Simulating Excited States of Antihydrogen within the Geant4 Simulation of the ASACUSA Experiment

Summer Student Report - *ASACUSA*

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Abstract

We have performed numerical calculations of decay rates for excited states of hydrogen in magnetic fields. The calculated decay rates were used to implement excited hydrogen states in a `Geant4`-simulation of an experimental setup intended to measure the hyperfine splitting of antihydrogen. The excited states could thereby decay to lower states in the simulation. Changes in the effective magnetic moment due to the decays were taken into account. The simulation was used to evaluate the efficiency of the experimental setup, depending on which initial antihydrogen state was created. The implementation of excited states also made possible more realistic evaluations of proposed changes in the experimental setup.

Contents

1 Introduction and Background

I have had the pleasure of working with the *ASACUSA* collaboration at CERN during the summer of 2013, with Chloe Malbrunot as supervisor. This report briefly outlines the work done and the results obtained during the duration of the Summer Student program.

The *ASACUSA* collaboration uses antiprotons from the Antiproton Decelerator (AD) at CERN to create antihydrogen[1]. The purpose of this is to measure its ground state hyperfine splitting, and to compare it to the hyperfine splitting of hydrogen. Since CPT symmetry states that hydrogen and antihydrogen should have the same hyperfine splitting, any observed difference would be an indication of CPT violation [1]. Violation of CPT has been included in some extensions of the Standard Model [2, 3].

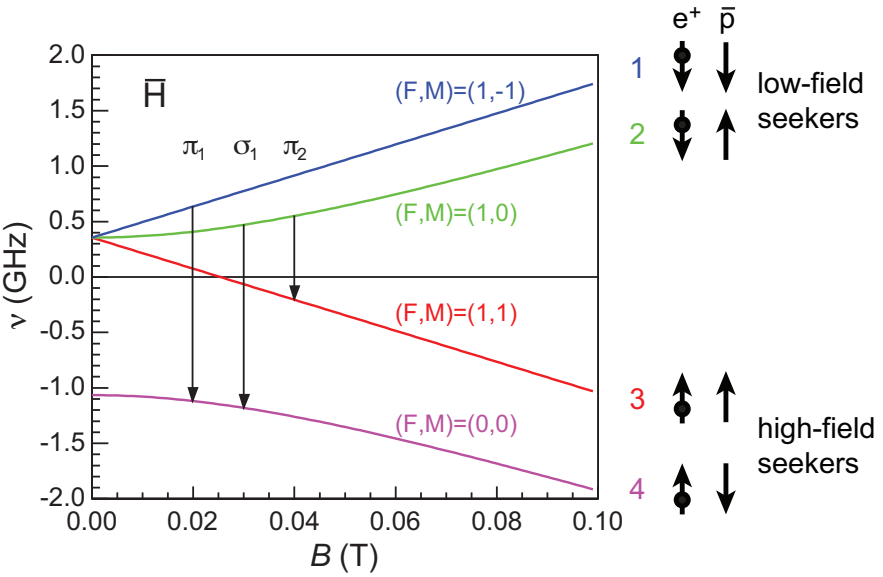


Figure 1. *The ground state hyperfine splitting of the energy levels in hydrogen [4].*

The proposed method for measuring the hyperfine structure is to use an atomic beam. This method works with antihydrogen at relatively high temperatures (up to 100 K), an advantage compared to experiments working with trapped atoms (e.g. *ALPHA* [5], *ATRAP* [6]) which require very cold antihydrogen (0.5 K) [1]. It utilizes the fact that the ground state energy levels split in an external magnetic field, as depicted in Figure 1. As seen in the figure, for some configurations the energy gets lower with increasing field strength, and in some configurations it gets higher. We denote the sooner as "high-field seeker" (HFS) states and the latter as "low-field seeker" (LFS) states, since they will be attracted to increasing and decreasing field strengths in an inhomogeneous field, respectively. The splitting of the energy levels and the attraction to high and low fields for different energy levels are key features of hydrogen, which are used in this experiment to characterize and precisely measure its physical properties.

The experimental setup is depicted in Figure 2. The basic principle of the setup is as follows. Antihydrogen is formed in a so-called CUSP trap [7], where an inhomogeneous magnetic field and an electric potential confines a positron-antiproton plasma. Antihydrogen forms by different types of recombination in this plasma. The idea is that the field lines in the CUSP trap will make LFS antihydrogen move forward towards the microwave cavity, while high field seeking antihydrogen would be bent away to a higher extent. In the microwave cavity, antihydrogen may flip from LFS to HFS if the radiofrequency matches the energy difference

[1]In this report, the word hydrogen and antihydrogen will be used interchangeably unless some specific difference between hydrogen and antihydrogen is pointed out.

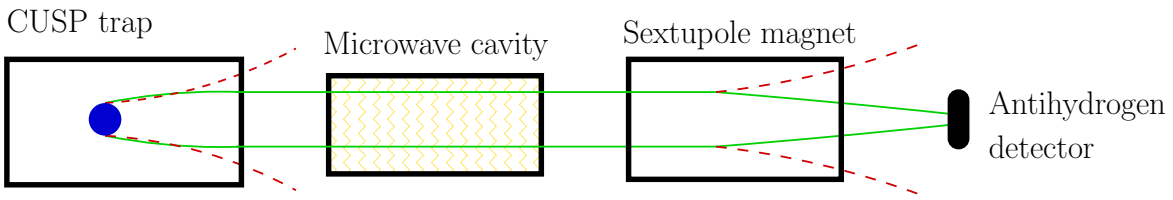


Figure 2. *Schematic view of the experimental setup.*

between the energy levels. The sextupole magnet will then focus LFS antihydrogen on the detector, and bend away HFS antihydrogen. By making a scan with the radiofrequency, one would be able to note a dip in the the number of detected antihydrogen atoms at the detector when the frequency matches the energy level splitting of antihydrogen, and thereby the level splitting can be determined [1].

If the antihydrogen is formed in an excited state rather than in the ground state, it might cause various problems, since it will behave differently in magnetic fields than if it were in the ground state. Antihydrogen placed in an inhomogeneous magnetic field may be affected by a force. This force is given by $\boldsymbol{F} = \nabla(\boldsymbol{\mu} \cdot \boldsymbol{B})$ where $\boldsymbol{\mu}$ is the magnetic moment of the atom.

In an excited state $\langle n, l, j, m_j \rangle$ the projection of $\boldsymbol{\mu}$ on the magnetic field is calculated as $\mu_z = m_j g_j \mu_B$ [8, p. 209] where

$$g_j = g_l \frac{j(j+1) - s(s+1) + l(l+1)}{2j(j+1)} + g_s \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}$$

using $g_l \approx 0.99946$ [8, p. 214] and $g_s \approx 2.0023$ [9], and $s = \pm\frac{1}{2}$.

Here, we approximated the contribution from the nuclear magnetic moment to zero. This is reasonable, since it is of the order of the electron mass divided by the proton mass ($\frac{1}{1836}$) smaller than the Bohr magneton [8, pp. 214-215].

In order to construct and run the experiment in an efficient way, it is of uttermost importance to make a simulation of the experimental setup. In this project, the behavior of excited states of antihydrogen has been implemented in the simulation. This required the decay rates for hydrogen to be calculated, which was also done.

2 Method

Calculating the decay rates for hydrogen in a magnetic field is non-trivial, since the decay rates depend on the field strength. In order to do the calculations, a modified version of a software package called `Flexible Atomic Code` (`FAC`) [10] was used. The methods used for the computations are described in more detail in documentation bundled with the software package itself [11]. The original `FAC` software was modified by Dr. Stambulchic [12] to calculate transition rates in electric and magnetic fields.

In order to enable us to use the software for our purposes, the `FAC` software was further modified so that selected parts of it did compile as `C++`-code. It was also modified to take orbital quantum numbers higher than $l = 22$ into account. Using a purpose-written software designed to invoke the `FAC` multiple times in parallel, for each possible transition and for many different magnetic fields, the decay rates were calculated. The `FAC` output was in the form of a large number ($O(10^5)$) of binary files. These were transferred to a `ROOT` tree, which was then used to create for the purpose optimized interpolation objects. These objects were saved in another `ROOT` tree, which could be used to simulate the decay of hydrogen. The data was also exported to a web interface, in which it was easy to read out and visualize the decay rates between specific states.

Using the `ROOT` file with the decay rates, excited states were implemented in the existing simulation of the experimental setup. This simulation was written using `Geant4`, a toolkit for simulating the passage of

particles through matter [13]. Particles are transported by numerically solving the equations of motion for particles in discrete steps, and Monte Carlo methods are used for the physical processes involved.

In `Geant4`, a particle is usually represented as a static singleton object which is not supposed to be modified. This poses a problem if the particle can have excited states, which is the case in atomic physics. Therefore, changeable quantum numbers were assigned to the particle. Using the database calculated with the `FAC`, the hydrogen atom was allowed to cascade down to lower states from an arbitrary initial state. This cascading could be made to depend on the external magnetic field in which the particle was, by making the particle itself keep track of its magnetic field in each step in the simulation. In each step, the particle was reminded of the time, and could cascade to lower states appropriately. Also, for each step additional tracking information about the hydrogen state had to be stored separately for analysis and track reconstruction since this information would otherwise be lost once the singleton particle changed state.

An excited state in hydrogen typically can have a radically different magnetic moment than a hydrogen atom in the ground state. This will give a different force on the antihydrogen atom, as discussed above. The standard `Geant4` equation of motion was modified to take this additional force into account for hydrogen atoms. This enabled us to simulate the tracks much more realistically.

Implementing the excited states in the simulation also adds a number of new variables, since it is not clear how the distribution of initial states will look. There are indications that the formation might be dominated by high field seeking states[14], nevertheless, there are too many unknown variables to assume any distribution for the current setup.

However, one can simulate with different initial quantum states and analyze how the result will depend on the initial conditions. It is also a natural step to characterize how different changes in the experimental setup will be more or less beneficial for different initial states.

3 Results and Discussion

The results presented in this section are currently preliminary, and might be subject to change.

3.1 Decay rates

The calculation of decay rates which were used in subsequent simulations, was for all allowed dipole transitions with $n \leq 25$. This amounts to a total of approximately 11,000 different quantum states. Filtering out very improbable transitions (with an Einstein coefficient less than $10^{-3}\,\mathrm{s}^{-1}$) reduced the database size by $\approx 93\,\%$ to approximately 60 Mb. The final result was a `ROOT` database with approximately $4 \cdot 10^5$ entries.

The Einstein coefficients ranged from very high (in the order of nanoseconds) for the most probable decay branches for low values of n, to lower ones (in the order of milliseconds) for the values of n closer to 25. The reason for setting $n \leq 25$ was that for higher n, there would be no realistic chance for the antihydrogen to reach ground state before arriving at the cavity.

The correctness of the calculations was verified for zero field strength using the NIST atomic database [15]. A sample of 10 values were selected from the ROOT data file, and these values were manually compared to the values in the NIST database. The mean relative error turned out to be $1.08 \cdot 10^{-3}$ (the NIST values were consistently larger), with a standard deviation of $1.57 \cdot 10^{-5}$. Thus, these errors should be negligible compared to the size of the error due to a limited sample size in the simulations. For decay in the magnetic field, there were no experimental data to use for the verification. However, the author of the software claimed [12] numerical uncertainties to dominate over methodological ones.

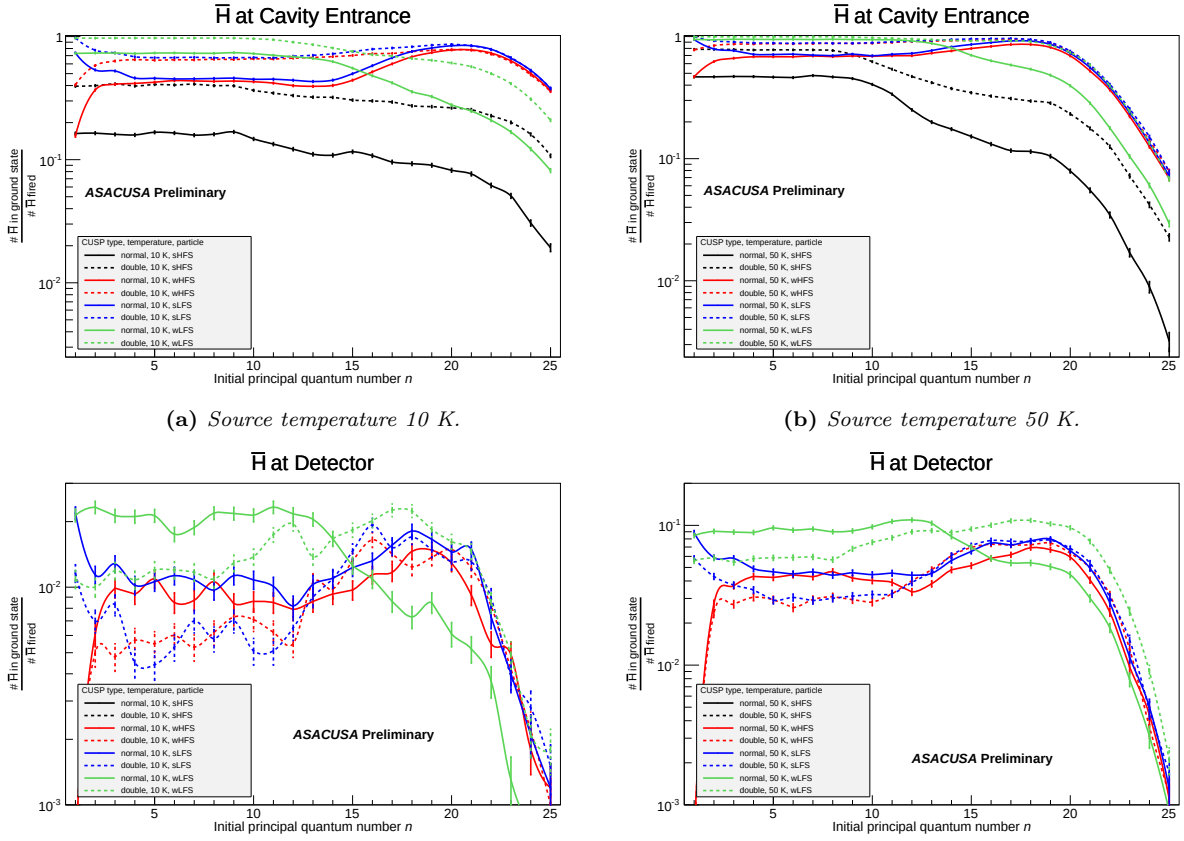
3.2 Simulations

The simulations were implemented in the existing `Geant4`-based simulation code that the collaboration developed. Thereafter, the behavior of different initial quantum states as well as other initial conditions in the

setup was studied. Some results are shown here. How well the setup behaved under certain conditions could be characterized using three key parameters:

- The number of hydrogen atoms reaching the cavity entrance in ground state.
- The number of hydrogen atoms reaching the detector in ground state, after passing the cavity in ground state (*signal*).
- The number of hydrogen atoms reaching the detector after passing the cavity in an excited state (*noise*).

Some important parameters to evaluate is the impact of different temperatures or positions for antihydrogen production inside the CUSP trap. The limited extent of this report unfortunately does not allow for a lot of results to be included. An example is described in Figure 3. The *ASACUSA* group is considering buying a new CUSP trap, called Double CUSP, to improve the performance. This will have a stronger field gradient in order to focus antihydrogen with a higher temperature. There are off course many other parameters one might characterize.



(a) *Source temperature 10 K.*

(b) *Source temperature 50 K.*

(c) *Source temperature 10 K.*

(d) *Source temperature 50 K.*

Figure 3. *Preliminary results: Relative number of $\bar{H}$ at the cavity entrance or at the detector, as a function of the initial quantum number, for the current CUSP trap (normal) and the suggested Double CUSP (double). HFS = High Field Seeking state ($m_j > 0$), LFS = Low Field Seeking state ($m_j < 0$), w = weak ($m_j = \pm\frac{1}{2}$), s = strong ($m_j = \pm j$).*

4 Conclusions

In this project, decay rates for hydrogen in a magnetic field have been computed. These have been used to implement deexcitation of antihydrogen in a simulation of an experimental setup. Using this implementation, different aspects of the experimental setup can be evaluated more realistically.

From the results, it is clear that if antihydrogen is created in a strong high field seeking state with a large principal quantum number (around $n = 25$ or larger), some kind of measures will have to be taken in order to speed up the deexcitation, since otherwise very few atoms will reach the cavity in the ground state. A suggestion that might be worth looking into is to use an electric field to induce deexcitation.

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