\vec{\mu} \cdot \vec{B}$ which will give low-field-seeking states. Thus, a crude estimate gives only $\sim 5\%$, $(60/260)^2$, of the atoms with low-field-seeking character. The situation is even worse than this estimate. In strong B fields, the canonical angular momentum and $m\vec{r} \times \vec{v}$ are not equal. Thus, while the change in energy with magnetic field strength, $dE/dB = -q\langle \hat{B} \cdot (\vec{r} \times \vec{v}) \rangle / 2$, may be positive, the canonical angular momentum in the field direction, $\hat{B} \cdot \vec{L} = m\hat{B} \cdot (\vec{r} \times \vec{v}) + q(\vec{B} \cdot \vec{r})^2 / (2B)$, can be of the wrong sign. This may cause the atoms to go through a series of states with negative dE/dB as the atom radiatively cascades to the ground state. As an example of the magnetic field introducing a bias in magnetic moment, a recent paper [9] investigated the properties of the Rydberg states formed in a double charge transfer and found that only $\sim 1/6$ of the $n=40$ atoms in a 1 T field formed with the sign of $\hat{B} \cdot \vec{L}$ giving low-field seekers.

The purpose of this paper is to report on the results of our calculations of three-body recombination for parameters similar to those used in the antihydrogen experiments. It has been found [6] that the properties of the \bar{H} depend on details of the actual antihydrogen experiments. Therefore, the relevance of these results to planned experiments will be specifically addressed in the Conclusions. For the sake of simplicity, we will refer to the calculation for matter (electrons and protons) since the results are the same as those for anti-

matter. The focus will be on the properties of the atoms relevant for trapping in strong magnetic field. Although the information is most directly relevant to future \bar{H} experiments, the atoms themselves show a nontrivial behavior worthy of wider interest.

II. NUMERICAL METHOD

A. Approximations

The states formed in TBR in strong B fields correspond to energies with principal quantum numbers greater than 30. Thus, we can simulate TBR using classical equations of motion. Electrons are fired at the proton with the distribution described below. The coupled equations for the motion of the electrons are solved using an adaptive step size, Runge-Kutta method. This ordinary differential equation (ODE) solver does not conserve energy and the canonical angular momentum in the B field direction, quantities conserved in the exact equations of motion. Thus, the numerical drift in these quantities is used as a gauge of the accuracy of a run. For example, the cumulative energy error during a run was required to be less than 0.01 K. Inevitably, some runs were rejected due to the too large drift in the conserved quantities. In principle, this could lead to bias in our results if the low-field-seeking states have a greater or lesser chance of giving error than the high-field seeking states. The largest fraction of errors in our final results were 56 failed runs out of 10 064 (roughly 0.55%) with the errors more typically being less than 10 out of 10 000. Thus, even complete bias in the errors should not affect the answers at more than the 0.005 level (and most at the 0.001 level). However, the bias appears to be very small. We compared the data from a run where 56 failed out of 10 064 to a run with larger δt that gave 1015 failed out of 10 871 and found that the distribution of atoms matched within statistical uncertainty (e.g., the fraction of low-field-seeking atoms was 0.312 in both runs).

The main approximation was treating the proton as being fixed in space, i.e., having infinite mass. Because the mass of the proton is ~ 1840 times larger than for the electron, this seems a reasonable approximation. For the states of interest, all of the motions of the electron have time scales over an order of magnitude shorter than those of the proton. This is another argument for treating the proton as stationary.

B. Initial distribution

The electron distribution is similar to that described in Ref. [5] with the addition of a thermal x, y velocity distribution. The distribution of trajectories is computed using the physical distributions for the electrons. Electrons are randomly fired at a proton located at the center of a cube. The time of firing an electron is random with a probability $\delta t/t_{av}$ during the time interval δt ; t_{av} is the average time an electron takes to cross the volume. The cube has edges of length $x_{max} = 10e^2/(4\pi\epsilon_0 k_B T_e)$ which is roughly 100 times larger than the radius of the recombined atom. The electrons are randomly fired from $z = \pm x_{max}/2$ with the x, y position randomly chosen in the range $-x_{max}/2 < x, y < x_{max}/2$ [10]. This prescription gives a varying number of electrons in the simu-

lation. The electrons have a Maxwell-Boltzmann distribution in \vec{v} .

In Ref. [5], we fired electrons until the binding energy was greater than a fixed multiple of the thermal energy. The time when this occurred is the recombination time. The TBR rate is the inverse of the average time for a recombination to occur. For the present simulation, this method is not practical due to the small time steps that are needed in the ODE solver. Instead we performed a two-step process similar in spirit to the method used in Ref. [4]. In the first step, we generated a distribution of one-electron initial conditions by randomly firing electrons at the proton until only one electron was inside the cube with an energy less than $-k_B T$. The time at which this occurred and the electron's position and velocity were stored. In the second stage, we randomly picked a bound electron from the first stage and randomly fired electrons at it until the atom was ionized or until an electron was bound by more than $\nu k_B T$. For a given ν , we then found the average time to recombination. The TBR rate is the inverse of this time [11].

The TBR rate depends on the binding energy $\nu k_B T$ because atoms with small ν can be ionized. We computed the TBR rate and the properties of the atoms for several values of ν . We computed the rates for $\nu=1, 2, 4,$ and 8 . The TBR is the rate for $\nu=8$ since the probability for reionization is very small for electrons so deeply bound. The statistical convergence of the TBR rate and the distribution of magnetic moments and angular momentum was ensured by increasing the number of trajectories in the simulation.

III. RESULTS

In this section, we compare the total rate of the present calculation with that obtained in previous work. We give the distribution of canonical angular momentum for different electron temperatures and binding energies. We also give the distribution of $\langle m\hat{B} \cdot (\vec{r} \times \vec{v}) \rangle$ for different temperatures and binding energies. All of the results are for a magnetic field of 1 T.

A. Total rate

Following the notation of Ref. [4], we will present our recombination rates in terms of $b = e^2/(4\pi\epsilon_0 k_B T_e)$ and $v_e = \sqrt{k_B T_e/m_e}$; the recombination rate is $C n_e^2 v_e b^5$ where C is a dimensionless constant. In Ref. [4], the authors determined $C = 0.070 \pm 0.01$ for the $B \rightarrow \infty$ approximation; the field-free coefficient is an order of magnitude larger: $C = 0.76$ [12]. In Ref. [5], we found the $B \rightarrow \infty$ equations of motion gave $C = 0.072$ with an uncertainty of 0.002 due to statistics and an estimated uncertainty of 0.004 due to systematic errors (volume effects and the soft-core potential are the main errors) which was in satisfactory agreement with Ref. [4]. We found $C = 0.11$ when we used a finite but large B within the guiding center approximation for the electron and full motion for the proton.

We compare these previous results using approximate equations of motion with the TBR rate using the full motion for the light particle. For all of the examples, the sample size

was greater than 10 000 which should give roughly 1% accuracy for total parameters (like the TBR rate). For a 1 T field, the present calculations give the TBR rate with $C = 0.11$ for 4 K electrons, 0.15 for 8 K electrons, and 0.19 for 16 K electrons. The 4 K rate is in good agreement with the guiding center approximation, but the 8 and 16 K rates are larger than the guiding center approximation with the difference increasing with temperature. This indicates that the guiding center approximation is breaking down at the higher temperatures. This should be expected because the radius of the cyclotron motion is increasing with temperature and the size of the atom is decreasing with temperature since the binding energy is proportional to temperature. Taking the cyclotron radius to be $r_{\text{cyc}} = \sqrt{2mk_B T}/eB$ and the radius of the atom for $8k_B T$ binding energy to be $r_{\text{at}} = e^2/(4\pi\epsilon_0 2 \times 8k_B T)$ demonstrates why the guiding center approximation breaks down. For 4 K, the ratio $r_{\text{at}}/r_{\text{cyc}} = 4.2$ and decreases to 1.5 at 8 K and 0.5 at 16 K. The guiding center approximation should only work well when the size of the atom is much larger than the cyclotron radius.

B. Distributions

The canonical angular momentum along the field is a conserved quantity. In a weak magnetic field, the canonical angular momentum goes to $m\vec{r} \times \vec{v}$ and becomes proportional to the magnetic moment. In strong fields, the canonical angular momentum in the direction of the field is

$$\hat{B} \cdot \vec{L} = m\hat{B} \cdot (\vec{r} \times \vec{v}) + \frac{qB}{2} (\hat{B} \cdot \vec{r})^2 \quad (1)$$

where m is the mass of the charge, $B = |\vec{B}|$, and q is the charge; this is a conserved quantity. Note that the quantity $\hat{B} \cdot (\vec{r} \times \vec{v})$ is not conserved. The change in internal energy of the atom with infinitesimal changes in the strength of the magnetic field is given by

$$\frac{dE}{dB} = -\frac{q}{2} \langle \hat{B} \cdot (\vec{r} \times \vec{v}) \rangle = -\frac{q}{2m} \hat{B} \cdot \vec{L} + \frac{q^2 B}{4m} \langle (\hat{B} \cdot \vec{r})^2 \rangle \quad (2)$$

where the angular brackets $\langle \dots \rangle$ indicate a time average. Because $q = -e$ for an electron, the time average of $\hat{B} \cdot (\vec{r} \times \vec{v})$ must be positive for the atom's internal energy to increase with increasing magnetic field strength (i.e., a low-field seeker). To some extent, the value of dE/dB depends on the duration of the time average. The duration of the average was chosen so that doubling the duration did not cause a substantial change in the distributions.

There are two possibilities for giving an atom whose internal energy increases with increasing B . The best case is when $\hat{B} \cdot \vec{L} > 0$ because both terms in Eq. (2) are positive. For this case, the atom will radiate more quickly [13] and it is likely the atom will maintain a positive magnetic moment during the radiative cascade. It is also possible that $dE/dB > 0$ but $\hat{B} \cdot \vec{L} < 0$. In this case, the atom starts as a low-field seeker. However, during the radiative cascade it is more likely to go through states that are high-field seekers. Thus, these states are less likely to reach the ground state as trapped atoms.

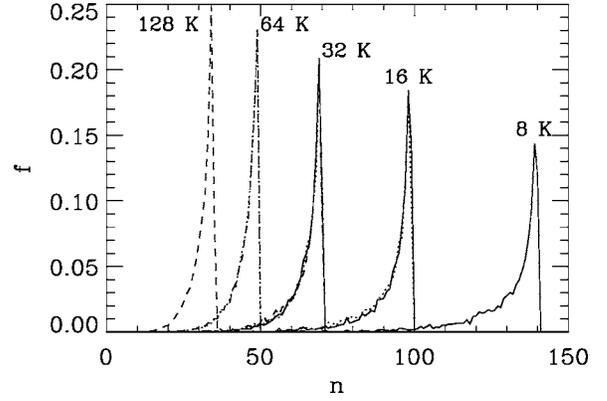


FIG. 1. The fraction of \bar{H} with a principal quantum number $n \equiv \sqrt{-13.6 \text{ eV}/E}$. Because the magnetic field is very strong (1 T), n is not simply related to the field-free levels. The solid lines correspond to results for 4 K plasma, the dotted lines to results for 8 K plasma, and the dashed lines to results for 16 K plasma. The different peaks correspond to stopping the simulation when an electron was bound by 8 K, 16 K, etc.

In the figures, we give results for atoms bound by less than $8k_B T$ because it has been found [6] that the short time the \bar{p} spends in the positron cloud allows some of the more weakly bound atoms to survive.

In Fig. 1, we show the n distribution of states when recombination is defined to be $2k_B T$, $4k_B T$, and $8k_B T$ for electron temperatures of 4, 8, and 16 K. In the simulations, electrons are fired at the atom until it is ionized or there is one electron in the region with a specific binding energy. This figure shows that the distribution peaks at the required binding energy but it extends to much lower n . A striking feature of the distributions is that the main dependence is from the binding energy condition; there is little dependence on the temperature of the electrons. We do not have a simple explanation of this phenomenon. The distribution is not well represented by the n^6 scaling seen in zero-field TBR; however, this may not be surprising because the n^6 is a steady-state property in a plasma whereas the distributions in Fig. 1 result from stopping the simulation when a particular condition is met.

In Fig. 2, we show the distribution of canonical angular momenta when recombination is defined to be $2k_B T$, $4k_B T$, and $8k_B T$ for electron temperatures of 4, 8, and 16 K. As in Fig. 1, the distributions depend most strongly on the required binding energy and much less strongly on the temperature of the electrons. The more weakly bound atoms have more negative distributions because the second term in Eq. (1) is larger. For more deeply bound atoms, the canonical angular momentum becomes closer to $m\vec{r} \times \vec{v}$. This trend can be seen in Table I where we show the fraction of atoms with positive L_z and with $L_z > 10\hbar$. For no magnetic field, half of the atoms should have positive L_z . The largest fraction, $\sim 1/4$, is for the atoms bound by $8k_B T$ from a 16 K plasma. This table also shows that there are very few atoms with large, positive L_z . Although the distributions for different temperature but the same binding energy are visually similar, the small populations of atoms for these parameters show a clear temperature dependence. For example, atoms with 32 K of binding

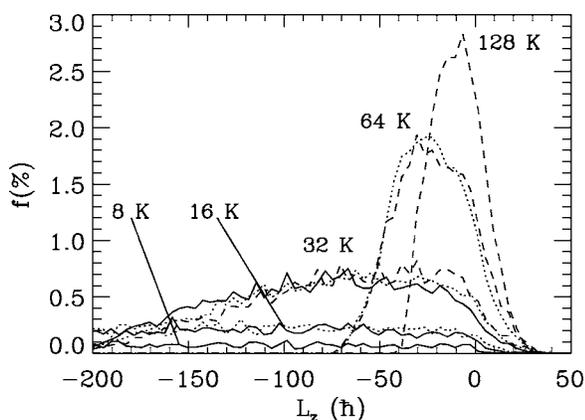


FIG. 2. The fraction of \bar{H} with a canonical angular momentum in the field direction. The canonical angular momentum is a conserved quantity but is progressively different from $m\vec{r}\times\vec{v}$ for weak binding. The line types and symbols are the same as for Fig. 1.

energy formed from the 4, 8, and 16 K plasmas have clearly different fractions of atoms with $L_z > 10\hbar$; the 16 K plasma gives the most favorable fraction. It seems likely this is due to the larger cyclotron orbit at 16 K.

In Fig. 3, we show the distribution of $\langle m\hat{B}\cdot(\vec{r}\times\vec{v}) \rangle$ when recombination is defined to be $2k_B T$, $4k_B T$, and $8k_B T$ for electron temperatures of 4, 8, and 16 K. As in Figs. 1 and 2, the distributions depend most strongly on the required binding energy and much less strongly on the temperature of the electrons. This quantity is proportional to dE/dB . Positive $\langle m\hat{B}\cdot(\vec{r}\times\vec{v}) \rangle$ gives low-field-seeking atoms. It is clear that the distribution is skewed to high-field-seeking atoms. The distribution has an interesting shape for weak binding giving a peak that moves progressively to negative values as the binding energy increases. The peak can be attributed to guiding center atoms that have very little $m\vec{r}\times\vec{v}$ because the motion of the electron is due to $\vec{E}\times\vec{B}$ drift. If the guiding center approximation holds, $mrv = me/(4\pi\epsilon_0 rB)$ which is roughly proportional to the binding energy. In Fig. 3, the peak is approximately at $-5.5\hbar$ for 8 K binding energy, $-10.5\hbar$ for 16 K binding energy, and $-21\hbar$ for 32 K binding energy, which is close to the expression for the guiding center approximation. The more deeply bound atoms do not show this peak.

In Table II, we give the fraction of atoms with $dE/dB > 0$ and > 10 K/T. The condition $dE/dB > 0$ means the atom energy increases with increasing B , which means it is low-field seeking. However, it does not indicate how strongly it is repelled from high B . The condition $dE/dB > 10$ K/T means these atoms are strongly repelled from high B . For small

TABLE I. Fraction of atoms with $L_z > 0$, $L_z > 10\hbar$.

	$2k_b T$	$4k_b T$	$8k_b T$
4 K	0.0015, 3.9×10^{-4}	0.009, 0.002	0.032, 0.013
8 K	0.016, 0.0045	0.052, 0.018	0.12, 0.040
16 K	0.058, 0.022	0.15, 0.058	0.26, 0.078

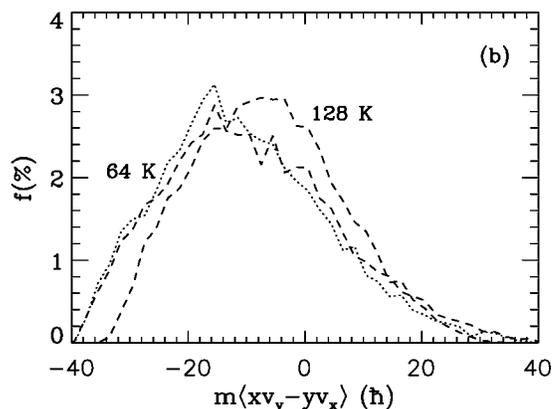
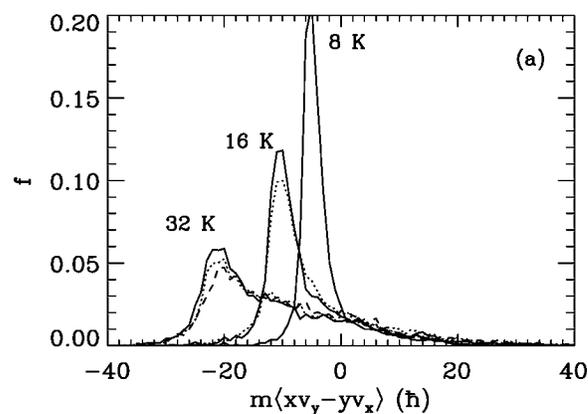


FIG. 3. The fraction of \bar{H} with $\langle m(\vec{r}\times\vec{v}) \rangle$ in the field direction. This is not a conserved quantity but is proportional to the magnetic moment. Positive values correspond to low-field seekers while negative values correspond to atoms attracted to high magnetic fields. The line types and symbols are the same as for Fig. 1; the separation into plots (a) and (b) is only for visual convenience.

changes in B , the energy change can be estimated from $\Delta E = \Delta B dE/dB$. The change in internal energy with larger changes in B will only be roughly approximated by dE/dB .

Table II does allow for some estimates. Suppose the e^+ plasma is at 4 K, the \bar{p} thermalizes with the e^+ , and an \bar{H} forms with a binding energy of 32 K (from past experiments, these are all optimistic suppositions). Then, the probability the \bar{H} could be trapped by a 0.1 T field change is $0.035 \times [(0.1 \text{ T} \times 10 \text{ K/T})/4 \text{ K}]^{5/2} \sim 1/230$. Since all assumptions were optimistic, it is likely the actual fraction of trapped \bar{H} will be less. It seems clear that the efficiency of trapping \bar{H} will be less than 1/100 if the properties are similar to previous experiments.

TABLE II. Fraction of atoms with $dE/dB > 0$, $dE/dB > 10$ K/T.

	$2k_b T$	$4k_b T$	$8k_b T$
4 K	0.16, 0.016	0.18, 0.027	0.17, 0.035
8 K	0.22, 0.035	0.21, 0.058	0.24, 0.055
16 K	0.25, 0.063	0.28, 0.074	0.31, 0.056

IV. CONCLUSIONS

We have computed the three-body recombination rate in a strong magnetic field using the full classical equations of motion for the light particles. The three-body recombination rate was in reasonable agreement with the results of previous calculations [4,5] that were based on larger approximations: the lowest temperatures produced the best agreement because the size of the cyclotron orbit is small compared to the size of the atom. Unlike the previous calculations, the current results allow us to make predictions about the magnetic moment of atoms formed through TBR. Besides being an interesting atomic physics question, the results have implications for experiments attempting to trap \bar{H} .

We have found that the atoms do not have randomly oriented magnetic moments and that a strong majority of atoms are *high-field seekers*. Although it is not surprising that the distribution of magnetic moments is not random, the extent of the asymmetry between high- and low-field seekers is striking. As the atoms become more deeply bound, a larger fraction of the atoms become low-field seekers but the magnetic moments are substantially smaller than expected from their principal quantum number. The atoms can reach more deeply bound states by collisions with cold e^+ . Radiation is not as effective because Rydberg states decay slowly and the angular momentum can only change by one \hbar for each decay.

We did find that the temperature of the light species plays a role in the magnetic moment of the atoms: higher-temperature plasmas produce a larger fraction of low-field seekers at a given binding energy. This appears to be due to the fact that the cyclotron radius increases with $T^{1/2}$.

In the \bar{H} experiments that used TBR for the formation of the atoms, the \bar{p} spent a short time inside the e^+ plasma. This

tended to give atoms less strongly bound than might be expected [6]. Because the more deeply bound atoms are more likely to be low-field seekers, the short exposure to the plasma will tend to give a higher proportion of high-field seekers than suggested by the results of this paper which assume the atoms reach a certain binding energy.

The next stage \bar{H} experiments will wish to maximize the number of trappable \bar{H} atoms. There are several conflicting trends to be considered. (1) Higher-temperature plasmas tend to give a larger fraction of low-field-seeking atoms at the same binding energy. (2) The fraction of low-field-seeking atoms and the fraction of atoms with positive canonical angular momentum increase as the binding energy increases to 64 K. (3) The maximum size of the magnetic moment decreases as n decreases from $n \sim 40$. The results of Ref. [6] suggest that the atoms are much less strongly bound than would be expected; thus the detrimental effect of trend 3 does not seem important unless the experimental arrangement drastically changes. Thus, the main question is whether trend 1 or 2 gives the more favorable results. The distribution of binding energies presented in Ref. [6] shows that lower-temperature plasmas are much more effective at giving more deeply bound atoms. Thus, it seems likely that lower-temperature plasmas will produce more low-field-seeking atoms. Unfortunately, the fraction of low-field-seeking atoms will be a few percent of the atoms made instead of roughly half.

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