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Three-body recombination for protons moving in a strong magnetic field

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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: $e+e+p \rightarrow \mathrm{H}+e$) in strong magnetic fields. The proton is allowed its full motion whereas the motion of the electron is given by the guiding center approximation. We investigate recombination for temperatures and fields similar to those used in recent experiments that generated anti-hydrogen. When the proton has the same temperature as the electrons, the recombination rate for the more elaborate equations of motion is roughly 60% larger than for the $B \rightarrow \infty$ approximation. The recombination rate decreases as the proton speed approaches the electron thermal speed; the variation of this rate has implications for the directionality of the anti-atoms formed in recent experiments. We report on several properties of the atoms formed by three-body recombination in strong magnetic fields.

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I. INTRODUCTION

Recently, two groups [1–3] have reported the formation of anti-hydrogen by having anti-protons traverse a positron plasma. Presumably [4], the anti-hydrogen is formed through three-body recombination: two positrons scatter in the field of the anti-proton so that one positron loses enough energy to become bound to the anti-proton and the other positron carries away the excess energy. 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 anti-hydrogen experiments. 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.

It was noted from the earliest studies that the three-body recombination rate is proportional to $n_e^2 T_e^{-9/2}$, where n_e is the electron density and T_e is the electron temperature. This form arises from simple dimensional arguments. The rate is proportional to the electron density times the electron velocity ($\propto T_e^{1/2}$) times the scattering cross section ($\propto r^2$) times the probability for finding a second electron within the size of the atom $\propto n_e r^3$; the size of the atom formed in the recombination step is proportional to T_e^{-1}. Three-body recombination was numerically studied during the 1970's. The main object of the numerical investigation was to obtain the proportionality factor in the recombination rate for no external fields (e.g., see Ref. [5]). For the parameters we investigate, classical mechanics will be sufficiently accurate since the process is classically allowed, populates high-n states ($n > 35$), and involves substantial averaging over initial conditions.

However, the recent anti-hydrogen experiments employ a strong magnetic field to confine the positrons and anti-protons. The zero-field recombination rates are not accurate for the anti-hydrogen experiments because the magnetic field strongly modifies the motion of the charged particles. To see that the results will be strongly modified we compare the size scale of the atom to the cyclotron radius for the electron and proton at $T_e = 4$ K and $B = 5.4$ T. (In all calculations we will use SI units.) The size scale of the hydrogen atom is $r_H = e^2/(4\pi\epsilon_0 k_B T_e) = 4.2\ \mu$m. The cyclotron radius scale is $r_{cyc} = mv/(eB) = \sqrt{2mk_B T_e}/(eB)$ and is 0.012 μm for an electron and 0.50 μm for the proton.

Glinsky and O'Neil [6] computed the proportionality coefficient for the three-body recombination [7] in the $B \rightarrow \infty$ limit. In this limit, the proton can be taken to be fixed in space and the electrons are only free to move along the magnetic-field direction; for definiteness we will take the magnetic field to be in the $+z$ direction. The electrons and protons interact through the z component of the $1/r^2$ electric forces. They used a clever method of extending the thermal distribution of the electrons to bound energies. The recombination rate was found by scattering electrons from these weakly bound atoms. Recombination was determined to have occurred if an electron was scattered to low enough energies that the probability for reionization was negligibly small. They found that electrons bound by roughly $10k_B T_e$ were rarely ionized. Thus, the recombination rate can be found from the rate that electrons are first scattered below $10k_B T_e$.

From the parameters above, it is clear that the detailed cyclotron motion of the electron can be ignored due to the small size of the electron cyclotron radius. However, it is not clear that two effects ignored in Ref. [6] can be neglected. The first is the motion of the proton, since the size of the cyclotron orbit for the proton ($r_{cyc} = 0.50\ \mu$m) is comparable to the size of an atom with a binding energy of $10k_B T_e$ ($\sim r_H/10 = 0.42\ \mu$m). The second effect is the $\vec{E} \times \vec{B}$ drift of the electron. In our calculations, we include both of these effects. We have performed calculations at 4, 8, and 16 K for magnetic fields of 3.0 and 5.4 T; the ATHENA experiment [1] runs at roughly 16 K and 3 T while the ATRAP experiment [2,3] runs at roughly 4 K and 5.4 T. We find that the recombination rate including these effects is roughly 60% larger than the $B \rightarrow \infty$ rate found by Glinsky and O'Neil [6]. Although this appears to be a sizeable difference, relatively small changes in temperature (11%) or density (26%) would

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compensate for this difference. As noted in Ref. [6], the $B \rightarrow \infty$ approximation works well because the fastest time scale is in the z direction. The motions from the $\vec{E}\times\vec{B}$ drift of the electrons and the cyclotron motion of the proton is more than an order of magnitude slower.

A more important effect is the decrease of the recombination rate with the increase of proton speed along the magnetic field. In the anti-hydrogen experiments, the anti-protons and positrons are contained in separate potential wells with depths of order 10 eV. Although the distribution of anti-proton speed in the positron cloud is not well characterized, it seems likely that the energy of the proton along the magnetic field is given by the trap depth. However, the transverse speed of the protons might be given by the temperature since longitudinal and transverse motions are largely decoupled. Because the temperatures are in Kelvin ($\sim 10^{-4}$ eV), the proton energy along the magnetic field can be sizeable even when it is only (1/100)th of the trap energy scale. Thus, it is possible that the anti-atoms have velocities mainly directed along the magnetic field. We have computed the recombination rate for proton speeds comparable to the electron thermal speed.

II. NUMERICAL METHOD

To provide an independent test of the previous calculations [6], we include higher terms in the equations of motion. We also generate the electron and proton distribution using a different method.

A. Equations of motion

The full equations of motion for electrons interacting with a proton require too much computational effort to solve. The electron cyclotron period $\tau_{cyc}=2\pi m/(eB)\simeq 6.7$ ps forces a numerical differential equation solver to take time steps of order 100 fs. Thus, the main effort would be devoted to the electron's helical motion.

Fortunately, the radius of the cyclotron orbit for electrons is very small compared to the other length scales. Also, the very fast cyclotron motion can be used to advantage. We average over a cyclotron period to obtain the well-known guiding center approximation. In this approximation, the center of the cyclotron orbit moves freely along the magnetic field. The motion of the center perpendicular to the field arises from $\vec{E}\times\vec{B}$ drift. For an electron whose cyclotron orbit is centered at $\vec{r}$, there are four coupled equations

$$\frac{dx}{dt}=E_y(\vec{r})/B, \quad \frac{dy}{dt}=-E_x(\vec{r})/B,$$

$$\frac{dz}{dt}=v_z, \quad m\frac{dv_z}{dt}=-eE_z(\vec{r}), \tag{1}$$

where x,y,z is the center of the cyclotron orbit.

We include the full equations of motion of the proton in the xy plane. In our simulations, we choose a frame where the proton speed along the field is initially 0. We do not include the subsequent motion of the proton along the field since this will only induce changes in the recombination rate proportional to the mass ratio. The four coupled equations for the proton are

$$\frac{dX}{dt}=V_x, \quad M\frac{dV_x}{dt}=e[E_x(\vec{R})+V_yB],$$

$$\frac{dY}{dt}=V_y, \quad M\frac{dV_y}{dt}=e[E_y(\vec{R})-V_xB]. \tag{2}$$

The coupled equations for the proton and electrons are solved using an adaptive step size, Runge-Kutta method.

The magnetic field is uniform and constant. The electric field is only due to the charged particles in the simulation. External fields from the traps are ignored. These simulations do not properly treat the motion of the electron and proton when the electron is within an electron cyclotron radius of the proton; two electrons are never within a cyclotron radius of each other because of the low temperature and the repelling Coulomb force. Not only are the equations of motion inaccurate for a close electron-proton approach but the simulation slows down because of the presence of large accelerations. Since the equations are already inaccurate, we *modify* the electric forces by ''softening'' the singularity. Instead of having the potential between two particles separated by r be proportional to $1/r$, we change the potential to $1/\sqrt{r^2+r_m^2}$ where we chose r_m to be the electron cyclotron radius; the electric fields are computed from $\vec{E}=-\vec{\nabla}V$.

We note that there are several conserved quantities for these equations of motion: an energy, the x and y components of a pseudomomentum, and an angular momentum in the z direction [8,9]. We use the conserved quantities as part of the error monitoring conditions in our adaptive step size ODE solver.

B. Distribution

The distribution of trajectories is computed using the physical distributions for the proton and 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 $\delta t/t_{\rm ave}$ during the time interval δt; $t_{\rm ave}$ 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 $-x_{max}/2<x,y<x_{max}/2$. This prescription gives a varying number of electrons in the simulation. Our simulations are in the rest frame of the proton in the z direction, and the electrons have a Maxwell-Boltzmann distribution in v_z. If we are simulating recombination onto a proton moving in z, then the electron velocity distribution in v_z is a shifted Maxwell-Boltzmann distribution.

The x,y proton distribution can be obtained more simply. It is assumed that the protons have a Maxwell-Boltzmann distribution with the same temperature as the electrons. This is probably not correct in some situations; however, it is probable that the transverse proton temperature is close to

the electron temperature in most cases of interest. Whenever the simulation makes a transition from 0 to 1 electron in the volume, a new set of initial velocities is chosen for the proton.

Whenever we launch an electron, we shift the position of the proton and any electrons that are already in the cube. The shift is chosen so that the estimated position of the proton will be at the center of the cube when the new electron crosses the xy plane; this prescription with choosing random x,y positions for the initial launch gives a uniform distribution of impact parameters around the position of the proton. Without this shift, the proton could drift out of the volume before the launched electron reaches the xy plane.

C. Recombination defined

In order to make the computation feasible, we only compute trajectories to the point where an electron has sufficient binding energy that it is unlikely to be reionized during subsequent collisions. For our definition of binding, we simulated the motion until there was one electron in the volume and the total energy of the electron plus proton,

$$E=\frac{1}{2}M(V_x^2+V_y^2)+\frac{1}{2}mv_z^2-\frac{e^2}{4\pi\epsilon_0\sqrt{r^2+r_{min}^2}}, \qquad (3)$$

is less than $-\nu k_B T_e$. We computed the average time to recombination for a few thousand events. We increased ν until the average time to recombination converged: $\nu=8$. Note this is similar to the definition of recombination in Ref. [6] since proton kinetic energy (roughly $k_B T_e$) is included in our definition of recombination. The three-body recombination rate is the inverse of the average time to recombination. The recombination rate for $\nu=6$ for which some reionization can still occur is roughly (10%) higher than for $\nu=8$.

We take the time to recombination to be the time at which the atom first has energy $E=-\nu k_B T_e$. We note that this time contains both the time to initially capture an electron (usually to $E>-\nu k_B T_e$) and the time to scatter the electron to deeper binding energies. For the parameters we have chosen the time to scatter to deeper binding is less than 1% of the time to recombination.

III. RESULTS

A. Thermal protons

Following the notation of Ref. [6], 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 $Cn_e^2 v_e b^5$ where C is a dimensionless constant. In Ref. [6], they determined $C=0.070\pm0.01$ for the $B\to\infty$ approximation; the field free coefficient is an order of magnitude larger: $C=0.76$. We found $C=0.072$ 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) when using the $B\to\infty$ equations of motion.

We computed the three-body recombination rates for three different temperatures (4, 8, and 16 K) and 2 different magnetic fields (3.0 and 5.4 T) and the results are presented in Table I. For all of the calculations the statistical uncertainty in C is less than 0.002. The main uncertainty is due to systematic errors and could be as high as 0.010. Note that the recombination coefficients are only weakly dependent on the temperature and magnetic field and the trends in this table are not significant. The rates are roughly 60% larger than the $B\to\infty$ rate.

TABLE I. Three-body recombination coefficient.

T_e	C at 3.0 T	C at 5.4 T
4 K	0.110	0.097
8 K	0.120	0.114
16 K	0.110	0.117

We have calculated the distribution of average transverse velocities of the recombined hydrogen atom for the three different temperatures in the 5.4 T magnetic field. The distribution of atomic velocities is close to the Maxwell-Boltzmann distribution of the original ions; the largest difference is for the 4 K data set which has transverse speeds roughly 30% larger than for a Maxwell-Boltzmann distribution. Thus, a rough estimate for the transverse speed of recombined atoms is $\sqrt{k_B T/M}$. At 4 K, this gives a transverse speed of roughly 200 m/s.

The transverse motion of a hydrogen atom through a magnetic field induces a nonzero time-average dipole moment. It is possible that this dipole moment could be used to guide the motion of the atom which would be useful in the anti-hydrogen experiments: the ability to guide their motion could enhance the delivery of anti-hydrogen to specified regions of the trap. We have computed the distributions of $\rho=\sqrt{(\langle x-X\rangle_t)^2+(\langle y-Y\rangle_t)^2}$ where $\langle\ \rangle_t$ is the time average. We compared the average displacement to the size of the atom $\rho_0=e^2/(4\pi\epsilon_0\ \ 8k_B T_e)=r_H/8$. At 4 K, the distribution of ρ extended to roughly $0.4\rho_0$ with a peak at $0.2\rho_0$ while at 8 K the distribution extended to roughly $0.2\rho_0$ with a peak at $0.07\rho_0$. This shows that the size of the time-average displacement of the electron from the proton is a fraction of the size of the atom and becomes a smaller fraction at higher temperatures.

For most experiments of interest, the anti-hydrogen needs to be in the ground state. One proposal is to expose the anti-hydrogen atoms formed in three-body recombination to laser light to stimulate transitions to lower-energy levels. One requirement for this proposal is that the electrons need to overlap the region of the final state. We took the final state to be $n=10$ and thus the relevant region to be a sphere with radius $r=2n^2\times0.529\times10^{-10}$ m. We examined the case when $B=5.4$ T and $T=4$ K which has a sample of 3905 atoms. We found only 10 out of 3905 atoms could be stimulated to $n=10$ [10]. However, it must be remembered that the recombined atoms in our sample are at $n\sim70$. Electron-Rydberg collisions in the experiments will stimulate the atoms to lower n; these lower-n atoms are more likely to overlap with the $n=10$. To understand this, we also computed the number that could be stimulated into $n=30$; in this case, 153 out of 3905 atoms could be stimulated to $n=30$. Unfortunately, this is still a small fraction: 4%.

TABLE II. Three-body recombination coefficient as a function of proton speed along the B field. $B=5.4$ T, $T_e=4$ K. The speed of the proton is given in units of electron thermal speed $V_0=\sqrt{2k_BT_e/m_e}=1.1\times10^4$ m/s. The energy of a proton with speed V_z is also given.

V_z/V_0	C	E (eV)
0.000	0.100	0.00
0.167	0.081	0.04
0.333	0.051	0.14
0.500	0.031	0.32
0.667	0.018	0.56
0.833	0.011	0.88
1.000	0.008	1.27

B. High-velocity protons

In Table II, we give the results of the three-body recombination when the electron velocities in the field direction are a shifted Maxwell-Boltzmann distribution. The velocity shift of the distribution is denoted by V_z. This rate is equivalent to recombination for a proton that is moving at a substantial speed V_z relative to the electron gas. We note that the anti-protons are launched through a positron gas in both of the anti-hydrogen experiments and it is likely that the velocity of the anti-proton along the field is large compared to the transverse velocity. The recombination rate decreases very rapidly as the proton speed approaches the electron thermal speed. However, a substantial amount of recombination can occur with V_z much larger than the transverse velocity of the atom. For example, V_z is 18 times larger than the transverse velocity, 200 m/s, at $V_0/3$. This means that after recombination the atoms could have a high degree of directionality which could be important for increasing the number of atoms that reach a particular area of the trap.

IV. CONCLUSIONS

We have generated data for three-body recombination in strong magnetic fields using more accurate equations of motion. The recombination rate for thermal protons is 60% higher than in previous calculations. We have also generated data when the proton has substantial velocity along the magnetic field. There exists a range of velocities with high recombination rate where the proton's speed along the field is substantially higher than proton speed perpendicular to the field. This could lead to directionality in the motion of the recombined atoms.

We have computed properties of the recombined atoms and found them to be roughly what might be expected from dimensional arguments. For example, the distribution of transverse speeds of the atoms is roughly Maxwell-Boltzmann with an average speed within 30% of the proton's average speed. Unfortunately, we found that only a small fraction of the atoms had properties suitable for laser stimulation to low-n states. We also found that the time-average displacement of the electron relative to the proton was a fraction of the possible size which does not bode well for using the dipole moment to guide the atom.

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